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Li, J., Lu, W., Zhang, S., Raabe, D.
Large strain synergetic material deformation enabled by hybrid nanolayer architectures
(2017) Scientific Reports, 7 (1), art. no. 11371, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85029286847&doi=10.1038%2fs41598-017-11001-w&partnerID=40&md5=7b0a4408aac1398a01f71d173ed7ec6e

DOI: 10.1038/s41598-017-11001-w
AFFILIATIONS: College of Mechanical and Electrical Engineering, Central South University, Changsha,Hunan, China;
Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Nanoanalytics and Interfaces, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: Nanolayered metallic composites are much stronger than pure nanocrystalline metals due to their high density of hetero-interfaces. However, they are usually mechanically instable due to the deformation incompatibility among the soft and hard constituent layers promoting shear instability. Here we designed a hybrid material with a heterogeneous multi-nanolayer architecture. It consists of alternating 10 nm and 100 nm-thick Cu/Zr bilayers which deform compatibly in both stress and strain by utilizing the layers' intrinsic strength, strain hardening and thickness, an effect referred to as synergetic deformation. Micropillar tests show that the 6.4 GPa-hard 10 nm Cu/Zr bilayers and the 3.3 GPa 100 nm Cu layers deform in a compatible fashion up to 50% strain. Shear instabilities are entirely suppressed. Synergetic strengthening of 768 MPa (83% increase) compared to the rule of mixture is observed, reaching a total strength of 1.69 GPa. We present a model that serves as a design guideline for such synergetically deforming nano-hybrid materials. © 2017 The Author(s).
DOCUMENT TYPE: Article
SOURCE: Scopus

Zhang, J., Raabe, D., Tasan, C.C.
Designing duplex, ultrafine-grained Fe-Mn-Al-C steels by tuning phase transformation and recrystallization kinetics
(2017) Acta Materialia, 141, pp. 374-387.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85029811123&doi=10.1016%2fj.actamat.2017.09.026&partnerID=40&md5=8c4314d10d12bbdb500d5f1699a71611

DOI: 10.1016/j.actamat.2017.09.026
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA, United States
ABSTRACT: A novel, lightweight Fe-25.7Mn-10.6Al-1.2C (wt.%) steel is designed by exploiting the concurrent progress of primary recrystallization and phase transformation, in order to produce an ultrafine-grained, duplex microstructure. The microstructure consists of recrystallized austenite grains surrounded by submicron-sized ferrite grains, and recovered austenite regions with preferential nano-κ-carbide precipitation. This partially recrystallized duplex microstructure demonstrates excellent strength-ductility combinations, e.g. a yield strength of 1251 MPa, an ultimate tensile strength of 1387 MPa, and a total elongation of 43%, arising from the composite response by virtue of diverging constituent strength and strain hardening behaviors. © 2017 Acta Materialia Inc.
AUTHOR KEYWORDS: Ferrite; Lightweight steels; Partial recrystallization; Strain partitioning; Ultrafine grain; κ-carbides
DOCUMENT TYPE: Article

SOURCE: Scopus

Luo, H., Li, Z., Raabe, D.
Hydrogen enhances strength and ductility of an equiatomic high-entropy alloy
(2017) Scientific Reports, 7 (1), art. no. 9892, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85028451950&doi=10.1038%2fs41598-017-10774-4&partnerID=40&md5=13003733848f7eb1f9c59792ece79cfc

DOI: 10.1038/s41598-017-10774-4
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: Metals are key materials for modern manufacturing and infrastructures as well as transpot and energy solutions owing to their strength and formability. These properties can severely deteriorate when they contain hydrogen, leading to unpredictable failure, an effect called hydrogen embrittlement. Here we report that hydrogen in an equiatomic CoCrFeMnNi high-entropy alloy (HEA) leads not to catastrophic weakening, but instead increases both, its strength and ductility. While HEAs originally aimed at entropy-driven phase stabilization, hydrogen blending acts opposite as it reduces phase stability. This effect, quantified by the alloy's stacking fault energy, enables nanotwinning which increases the material's work-hardening. These results turn a bane into a boon: hydrogen does not generally act as a harmful impurity, but can be utilized for tuning beneficial hardening mechanisms. This opens new pathways for the design of strong, ductile, and hydrogen tolerant materials.
DOCUMENT TYPE: Article
SOURCE: Scopus

Kim, J.-K., Jin, L., Sandlöbes, S., Raabe, D.
Diffusional-displacive transformation enables formation of long-period stacking order in magnesium
(2017) Scientific Reports, 7 (1), art. no. 4046, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85021107140&doi=10.1038%2fs41598-017-04343-y&partnerID=40&md5=e40ce3aa35bdd211f1b30c37719e49b8

DOI: 10.1038/s41598-017-04343-y
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ER-C), Peter Grünberg Institute (PGI-5), Research Centre Jülich, Jülich, Germany;
Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Aachen, Germany;
Graduate Institute of Ferrous Technology, Pohang University of Science and Technology, 77 Cheongam-Ro, Pohang, South Korea
ABSTRACT: Mg is the most important lightweight engineering alloy enabling future weight-reduced and fuel-saving engineering solutions. Yet, Mg is soft. Long-period stacking ordered (LPSO) structures in Mg alloys have unique crystal structures, characterized by both complex chemical and stacking order. They are essential for strengthening of Mg alloys. The formation mechanism of these LPSO structures is still under discussion. Here we report that Y/Zn enriched Guinier-Preston (GP) zones observed in a lean Mg-Y-Zn model alloy are precursors of early stage LPSO structures. We provide evidence of a new type of phase transformation mechanism which comprises the diffusional formation of Y/Zn enriched GP zones and their subsequent shear transformation into LPSO building blocks. The mechanism constitutes a new type of coupled diffusional-displacive phase formation sequence which may also be applicable to other alloy systems.
DOCUMENT TYPE: Article

SOURCE: Scopus

Springer, H., Baron, C., Szczepaniak, A., Uhlenwinkel, V., Raabe, D.
Stiff, light, strong and ductile: nano-structured High Modulus Steel
(2017) Scientific Reports, 7 (1), art. no. 2757, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85020412282&doi=10.1038%2fs41598-017-02861-3&partnerID=40&md5=a79952e03c27cd88857f5d40ed01d338

DOI: 10.1038/s41598-017-02861-3
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Foundation Institute of Material Science (IWT), Department of Production Engineering, University of Bremen, Badgasteiner Straße 3, Bremen, Germany
ABSTRACT: Structural material development for lightweight applications aims at improving the key parameters strength, stiffness and ductility at low density, but these properties are typically mutually exclusive. Here we present how we overcome this trade-off with a new class of nano-structured steel - TiB2 composites synthesised in-situ via bulk metallurgical spray-forming. Owing to the nano-sized dispersion of the TiB2 particles of extreme stiffness and low density - obtained by the in-situ formation with rapid solidification kinetics - the new material has the mechanical performance of advanced high strength steels, and a 25% higher stiffness/density ratio than any of the currently used high strength steels, aluminium, magnesium and titanium alloys. This renders this High Modulus Steel the first density-reduced, high stiffness, high strength and yet ductile material which can be produced on an industrial scale. Also ideally suited for 3D printing technology, this material addresses all key requirements for high performance and cost effective lightweight design. © The Author(s) 2017.
DOCUMENT TYPE: Article
SOURCE: Scopus

Jafari, M., Jamshidian, M., Ziaei-Rad, S., Raabe, D., Roters, F.
Constitutive modeling of strain induced grain boundary migration via coupling crystal plasticity and phase-field methods
(2017) International Journal of Plasticity, 99, pp. 19-42.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85028989353&doi=10.1016%2fj.ijplas.2017.08.004&partnerID=40&md5=2c7d2cc8f25c13d6ff6df15b187a559a

DOI: 10.1016/j.ijplas.2017.08.004
AFFILIATIONS: Department of Mechanical Engineering, Isfahan University of Technology, Isfahan, Iran;
Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: We have developed a thermodynamically-consistent finite-deformation-based constitutive theory to describe strain induced grain boundary migration due to the heterogeneity of stored deformation energy in a plastically deformed polycrystalline cubic metal. Considering a representative volume element, a mesoscale continuum theory is developed based on the coupling between dislocation density-based crystal plasticity and phase field methods. Using the Taylor model-based homogenization method, a multiscale coupled finite-element and phase-field staggered time integration procedure is developed and implemented into the Abaqus/Standard finite element package via a user-defined material subroutine. The developed constitutive model is then used to perform numerical simulations of strain induced grain boundary migration in polycrystalline tantalum. The simulation results are shown to qualitatively and quantitatively agree with experimental results. © 2017 Elsevier Ltd.
AUTHOR KEYWORDS: Constitutive modeling; Crystal plasticity; Finite elements; Phase field; Strain induced boundary migration
DOCUMENT TYPE: Article

SOURCE: Scopus

Sandlöbes, S., Friák, M., Korte-Kerzel, S., Pei, Z., Neugebauer, J., Raabe, D.
A rare-earth free magnesium alloy with improved intrinsic ductility
(2017) Scientific Reports, 7 (1), art. no. 10458, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85028951021&doi=10.1038%2fs41598-017-10384-0&partnerID=40&md5=921f1048c3b63a93fe21bcdba21d586c

DOI: 10.1038/s41598-017-10384-0
AFFILIATIONS: Institut für Metallkunde und Metallphysik, RWTH Aachen University, Kopernikusstr. 14, Aachen, Germany;
Institute of Physics of Materials, Academy of Sciences of the Czech Republic, v.v.i., Žižkova 22, Brno, Czech Republic;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: Metals are the backbone of manufacturing owing to their strength and formability. Compared to polymers they have high mass density. There is, however, one exception: magnesium. It has a density of only 1.7 g/cm3, making it the lightest structural material, 4.5 times lighter than steels, 1.7 times lighter than aluminum, and even slightly lighter than carbon fibers. Yet, the widespread use of magnesium is hampered by its intrinsic brittleness. While other metallic alloys have multiple dislocation slip systems, enabling their well-known ductility, the hexagonal lattice of magnesium offers insufficient modes of deformation, rendering it intrinsically brittle. We have developed a quantum-mechanically derived treasure map which screens solid solution combinations with electronic bonding, structure and volume descriptors for similarity to the ductile magnesium-rare earth alloys. Using this insight we synthesized a surprisingly simple, compositionally lean, low-cost and industry-compatible new alloy which is over 4 times more ductile and 40% stronger than pure magnesium. The alloy contains 1 wt.% aluminum and 0.1 wt.% calcium, two inexpensive elements which are compatible with downstream recycling constraints. © 2017 The Author(s).
DOCUMENT TYPE: Article
SOURCE: Scopus

Han, J., Kang, S.-H., Lee, S.-J., Kawasaki, M., Lee, H.-J., Ponge, D., Raabe, D., Lee, Y.-K.
Superplasticity in a lean Fe-Mn-Al steel
(2017) Nature Communications, 8 (1), art. no. 751, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85030319437&doi=10.1038%2fs41467-017-00814-y&partnerID=40&md5=fa2767e4bdcc5571a6b88ea60921191a

DOI: 10.1038/s41467-017-00814-y
AFFILIATIONS: Department of Materials Science and Engineering, Yonsei University, Seoul, South Korea;
Division of Materials Science and Engineering, Hanyang University, Seoul, South Korea;
Max-Planck-Institut für Eisenforschung Germany, Max-Planck-Straße 1, Düsseldorf, South Korea;
Department of Materials Science and Engineering, Chungnam National University, Daejeon, South Korea;
Joining and Welding Research Institute, Osaka University, Osaka, Japan
ABSTRACT: Superplastic alloys exhibit extremely high ductility (>300%) without cracks when tensile-strained at temperatures above half of their melting point. Superplasticity, which resembles the flow behavior of honey, is caused by grain boundary sliding in metals. Although several non-ferrous and ferrous superplastic alloys are reported, their practical applications are limited due to high material cost, low strength after forming, high deformation temperature, and complicated fabrication process. Here we

introduce a new compositionally lean (Fe-6.6Mn-2.3Al, wt.%) superplastic medium Mn steel that resolves these limitations. The medium Mn steel is characterized by ultrafine grains, low material costs, simple fabrication, i.e., conventional hot and cold rolling, low deformation temperature (ca. 650 °C) and superior ductility above 1300% at 850 °C. We suggest that this ultrafine-grained medium Mn steel may accelerate the commercialization of superplastic ferrous alloys. © 2017 The Author(s).
DOCUMENT TYPE: Article
SOURCE: Scopus

Li, Z., Raabe, D.
Strong and Ductile Non-equiatomic High-Entropy Alloys: Design, Processing, Microstructure, and Mechanical Properties
(2017) JOM, 69 (11), pp. 2099-2106.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85028014616&doi=10.1007%2fs11837-017-2540-2&partnerID=40&md5=22df761f795f9751e9e1f58b7cc7c5cd

DOI: 10.1007/s11837-017-2540-2
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: We present a brief overview on recent developments in the field of strong and ductile non-equiatomic high-entropy alloys (HEAs). The materials reviewed are mainly based on massive transition-metal solute solutions and exhibit a broad spectrum of microstructures and mechanical properties. Three relevant aspects of such non-equiatomic HEAs with excellent strength–ductility combination are addressed in detail, namely phase stability-guided design, controlled and inexpensive bulk metallurgical processing routes for appropriate microstructure and compositional homogeneity, and the resultant microstructure–property relations. In addition to the multiple principal substitutional elements used in these alloys, minor interstitial alloying elements are also considered. We show that various groups of strong and ductile HEAs can be obtained by shifting the alloy design strategy from single-phase equiatomic to dual- or multiphase non-equiatomic compositional configurations with carefully designed phase instability. This design direction provides ample possibilities for joint activation of a number of strengthening and toughening mechanisms. Some potential research efforts which can be conducted in the future are also proposed. © 2017, The Author(s).
DOCUMENT TYPE: Review
SOURCE: Scopus

Kim, J., Oh, H.S., Kim, W., Choi, P.-P., Raabe, D., Park, E.S.
Modulation of plastic flow in metallic glasses via nanoscale networks of chemical heterogeneities
(2017) Acta Materialia, 140, pp. 116-129.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85027966128&doi=10.1016%2fj.actamat.2017.08.002&partnerID=40&md5=d5cdfcaee085e8cb387dfd63e82815bc

DOI: 10.1016/j.actamat.2017.08.002
AFFILIATIONS: Research Institute of Advanced Materials, Department of Materials Science and Engineering, Seoul National University, Seoul, South Korea;
Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology, Daejeon, South Korea;
Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: We systematically investigate the microstructures of metallic glasses with nanoscale networks of chemical heterogeneities introduced by the presence of a metastable miscibility gap, and their effects on modulating plastic flow of the alloys. Microstructural analysis of as-quenched alloys and the associated thermodynamic assessment in Cu-Zr-Al-Y

metallic glass-forming system suggest that the existence of a metastable miscibility gap can induce not only phase-separated microstructures with sharp phase interfaces but also compositional fluctuations without a clear interface ranging from atomic scale to a few-nanometer scale in the fully amorphous alloys. The statistical analysis of shear avalanches in such compositionally heterogeneous metallic glasses reveals that chemical heterogeneities extending over a few nanometers promote a relatively large population of shear deformation units jammed before the nucleation of mature shear bands. This leads to the multiple nucleation of shear bands and sluggish deformation behavior along them. However, phase interfaces formed by phase separation inside the miscibility gap promote rapid propagation of shear bands at low flow stress, while compositional fluctuations creating non-sharp interfaces emerging at the outside of miscibility gap have relatively high resistance against shear band propagation. We hence suggest that the optimization of nanoscale compositional fluctuations in metallic glasses in terms of topology, percolation and magnitude can be an effective route for improving the materials' damage tolerance upon plastic flow. © 2017 Acta Materialia Inc.
AUTHOR KEYWORDS: Chemical heterogeneity; Metallic glass; Metastable miscibility gap; Plasticity; Shear avalanche
DOCUMENT TYPE: Article
SOURCE: Scopus

Yao, M.J., Welsch, E., Ponge, D., Haghighat, S.M.H., Sandlöbes, S., Choi, P., Herbig, M., Bleskov, I., Hickel, T., Lipinska-Chwalek, M., Shanthraj, P., Scheu, C., Zaefferer, S., Gault, B., Raabe, D.
Strengthening and strain hardening mechanisms in a precipitation-hardened high-Mn lightweight steel
(2017) Acta Materialia, 140, pp. 258-273.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85028459396&doi=10.1016%2fj.actamat.2017.08.049&partnerID=40&md5=f86a8976ba4113ea1edaf2c0eb675ab5

DOI: 10.1016/j.actamat.2017.08.049
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, Düsseldorf, Germany;
Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Aachen, Germany;
Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon, South Korea;
Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich GmbH, Jülich, Germany;
Central Facility for Electron Microscopy (GFE), RWTH Aachen University, Aachen, Germany
ABSTRACT: We report on the strengthening and strain hardening mechanisms in an aged high-Mn lightweight steel (Fe-30.4Mn-8Al-1.2C, wt.%) studied by electron channeling contrast imaging (ECCI), transmission electron microscopy (TEM), atom probe tomography (APT) and correlative TEM/APT. Upon isothermal annealing at 600 °C, nano-sized κ-carbides form, as characterized by TEM and APT. The resultant alloy exhibits high strength and excellent ductility accompanied by a high constant strain hardening rate. In comparison to the as-quenched κ-free state, the precipitation of κ-carbides leads to a significant increase in yield strength (~480 MPa) without sacrificing much tensile elongation. To study the strengthening and strain hardening behavior of the precipitation-hardened material, deformation microstructures were analyzed at different strain levels. TEM and correlative TEM/APT results show that the κ-carbides are primarily sheared by lattice dislocations, gliding on the typical face-centered-cubic (fcc) slip system {111}<110>, leading to particle dissolution and solute segregation. Ordering strengthening is the predominant strengthening mechanism. As the deformation substructure is characterized by planar slip bands, we quantitatively studied the evolution of the slip band spacing

during straining to understand the strain hardening behavior. A good agreement between the calculated flow stresses and the experimental data suggests that dynamic slip band refinement is the main strain hardening mechanism. The influence of κ-carbides on mechanical properties is discussed by comparing the results with that of the same alloy in the as-quenched, κ-free state. © 2017 Acta Materialia Inc.
AUTHOR KEYWORDS: Antiphase boundary; Lightweight; Precipitation; Strain hardening; Strengthening
DOCUMENT TYPE: Article
SOURCE: Scopus

Tang, S., Wang, J.C., Svendsen, B., Raabe, D.
Competitive bcc and fcc crystal nucleation from non-equilibrium liquids studied by phase-field crystal simulation
(2017) Acta Materialia, 139, pp. 196-204.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85028302200&doi=10.1016%2fj.actamat.2017.08.015&partnerID=40&md5=2f606acd48671d8c963b128fbd39fb78

DOI: 10.1016/j.actamat.2017.08.015
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany;
State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Youyi Western Road 127, Xi'an, China;
Material Mechanics, RWTH Aachen University, Aachen, Germany
ABSTRACT: Crystal nucleation is among the most important processes in the synthesis of materials. Here we study the competitive and multistep nucleation process of body centered cubic (bcc) and face centered cubic (fcc) crystals using phase-field crystal simulations. The initial state is a non-equilibrium liquid. This transforms into an amorphous phase composed of clusters with short-range order (SRO) and medium-range order (MRO). Crystal nucleation begins with the formation of MRO clusters structurally similar to the subsequently nucleated crystal. The formation of bcc and fcc nuclei from MRO clusters involves the following steps: (1) formation of a small thin platelet with MRO; (2) its subsequent growth into 3D MRO clusters; (3) development of crystal embryos from MRO clusters; and (4) crystal embryos transformation into a stable crystal nuclei. In addition, the role of bcc precursors in the formation of fcc nuclei is clarified. In particular, {112} surfaces and steps on {110} surfaces of bcc precursors serve as energetically favorable sites for fcc nucleation. This is also reflected in the resulting orientation relationships, i.e., Pitsch, Nishiyama-Wassermann and Kurdjumov-Sachs, between the bcc precursor and fcc nucleus. © 2017 Acta Materialia Inc.
AUTHOR KEYWORDS: Atomistic simulation; Crystallization; Nucleation; Phase-field crystal modeling
DOCUMENT TYPE: Article
SOURCE: Scopus

Bernardi, H.H., Sandim, H.R.Z., Zilnyk, K.D., Verlinden, B., Raabe, D.
Microstructural stability of a niobium single crystal deformed by equal channel angular pressing
(2017) Materials Research, 20 (5), pp. 1238-1247.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85031289302&doi=10.1590%2f1980-5373-MR-2017-0288&partnerID=40&md5=a061ff56ced2df9abc770015d04d7c62

DOI: 10.1590/1980-5373-MR-2017-0288
AFFILIATIONS: Escola de Engenharia de Lorena, Universidade de São Paulo (USP), Lorena, SP, Brazil;
Faculdade de Tecnologia de São José dos Campos, Prof. Jessen Vidal - FATEC-SJC, São José dos Campos, SP, Brazil;
Instituto Federal de Educaçãociência e Tecnologia de São Paulo, Itapetininga, SP, Brazil;

Department of Materials Engineering, Katholieke Universiteit Leuven 3001, Leuven, Belgium;
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
ABSTRACT: A [211]-oriented niobium single crystal was deformed by equal channel angular pressing (ECAP) at room temperature using the route Bc to a total strain of 9.2. A sharp cube texture develops after ECAP processing. The deformed samples were annealed in vacuum from 400°C (673 K) to 900°C (1173 K) for 1 h to evaluate their microstructural stability. Scanning electron microscopy (SEM) was used to image the microstructures of as-deformed and annealed specimens. Electron backscatter diffraction (EBSD) was employed to determine the respective microtextures before and after annealing. Coarsening of the microstructure occurs at a maximum rate at 550°C (823 K) due to discontinuous recrystallization. Normal grain growth replaces discontinuous recrystallization as the main coarsening mechanism above 700°C (973 K).
AUTHOR KEYWORDS: EBSD; ECAP; Grain growth; Niobium; Recrystallization
DOCUMENT TYPE: Article
SOURCE: Scopus

Koyama, M., Rohwerder, M., Tasan, C.C., Bashir, A., Akiyama, E., Takai, K., Raabe, D., Tsuzaki, K.
Recent progress in microstructural hydrogen mapping in steels: quantification, kinetic analysis, and multi-scale characterisation
(2017) Materials Science and Technology (United Kingdom), 33 (13), pp. 1481-1496. Cited 3 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85014524937&doi=10.1080%2f02670836.2017.1299276&partnerID=40&md5=31c552bbe27871fd373f2f942549d2b0

DOI: 10.1080/02670836.2017.1299276
AFFILIATIONS: Department of Mechanical Engineering, Faculty of Engineering, Kyushu University, Fukuoka, Japan;
Department of Interface Chemistry and Surface Engineering, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA, United States;
Thyssenkrupp Bilstein GmbH, Mandern, Germany;
Institute for Materials Research, Tohoku University, Sendai, Japan;
Department of Engineering and Applied Science, Sophia University, Tokyo, Japan;
Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
HYDROGENIUS, Kyushu University, Fukuoka, Japan
ABSTRACT: This paper gives an overview of recent progress in microstructure-specific hydrogen mapping techniques. The challenging nature of mapping hydrogen with high spatial resolution, i.e. at the scale of finest microstructural features, led to the development of various methodologies: thermal desorption spectrometry, silver decoration, the hydrogen microprint technique, secondary ion mass spectroscopy, atom probe tomography, neutron radiography, and the scanning Kelvin probe. These techniques have different characteristics regarding spatial and temporal resolution associated with microstructure-sensitive hydrogen detection. Employing these techniques in a site-specific manner together with other microstructure probing methods enables multi-scale, quantitative, three-dimensional, high spatial, and kinetic resolution hydrogen mapping, depending on the specific multi-probe approaches used. Here, we present a brief overview of the specific characteristics of each method and the progress resulting from their combined application to the field of hydrogen embrittlement. This paper is part of a thematic issue on Hydrogen in Metallic Alloys.

AUTHOR KEYWORDS: atom probe tomography; hydrogen embrittlement; Hydrogen mapping; hydrogen microprinting; kelvin probe; secondary ion mass spectroscopy; silver decoration; thermal desorption spectrometry
DOCUMENT TYPE: Article
SOURCE: Scopus

Raabe, D., Dehm, G., Neugebauer, J., Rohwerder, M.
100 years public–private partnership in metallurgical and materials science research
(2017) Materials Today, 20 (7), pp. 335-337.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85016474327&doi=10.1016%2fj.mattod.2017.02.005&partnerID=40&md5=aadf104ee8fc9b9243a35ad2d632f825

DOI: 10.1016/j.mattod.2017.02.005
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max Planck Str. 1, Düsseldorf, Germany
DOCUMENT TYPE: Letter
SOURCE: Scopus

Li, Z., Körmann, F., Grabowski, B., Neugebauer, J., Raabe, D.
Ab initio assisted design of quinary dual-phase high-entropy alloys with transformation-induced plasticity
(2017) Acta Materialia, 136, pp. 262-270. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85022346760&doi=10.1016%2fj.actamat.2017.07.023&partnerID=40&md5=4a302d84e1bd8724fccdb50a9a047783

DOI: 10.1016/j.actamat.2017.07.023
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany;
Delft University of Technology, Mekelweg 2, Delft, Netherlands
ABSTRACT: We introduce a new class of high-entropy alloys (HEAs), i.e., quinary (five-component) dual-phase (DP) HEAs revealing transformation-induced plasticity (TRIP), designed by using a quantum mechanically based and experimentally validated approach. Ab initio simulations of thermodynamic phase stabilities of Co20Cr20Fe40-xMn20Nix (x = 0–20 at. %) HEAs were performed to screen for promising compositions showing the TRIP-DP effect. The theoretical predictions reveal several promising alloys, which have been cast and systematically characterized with respect to their room temperature phase constituents, microstructures, element distributions and compositional homogeneity, tensile properties and deformation mechanisms. The study demonstrates the strength of ab initio calculations to predict the behavior of multi-component HEAs on the macroscopic scale from the atomistic level. As a prototype example a non-equiatomic Co20Cr20Fe34Mn20Ni6 HEA, selected based on our ab initio simulations, reveals the TRIP-DP effect and hence exhibits higher tensile strength and strain-hardening ability compared to the corresponding equiatomic CoCrFeMnNi alloy. © 2017 Acta Materialia Inc.
AUTHOR KEYWORDS: Ab initio calculation; Dual-phase; High-entropy alloys; Mechanical properties; Phase transformations
DOCUMENT TYPE: Article
SOURCE: Scopus

Ponge, D., Diehl, M., Archie, F., Zaefferer, S., Roters, F., Raabe, D.
Development of damage-resistant dual-phase steels
(2017) Chernye Metally, (9), pp. 40-41.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85030869801&partnerID=40&md5=98241adcbcb4284a82b42218b5626fef

AFFILIATIONS: Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: Dual-phase steels are characterized by high level of mechanical properties and thereby are used in automotive industry for the components

with responsible applications. They are not leaders in the wide spectrum of used high-strength steels, but their potential is not completely used yet. The paper presents development of damage mechanisms of the components made of such steels by the specialists from the Institute of iron and steel research. The correct understanding of such mechanisms allows to improve computer simulation and to optimize technological parameters of dual-phase steels.
AUTHOR KEYWORDS: Cracks; Damage mechanisms; Dual-phase steels; Ferrite; Martensite; Simulation
DOCUMENT TYPE: Article
SOURCE: Scopus

Zhang, J.-L., Tasan, C.C., Lai, M.J., Yan, D., Raabe, D.
Partial recrystallization of gum metal to achieve enhanced strength and ductility
(2017) Acta Materialia, 135, pp. 400-410.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85021446960&doi=10.1016%2fj.actamat.2017.06.051&partnerID=40&md5=1388c7afe119a85423502e625e188f8b

DOI: 10.1016/j.actamat.2017.06.051
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA, United States
ABSTRACT: Here we present a microstructure design approach which leads to partial recrystallization and nano-precipitation within the same single-step heat treatment. This produces a dual-constituent microstructure in Ti-Nb based gum metal, which consists of nano-ω-particle-rich ultrafine recrystallized grain chains embedded in ω-lean subgrain-containing recovered zones. This partially recrystallized microstructure exhibits an improved strength-ductility combination that surpasses the inverse strength-ductility relationship exhibited by materials with similar composition. The strengthening effects due to precipitates and grain refinement were studied by nanoindentation. The deformation mechanisms of the partially recrystallized material were investigated by in-situ scanning electron microscope tensile tests, micro-strain mapping and post-mortem microstructure characterization. The improved mechanical properties are attributed to the high yield strength of the recrystallized grains and the sequential activation of dislocation slip and dislocation channeling. © 2017 Acta Materialia Inc.
AUTHOR KEYWORDS: Dislocation channeling; Gum metal; Microstructure heterogeneity; Partial recrystallization; ω-Phase
DOCUMENT TYPE: Article
SOURCE: Scopus

Zilnyk, K.D., Pradeep, K.G., Choi, P., Sandim, H.R.Z., Raabe, D.
Long-term thermal stability of nanoclusters in ODS-Eurofer steel: An atom probe tomography study
(2017) Journal of Nuclear Materials, 492, pp. 142-147.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85019891782&doi=10.1016%2fj.jnucmat.2017.05.027&partnerID=40&md5=537dff3d40cc8ab2912ba47782ca17d4

DOI: 10.1016/j.jnucmat.2017.05.027
AFFILIATIONS: Escola de Engenharia de Lorena - USP, Lorena, Brazil;
Federal Institute of São Paulo, Itapetininga, Brazil;
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany;
Materials Chemistry, RWTH Aachen University, Kopernikusstr.10, Aachen, Germany;
Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology, 291 Daehak-ro, Yuseong-gu, Daejeon, South Korea

ABSTRACT: Oxide-dispersion strengthened materials are important candidates for several high-temperature structural applications in advanced nuclear power plants. Most of the desirable mechanical properties presented by these materials are due to the dispersion of stable nanoparticles in the matrix. Samples of ODS-Eurofer steel were annealed for 4320 h (6 months) at 800 °C. The material was characterized using atom probe tomography in both conditions (prior and after heat treatment). The particles number density, size distribution, and chemical compositions were determined. No significant changes were observed between the two conditions indicating a high thermal stability of the Y-rich nanoparticles at 800 °C. © 2017 Elsevier B.V.
AUTHOR KEYWORDS: Atom probe tomography; Microstructural stability; Nanoclusters; ODS-Eurofer steel
DOCUMENT TYPE: Article
SOURCE: Scopus

Zenk, C.H., Povstugar, I., Li, R., Rinaldi, F., Neumeier, S., Raabe, D., Göken, M.
A novel type of Co–Ti–Cr-base γ/γ′ superalloys with low mass density
(2017) Acta Materialia, 135, pp. 244-251. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85021105229&doi=10.1016%2fj.actamat.2017.06.024&partnerID=40&md5=201d4a1fc184b346decb5d4cf4dd960d

DOI: 10.1016/j.actamat.2017.06.024
AFFILIATIONS: Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Materials Science & Engineering, Institute I, Martensstr. 5, Erlangen, Germany;
Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany;
Bruker AXS GmbH, Östliche Rheinbrückenstraße 49, Karlsruhe, Germany
ABSTRACT: A γ′ strengthened Co–Ti–Cr superalloy is presented with a mass density ~14 % below that of typical Co–Al–W-based alloys. The lattice misfit is sufficiently low to form coherent cuboidal γ′ precipitates. Atom probe tomography shows that Cr partitions to the γ phase, but increases the γ′ volume fraction compared to a binary Co-Ti alloy to more than 60 %. The solubility of Cr in the γ′ phase is significantly higher than expected from previously published values. The γ′ solvus temperature is above 1100 °C. The yield strength shows a distinct increase above 600 °C surpassing that of Co–9Al–8W (at.%) and conventional Co-base superalloys, even more so when it is normalized by the mass density. © 2017 Acta Materialia Inc.
AUTHOR KEYWORDS: Atom probe tomography (APT); Co-base superalloys; High-temperature deformation; Phase diagram calculation; X-ray diffraction (XRD)
DOCUMENT TYPE: Article
SOURCE: Scopus

Liu, J., Chen, C., Feng, Q., Fang, X., Wang, H., Liu, F., Lu, J., Raabe, D.
Dislocation activities at the martensite phase transformation interface in metastable austenitic stainless steel: An in-situ TEM study
(2017) Materials Science and Engineering A, 703, pp. 236-243.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85025830160&doi=10.1016%2fj.msea.2017.06.107&partnerID=40&md5=d19984dbfafb8e15ad6cd63f54e4e6da

DOI: 10.1016/j.msea.2017.06.107
AFFILIATIONS: Institute of Applied Mechanics, Zhejiang University, Hangzhou, China;
College of Materials Science and Engineering, Zhejiang University, Hangzhou, China;
China Railway Electrification Survey Design & Research Institute Co. Ltd, Tianjing, China;

Northwestern Polytechnical University, Xi'an, China;
Department of Mechanical and Biomedical Engineering, City University of Hong Kong, Hong Kong, China;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: Understanding the mechanism of martensitic transformation is of great importance in developing advanced high strength steels, especially TRansformation-Induced Plasticity (TRIP) steels. The TRIP effect leads to enhanced work-hardening rate, postponed onset of necking and excellent formability. In-situ transmission electron microscopy has been performed to systematically investigate the dynamic interactions between dislocations and α′ martensite at microscale. Local stress concentrations, e.g. from notches or dislocation pile-ups, render free edges and grain boundaries favorable nucleation sites for α′ martensite. Its growth leads to partial dislocation emission on two independent slip planes from the hetero-interface when the austenite matrix is initially free of dislocations. The kinematic analysis reveals that activating slip systems on two independent {111} planes of austenite are necessary in accommodating the interfacial mismatch strain. Full dislocation emission is generally observed inside of austenite regions that contain high density of dislocations. In both situations, phase boundary propagation generates large amounts of dislocations entering into the matrix, which renders the total deformation compatible and provide substantial strain hardening of the host phase. These moving dislocation sources enable plastic relaxation and prevent local damage accumulation by intense slipping on the softer side of the interfacial region. Thus, finely dispersed martensite distribution renders plastic deformation more uniform throughout the austenitic matrix, which explains the exceptional combination of strength and ductility of TRIP steels. © 2017 Elsevier B.V.
AUTHOR KEYWORDS: Deformation; Dislocations; In-situ transmission electron microscopy; Martensitic transformation
DOCUMENT TYPE: Article
SOURCE: Scopus

Fischle, A., Neff, P., Raabe, D.
The relaxed-polar mechanism of locally optimal Cosserat rotations for an idealized nanoindentation and comparison with 3D-EBSD experiments
(2017) Zeitschrift fur Angewandte Mathematik und Physik, 68 (4), art. no. 90, . Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85026744572&doi=10.1007%2fs00033-017-0834-4&partnerID=40&md5=3d092e7ab6b79c426b68211fdcbe389e

DOI: 10.1007/s00033-017-0834-4
AFFILIATIONS: Institut für Numerische Mathematik, TU Dresden, Zellescher Weg 12-14, Dresden, Germany;
Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany;
Head of Lehrstuhl für Nichtlineare Analysis und Modellierung Fakultät für Mathematik, Universität Duisburg-Essen, Thea-Leymann Str. 9, Essen, Germany;
Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: The rotation polar (F) ∈ SO (3) arises as the unique orthogonal factor of the right polar decomposition F=polar(F)U of a given invertible matrix F∈ GL +(3). In the context of nonlinear elasticity Grioli (Boll Un Math Ital 2:252–255, 1940) discovered a geometric variational characterization of polar (F) as a unique energy-minimizing rotation. In preceding works, we have analyzed a generalization of Grioli’s variational approach with weights (material parameters) μ> 0 and μc≥ 0 (Grioli: μ= μc). The energy subject to minimization coincides with the Cosserat shear-stretch contribution arising in any geometrically nonlinear, isotropic and

quadratic Cosserat continuum model formulated in the deformation gradient field F: = ∇ φ: Ω → GL +(3) and the microrotation field R: Ω → SO (3). The corresponding set of non-classical energy-minimizing rotations rpolarμ,μc±(F):=arg minR∈SO(3){Wμ,μc(R;F):=μ||sym(RTF-1)||2+μc||skew(RTF-1)||2}represents a new relaxed-polar mechanism. Our goal is to motivate this mechanism by presenting it in a relevant setting. To this end, we explicitly construct a deformation mapping φnano which models an idealized nanoindentation and compare the corresponding optimal rotation patterns rpolar1,0±(Fnano) with experimentally obtained 3D-EBSD measurements of the disorientation angle of lattice rotations due to a nanoindentation in solid copper. We observe that the non-classical relaxed-polar mechanism can produce interesting counter-rotations. A possible link between Cosserat theory and finite multiplicative plasticity theory on small scales is also explored. © 2017, Springer International Publishing AG.
AUTHOR KEYWORDS: 3D-EBSD; Cosserat; Cosserat couple modulus; Counter-rotations; Grioli's theorem; Micropolar; Nanoindentation; Non-symmetric stretch; Relaxed-polar mechanism; Rotations
DOCUMENT TYPE: Article
SOURCE: Scopus

Raabe, D., Ponge, D., Wang, M.-M., Herbig, M., Belde, M., Springer, H.
1 billion tons of nanostructure - Segregation engineering enables confined transformation effects at lattice defects in steels
(2017) IOP Conference Series: Materials Science and Engineering, 219 (1), art. no. 012006, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85028313345&doi=10.1088%2f1757-899X%2f219%2f1%2f012006&partnerID=40&md5=7daa10a6e471b62510c2eba7e2093414

DOI: 10.1088/1757-899X/219/1/012006
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: The microstructure of complex steels can be manipulated by utilising the interaction between the local mechanical distortions associated with lattice defects, such as dislocations and grain boundaries, and solute components that segregate to them. Phenomenologically these phenomena can be interpreted in terms of the classical Gibbs adsorption isotherm, which states that the total system energy can be reduced by removing solute atoms from the bulk and segregating them at lattice defects. Here we show how this principle can be utilised through appropriate heat treatments not only to enrich lattice defects by solute atoms, but also to further change these decorated regions into confined ordered structural states or even to trigger localized decomposition and phase transformations. This principle, which is based on the interplay between the structure and mechanics of lattice defects on the one hand and the chemistry of the alloy's solute components on the other hand, is referred to as segregation engineering. In this concept solute decoration to specific microstructural traps, viz. lattice defects, is not taken as an undesired effect, but instead seen as a tool for manipulating specific lattice defect structures, compositions and properties that lead to beneficial material behavior. Owing to the fairly well established underlying thermodynamic and kinetic principles, such local decoration and transformation effects can be tuned to proceed in a self-organised manner by adjusting (i) the heat treatment temperatures for matching the desired trapping, transformation or reversion regimes, and (ii) the corresponding timescales for sufficient solute diffusion to the targeted defects. Here we show how this segregation engineering principle can be applied to design self-organized nano- and microstructures in complex steels for improving their mechanical properties.
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Knoll, H., Ocylok, S., Weisheit, A., Springer, H., Jägle, E., Raabe, D.
Combinatorial Alloy Design by Laser Additive Manufacturing
(2017) Steel Research International, 88 (8), art. no. 1600416, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85006965989&doi=10.1002%2fsrin.201600416&partnerID=40&md5=4aff33963a10bad60aa8a128398e5e71

DOI: 10.1002/srin.201600416
AFFILIATIONS: Department for Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany; Fraunhofer Institut für Lasertechnik (FhG - ILT), Steinbachstraße 15, Aachen, Germany
ABSTRACT: The authors uses laser additive manufacturing (LAM) as a combinatorial method for synthesizing microstructurally and compositionally piecewise graded bulk alloys. Authors fabricate blocks consisting of a sequence of ≈500 μm thick tool steel layers, each with different chemical composition, by laser metal deposition where alloy powders are deposited layer-wise on a substrate. The reference materials are a Cr–Mo–V hot working tool steel and a Ni-based maraging steel. The layers between them consist of corresponding blends of the two materials with varying composition from layer to layer (alloy volume fractions 80:20, 60:40, 40:60, and 20:80). The bulk alloy is hot rolled and heat treated. Subsequently each layer is characterized for microstructure, chemical composition and mechanical properties using electron back scatter diffraction, tensile testing, and indentation. The approach is an efficient high-throughput method enabling rapid probing of novel compositional alloy blends. It can be applied for finding new alloys both, by LAM and for LAM. For the tool steel blends synthesized here, authors observe that the Cr–Mo–V tool steel, when mixed with the Ni-base maraging steel, can be continuously tuned for a strength-ductility profile in the range of 800–1650 MPa strength and 15–25% tensile elongation.
AUTHOR KEYWORDS: alloy design; combinatorial synthesis; laser additive manufacturing; maraging steel; tool steel
DOCUMENT TYPE: Article
SOURCE: Scopus

Kirchlechner, C., Djaziri, S., Li, Y., Herbig, M., Grabowski, B., Nematollahi, G.A., Goto, S., Kirchheim, R., Neugebauer, J., Raabe, D., Dehm, G.
Konlcurrenzlose Festiglceit durch extremes Umformen von Stahl
(2017) Stahl und Eisen, 137 (8), pp. 58-63.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85028876849&partnerID=40&md5=e1ad13596a82a54c02fb316e6b0fc826

AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Diisseldorf, Germany
DOCUMENT TYPE: Article
SOURCE: Scopus

Kolb, M., Zenk, C.H., Kirzinger, A., Povstugar, I., Raabe, D., Neumeier, S., Göken, M.
Influence of rhenium on γ′-strengthened cobalt-base superalloys
(2017) Journal of Materials Research, 32 (13), pp. 2551-2559.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85024124276&doi=10.1557%2fjmr.2017.242&partnerID=40&md5=8f2722bc2fd5b375afc2b1a9d0a62c3c

DOI: 10.1557/jmr.2017.242
AFFILIATIONS: Friedrich-Alexander-Universität Erlangen-Nürnberg, Materials Science and Engineering, Institute i, Erlangen, Germany;
Max-Planck-Institut für Eisenforschung, Department of Microstructure Physics and Alloy Design, Düsseldorf, Germany

ABSTRACT: The element Re is known to be a very potent strengthener concerning the creep properties of Ni-base superalloys. In this paper the influence of Re on the properties of new γ′-strengthened Co-base superalloys is addressed. Atom probe tomography reveals that Re partitions preferentially to the γ phase, but not as pronounced as in ni-base superalloys. Nanoindentation and micro-pillar compression tests of the γ′ phase indicate an increase of the hardness and the critical resolved shear stress caused by a considerable concentration of Re in the γ′ phase. Creep investigations show that the positive effect of Re is by far not as pronounced as in Ni-base superalloys. Several effects, which can contribute to this behavior, such as the lower Re concentration in γ and hence a slightly reduced effective diffusion coefficient, a smaller diffusion barrier of Re in Co compared to Ni, a slightly lower lattice misfit and γ′ volume fraction of the Re-containing alloy, are discussed.
AUTHOR KEYWORDS: Co; microstructure; nano-indentation; transmission electron microscopy (TEM)
DOCUMENT TYPE: Article
SOURCE: Scopus

Diehl, M., An, D., Shanthraj, P., Zaefferer, S., Roters, F., Raabe, D.
Crystal plasticity study on stress and strain partitioning in a measured 3D dual phase steel microstructure
(2017) Physical Mesomechanics, 20 (3), pp. 311-323.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85029607682&doi=10.1134%2fS1029959917030079&partnerID=40&md5=4da7ef71d32ab05d7da5191a39ff018d

DOI: 10.1134/S1029959917030079
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: Dual phase steels are advanced high strength alloys typically used for structural parts and reinforcements in car bodies. Their good combination of strength and ductility and their lean composition render them an economically competitive option for realizing multiple lightweight design options in automotive engineering. The mechanical response of dual phase steels is the result of the strain and stress partitioning among the ferritic and martensitic phases and the individual crystallographic grains and subgrains of these phases. Therefore, understanding how these microstructural features influence the global and local mechanical properties is of utmost importance for the design of improved dual phase steel grades. While multiple corresponding simulation studies have been dedicated to the investigation of dual phase steel micromechanics, numerical tools and experiment techniques for characterizing and simulating real 3D microstructures of such complex materials have been emerged only recently. Here we present a crystal plasticity simulation study based on a 3D dual phase microstructure which is obtained by EBdD tomography, also referred to as 3D EBdD (EBdD—electron backscatter diffraction). In the present case we utilized a 3D EBdD serial sectioning approach based on mechanical polishing. Moreover, sections of the 3D microstructure are used as 2D models to study the effect of this simplification on the stress and strain distribution. The simulations are conducted using a phenomenological crystal plasticity model and a spectral method approach implemented in the Düsseldorf Advanced Material Simulation Kit (DAMAdK).
AUTHOR KEYWORDS: 3D EBdD; crystal plasticity; DAMAdK; dual phase steel; microstructure; spectral method
DOCUMENT TYPE: Article
SOURCE: Scopus

Stechmann, G., Zaefferer, S., Schwarz, T., Konijnenberg, P., Raabe, D., Gretener, C., Kranz, L., Perrenoud, J., Buecheler, S., Nath Tiwari, A.

A correlative investigation of grain boundary crystallography and electronic properties in CdTe thin film solar cells
(2017) Solar Energy Materials and Solar Cells, 166, pp. 108-120. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85015925825&doi=10.1016%2fj.solmat.2017.03.022&partnerID=40&md5=b33f93042db38e3a8631f0824d3cfb47

DOI: 10.1016/j.solmat.2017.03.022
AFFILIATIONS: Max-Planck-Institut Für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany;
Bruker Nano GmbH Am Studio 2D, Berlin, Germany;
Empa – Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, Dübendorf, Switzerland
ABSTRACT: Evaluating the impact of grain boundaries on the functional properties of CdTe thin films, consistent with processes used in photovoltaic solar cells, requires a direct correlation between their crystallography and electronic behavior. In the present work, we propose a novel comprehensive approach, combining focused ion beam/electron backscatter diffraction tomography (3D-EBSD) and quantitative cathodoluminescence (CL). While the former enables a full five parameter characterization of the interfaces, the latter is used to probe the spatial distribution of recombination centers and their characteristics. In addition, critical issues associated with sample preparation are also discussed. Monte Carlo simulations, together with electron channeling contrast imaging (ECCI), are employed to evaluate the effects of ion-sputtering damage on the CL response of CdTe thin films, as well as to overcome the resolution limit of EBSD characterization. The results obtained show that, at the exception of coherent twin boundaries, all interfaces behave as non-radiative recombination centers, exhibiting significant recombination velocities. Furthermore, there is no direct correlation between the misorientation parameters of the interfaces and their recombination properties. In contrast, trends can be observed when considering the crystallography of the boundary planes.
AUTHOR KEYWORDS: Cathodoluminescence; CdTe; EBSD; ECCI; Grain boundary
DOCUMENT TYPE: Article
SOURCE: Scopus

Szczepaniak, A., Springer, H., Aparicio-Fernández, R., Baron, C., Raabe, D.
Strengthening Fe – TiB2 based high modulus steels by precipitations
(2017) Materials and Design, 124, pp. 183-193. Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85016515821&doi=10.1016%2fj.matdes.2017.03.042&partnerID=40&md5=ec27aed12879d5937d14f890853c55b5

DOI: 10.1016/j.matdes.2017.03.042
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: We systematically studied the microstructure, mechanical and physical properties of hyper-eutectic Fe – TiB2 high modulus steels (20 vol% TiB2) with (Si, Mn, Ni) and Cu additions for the formation of G-phase and Cu precipitates during ageing treatments. Alloying with Si, Mn and Ni led predominantly to pronounced solid solution strengthening, reaching tensile strength (UTS) values up to 1100 MPa after quenching. While G-phase formation could be observed in aged materials, its preferential formation on grain boundaries significantly deteriorated ductility. Its effects on strength were partially balanced by a decrease of grain boundary density. Additions of 1 and 2 wt% Cu, respectively, led to lower strength in the as quenched state, but also to significant strengthening via ageing. The peak ageing conditions as well as the Cu particle structure and size are comparable to values reported for Cu strengthened interstitial free steels and Fe-Cu alloys. Both alloying additions slightly lowered the specific

elastic modulus of the HMS, most pronounced for Cu addition with a drop of about 3 GPa cm3 g− 1 per wt% and also promoted embrittlement. Microstructure-property relationships and consequences for future alloy design, especially towards more ductile hypo-eutectic HMS, are outlined and discussed. © 2017
AUTHOR KEYWORDS: Cu precipitation; Density; G-phase; Steel; Stiffness
DOCUMENT TYPE: Article
SOURCE: Scopus

Lemmens, B., Springer, H., De Graeve, I., De Strycker, J., Raabe, D., Verbeken, K.
Effect of silicon on the microstructure and growth kinetics of intermetallic phases formed during hot-dip aluminizing of ferritic steel
(2017) Surface and Coatings Technology, 319, pp. 104-109. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85017158089&doi=10.1016%2fj.surfcoat.2017.03.040&partnerID=40&md5=b1bffc2b29d1343906733dad22d4487d

DOI: 10.1016/j.surfcoat.2017.03.040
AFFILIATIONS: Department of Materials, Textiles and Chemical Engineering, Ghent University (UGent), Tech Lane Ghent Science Park – Campus A, Technologiepark 903, Zwijnaarde, Belgium;
Research group of Electrochemical and Surface Engineering (SURF), Vrije Universiteit Brussel (VUB), Pleinlaan 2, Brussels, Belgium;
Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
ArcelorMittal Global R&D Gent, J.F.Kennedylaan 3, Zelzate, Belgium
DOCUMENT TYPE: Article
SOURCE: Scopus

Schwarz, T., Cojocaru-Mirédin, O., Mousel, M., Redinger, A., Raabe, D., Choi, P.-P.
Formation of nanometer-sized Cu-Sn-Se particles in Cu2ZnSnSe4 thin-films and their effect on solar cell efficiency
(2017) Acta Materialia, 132, pp. 276-284.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85018281189&doi=10.1016%2fj.actamat.2017.04.056&partnerID=40&md5=8e9df14042f17162cdaad60183f6d5b8

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AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany;
RWTH Aachen University, I. Physikalisches Institut IA, Aachen, Germany;
University of Luxembourg, Laboratory for Photovoltaics, 41, Rue du Brill, Belvaux, Luxembourg;
Helmholtz-Zentrum Berlin, Department Complex Compound Semiconductor Materials for Photovoltaics, Berlin, Germany;
Korea Advanced Institute of Science and Technology, Department of Materials Science and Engineering, Daejeon, South Korea
ABSTRACT: Atom probe tomography and transmission electron microscopy are used to study the formation of nano-sized Cu-Sn-Se particles in Cu2ZnSnSe4 thin-films. For a Cu-rich precursor, which was deposited at 320 °C under Cu- and Zn-rich growth conditions, Cu2-xSe grains at the surface are detected. During annealing the precursor at 500 °C in a SnSe + Se atmosphere most of the Cu2-xSe is transformed to Cu2ZnSnSe4 via the consumption of excessive ZnSe and incorporation of Sn. However, atom probe tomography studies also reveal the formation of various nanometer-sized Cu-Sn-Se particles close to the CdS/Cu2ZnSnSe4 interface. One of those particles has a composition close to the Cu2SnSe3 compound. This phase has a smaller band gap than Cu2ZnSnSe4 and is proposed to lead to a significant drop in the open-circuit voltage and could be the main cause for a detrimental p-n junction and the zero efficiency of the final device. Possible effects of the other phases on solar cell performance and formation mechanisms are discussed as well. © 2017 Acta Materialia Inc.

AUTHOR KEYWORDS: Atom probe tomography; Microstructure; Precipitates; Thin films; Transmission electron microscopy
DOCUMENT TYPE: Article
SOURCE: Scopus

Choi, W.S., Sandlöbes, S., Malyar, N.V., Kirchlechner, C., Korte-Kerzel, S., Dehm, G., De Cooman, B.C., Raabe, D.
Dislocation interaction and twinning-induced plasticity in face-centered cubic Fe-Mn-C micro-pillars
(2017) Acta Materialia, 132, pp. 162-173.
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AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Institut für Metallkunde und Metallphysik, RWTH Aachen University, Aachen, Germany;
Graduate Institute of Ferrous Technology, Pohang University of Science and Technology, Pohang, South Korea
ABSTRACT: Deformation twinning contributes to a high work-hardening rate through modification of the dislocation structure and a dynamic Hall-Petch effect in polycrystalline steel. Due to the well-defined compression axis and limited deformation volume of micro-pillars, micro-compression testing is a suitable method to investigate the mechanisms of deformation twinning and the interactions of dislocations with twin boundaries. The material investigated is an austenitic Fe-22 wt%Mn-0.6 wt%C twining-induced plasticity steel. Micro-pillars oriented preferentially for deformation twinning and dislocation glide are compressed and the activated deformation systems are characterized. We observe that deformation twinning induces higher flow stresses and a more unstable work-hardening behavior than dislocation glide, while dislocation glide dominated deformation results in a stable work-hardening behavior. The higher flow stresses and unstable work-hardening behavior in micro-pillars oriented for deformation twinning are assumed to be caused by the activation of secondary slip systems and accumulated plastic deformation. © 2017 Acta Materialia Inc.
AUTHOR KEYWORDS: Deformation twinning; Dislocation interaction; Micro-pillar compression; Transmission electron microscopy; TWIP steel; Work-hardening
DOCUMENT TYPE: Article
SOURCE: Scopus

Li, Z., Tasan, C.C., Pradeep, K.G., Raabe, D.
A TRIP-assisted dual-phase high-entropy alloy: Grain size and phase fraction effects on deformation behavior
(2017) Acta Materialia, 131, pp. 323-335. Cited 4 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85017382396&doi=10.1016%2fj.actamat.2017.03.069&partnerID=40&md5=9c3837db87624e9e37014d59656e7da5

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AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany;
Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA, United States;
Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, Aachen, Germany
ABSTRACT: We present a systematic microstructure oriented mechanical property investigation for a newly developed class of transformation-induced plasticity-assisted dual-phase high-entropy alloys (TRIP-DP-HEAs) with varying grain sizes and phase fractions. The DP-HEAs in both, as-homogenized and recrystallized states consist of a face-centered cubic

(FCC) matrix containing a high-density of stacking faults and a laminate hexagonal close-packed (HCP) phase. No elemental segregation was observed in grain interiors or at interfaces even down to near-atomic resolution, as confirmed by energy-dispersive X-ray spectroscopy and atom probe tomography. The strength-ductility combinations of the recrystallized DP-HEAs (Fe50Mn30Co10Cr10) with varying FCC grain sizes and HCP phase fractions prior to deformation are superior to those of the recrystallized equiatomic single-phase Cantor reference HEA (Fe20Mn20Ni20Co20Cr20). The multiple deformation micro-mechanisms (including strain-induced transformation from FCC to HCP phase) and dynamic strain partitioning behavior among the two phases are revealed in detail. Both, strength and ductility of the DP-HEAs increase with decreasing the average FCC matrix grain size and increasing the HCP phase fraction prior to loading (in the range of 10–35%) due to the resulting enhanced stability of the FCC matrix. These insights are used to project some future directions for designing advanced TRIP-HEAs through the adjustment of the matrix phase's stability by alloy tuning and grain size effects. © 2017 Acta Materialia Inc.
AUTHOR KEYWORDS: Dual phase; Grain refining; High-entropy alloy; Mechanical properties; Phase transformations
DOCUMENT TYPE: Article
SOURCE: Scopus

Luo, H., Li, Z., Chen, Y.-H., Ponge, D., Rohwerder, M., Raabe, D.
Hydrogen effects on microstructural evolution and passive film characteristics of a duplex stainless steel
(2017) Electrochemistry Communications, 79, pp. 28-32. Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85018652362&doi=10.1016%2fj.elecom.2017.04.013&partnerID=40&md5=fa6dd6afd74019fb1105aabbd384598b

DOI: 10.1016/j.elecom.2017.04.013
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, Düsseldorf, Germany
ABSTRACT: We revealed the effects of hydrogen on the microstructural evolution and passive film properties of a 2205 duplex stainless steel by the joint use of electron backscatter diffraction (EBSD), electron channeling contrast imaging (ECCI), X-ray photoelectron spectroscopy (XPS) and electrochemical measurements. The microstructural analysis results show that effects of hydrogen on the two phases are different: (i) in austenite, stacking faults are induced by hydrogen, and (ii) in ferrite, hydrogen causes an increase of the dislocation density. The XPS analysis revealed that hydrogen reduced the occurrence of Cr2O3 and nitrogen in the passive film, leading to the reduction of their overall thickness. Furthermore, for the first time we demonstrated that the hydrogen release time plays an important role in the electrochemical behavior of the hydrogen charged steel. © 2017 Elsevier B.V.
AUTHOR KEYWORDS: Corrosion; Duplex stainless steel; Hydrogen; Microstructure; Passive film
DOCUMENT TYPE: Article
SOURCE: Scopus

Schnabel, V., Köhler, M., Music, D., Bednarcik, J., Clegg, W.J., Raabe, D., Schneider, J.M.
Ultra-stiff metallic glasses through bond energy density design
(2017) Journal of Physics Condensed Matter, 29 (26), art. no. 265502, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85020469275&doi=10.1088%2f1361-648X%2faa72cb&partnerID=40&md5=04ca127b6eb05d64855d8505dbd6dd39

DOI: 10.1088/1361-648X/aa72cb
AFFILIATIONS: Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, Aachen, Germany;

Laboratory for Nanometallurgy, ETH Zürich, Vladimir-Prelog-Weg 5, Zürich, Switzerland;
Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
Deutsches Elektronen Synchrotron DESY, FS-PE Group, Notkestrasse 85, Hamburg, Germany;
Department of Materials Science and Metallurgy, Cambridge University, 27 Charles Babbage Rd, Cambridge, United Kingdom
ABSTRACT: The elastic properties of crystalline metals scale with their valence electron density. Similar observations have been made for metallic glasses. However, for metallic glasses where covalent bonding predominates, such as metalloid metallic glasses, this relationship appears to break down. At present, the reasons for this are not understood. Using high energy x-ray diffraction analysis of melt spun and thin film metallic glasses combined with density functional theory based molecular dynamics simulations, we show that the physical origin of the ultrahigh stiffness in both metalloid and non-metalloid metallic glasses is best understood in terms of the bond energy density. Using the bond energy density as novel materials design criterion for ultra-stiff metallic glasses, we are able to predict a Co33.0Ta3.5B63.5 short range ordered material by density functional theory based molecular dynamics simulations with a high bond energy density of 0.94 eV Å-3 and a bulk modulus of 263 GPa, which is 17% greater than the stiffest Co-B based metallic glasses reported in literature. © 2017 IOP Publishing Ltd.
AUTHOR KEYWORDS: electronic structure; metallic glass; stiffness; topology
DOCUMENT TYPE: Article
SOURCE: Scopus

Peng, Z., Rohwerder, M., Choi, P.-P., Gault, B., Meiners, T., Friedrichs, M., Kreilkamp, H., Klocke, F., Raabe, D.
Atomic diffusion induced degradation in bimetallic layer coated cemented tungsten carbide
(2017) Corrosion Science, 120, pp. 1-13.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85014320014&doi=10.1016%2fj.corsci.2017.01.007&partnerID=40&md5=8994a89f0c6aed6950be61a096cff797

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AFFILIATIONS: Max-Planck Institut für Eisenforschung GmbH, Max-Planck Str. 1, Düsseldorf, Germany;
Korea Advanced Institute of Science and Technology (KAIST), Department of Materials Science and Engineering, Daejeon, South Korea;
Fraunhofer Institute for Production Technology (IPT), Steinbachstrasse 17, Aachen, Germany
ABSTRACT: We investigated the temporal degradation of glass moulding dies, made of cemented tungsten carbide coated with PtIr on an adhesive Cr or Ni interlayer, by electron microscopy and atom probe tomography. During the exposure treatments at 630 °C under an oxygen partial pressure of 1.12 × 10−23 bar, Cr (Ni) was found to diffuse outwards via grain boundaries in the PtIr, altering the surface morphology. Upon dissolution of the interlayer, the WC substrate also started degrading. Extensive interdiffusion processes involving PtIr, Cr (Ni) and WC took place, leading to the formation of intermetallic phases and voids, deteriorating the adhesion of the coating. © 2017 The Authors
AUTHOR KEYWORDS: A. Metal coatings; A. Sputtered film; B. TEM; C. Interfaces; C. Oxidation
DOCUMENT TYPE: Article
SOURCE: Scopus

Cojocaru-Mirédin, O., Abdellaoui, L., Nagli, M., Zhang, S., Yu, Y., Scheu, C., Raabe, D., Wuttig, M., Amouyal, Y.

Role of Nanostructuring and Microstructuring in Silver Antimony Telluride Compounds for Thermoelectric Applications
(2017) ACS Applied Materials and Interfaces, 9 (17), pp. 14779-14790. Cited 1 time.
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DOI: 10.1021/acsami.7b00689
AFFILIATIONS: I. Institut of Physics, RWTH Aachen University, Sommerfeldstraße 14, Aachen, Germany;
Max-Planck Institut für Eisenforschung GmbH, Max-Planck Straße 1, Düsseldorf, Germany;
Materials Analytics, RWTH Aachen University, Kopernikusstraße 10, Aachen, Germany;
Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Technion City, Haifa, Israel
ABSTRACT: Thermoelectric (TE) materials are of utmost significance for conversion of heat flux into electrical power in the low-power regime. Their conversion efficiency depends strongly on the microstructure. AgSbTe2-based compounds are high-efficiency TE materials suitable for the mid-temperature range. Herein, we explore an Ag16.7Sb30Te53.3 alloy (at %) subjected to heat treatments at 380 °C for different durations aimed at nucleation and coarsening of Sb2Te3-precipitates. To characterize the Sb2Te3-precipitation, we use a set of methods combining thermal and electrical measurements in concert with transmission electron microscopy and atom probe tomography. We find correlations between the measured TE transport coefficients and the applied heat treatments. Specifically, the lowest electrical and thermal conductivity values are obtained for the as-quenched state, whereas the highest values are observed for alloys aged for 8 h. In turn, long-term heat treatments result in intermediate values of transport coefficients. We explain these findings in terms of interplay between precipitate formation and variations in the matrix composition, highlighting the importance of thermal stability of the material under service conditions. © 2017 American Chemical Society.
AUTHOR KEYWORDS: atom probe tomography; electron microscopy; silver-antimony-telluride compounds; thermal conductivity; thermoelectric materials
DOCUMENT TYPE: Article
SOURCE: Scopus

Kürnsteiner, P., Wilms, M.B., Weisheit, A., Barriobero-Vila, P., Jägle, E.A., Raabe, D.
Massive nanoprecipitation in an Fe-19Ni-xAl maraging steel triggered by the intrinsic heat treatment during laser metal deposition
(2017) Acta Materialia, 129, pp. 52-60. Cited 2 times.
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AFFILIATIONS: Department Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Fraunhofer Institute for Laser Technology ILT, Aachen, Germany;
Institute of Materials Science and Technology, Vienna University of Technology, Vienna, Austria
ABSTRACT: Due to the layer-by-layer build-up of additively manufactured parts, the deposited material experiences a cyclic re-heating in the form of a sequence of temperature pulses. In the current work, this “intrinsic heat treatment (IHT)” was exploited to induce the precipitation of NiAl nanoparticles in an Fe-19Ni-xAl (at%) model maraging steel, a system known for rapid clustering. We used Laser Metal Deposition (LMD) to synthesize compositionally graded specimens. This allowed for the efficient screening

of effects associated with varying Al contents ranging from 0 to 25 at% and for identifying promising concentrations for further studies. Based on the existence of the desired martensitic matrix, an upper bound for the Al concentration of 15 at% was defined. Owing to the presence of NiAl precipitates as observed by Atom Probe Tomography (APT), a lower bound of 3–5 at% Al was established. Within this concentration window, increasing the Al concentration gave rise to an increase in hardness by 225 HV due to an exceptionally high number density of 1025 NiAl precipitates per m3, as measured by APT. This work demonstrates the possibility of exploiting the IHT of the LMD process for the production of samples that are precipitation strengthened during the additive manufacturing process without need for any further heat treatment. © 2017
AUTHOR KEYWORDS: Additive manufacturing; Atom Probe Tomography; High-energy X-ray diffraction; Nanoparticles; Precipitation strengthening
DOCUMENT TYPE: Article
SOURCE: Scopus

Diehl, M., Wicke, M., Shanthraj, P., Roters, F., Brueckner-Foit, A., Raabe, D.
Coupled Crystal Plasticity–Phase Field Fracture Simulation Study on Damage Evolution Around a Void: Pore Shape Versus Crystallographic Orientation
(2017) JOM, 69 (5), pp. 872-878. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85015630485&doi=10.1007%2fs11837-017-2308-8&partnerID=40&md5=7f93e60f350dfd72dd80b185749d6477

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AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany;
Institute for Materials Engineering, University of Kassel, Moenchebergstraße 3, Kassel, Germany
ABSTRACT: Various mechanisms such as anisotropic plastic flow, damage nucleation, and crack propagation govern the overall mechanical response of structural materials. Understanding how these mechanisms interact, i.e. if they amplify mutually or compete with each other, is an essential prerequisite for the design of improved alloys. This study shows—by using the free and open source software DAMASK (the Düsseldorf Advanced Material Simulation Kit)—how the coupling of crystal plasticity and phase field fracture methods can increase the understanding of the complex interplay between crystallographic orientation and the geometry of a void. To this end, crack initiation and propagation around an experimentally obtained pore with complex shape is investigated and compared to the situation of a simplified spherical void. Three different crystallographic orientations of the aluminum matrix hosting the defects are considered. It is shown that crack initiation and propagation depend in a non-trivial way on crystallographic orientation and its associated plastic behavior as well as on the shape of the pore. © 2017, The Author(s).
DOCUMENT TYPE: Article
SOURCE: Scopus

Diehl, M., Groeber, M., Haase, C., Molodov, D.A., Roters, F., Raabe, D.
Identifying Structure–Property Relationships Through DREAM.3D Representative Volume Elements and DAMASK Crystal Plasticity Simulations: An Integrated Computational Materials Engineering Approach
(2017) JOM, 69 (5), pp. 848-855. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85015212435&doi=10.1007%2fs11837-017-2303-0&partnerID=40&md5=1565bfb48a7173728ea7bcfa670a64ca

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AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany;
Air Force Research Laboratory, WPAFB, 2230 Tenth StreetOH, United States;

Institut für Eisenhüttenkunde der RWTH Aachen, RWTH Aachen, Intzestraße 1, Aachen, Germany;
Institut für Metallkunde und Metallphysik, RWTH Aachen, Kopernikusstraße 14, Aachen, Germany
ABSTRACT: Predicting, understanding, and controlling the mechanical behavior is the most important task when designing structural materials. Modern alloy systems—in which multiple deformation mechanisms, phases, and defects are introduced to overcome the inverse strength–ductility relationship—give raise to multiple possibilities for modifying the deformation behavior, rendering traditional, exclusively experimentally-based alloy development workflows inappropriate. For fast and efficient alloy design, it is therefore desirable to predict the mechanical performance of candidate alloys by simulation studies to replace time- and resource-consuming mechanical tests. Simulation tools suitable for this task need to correctly predict the mechanical behavior in dependence of alloy composition, microstructure, texture, phase fractions, and processing history. Here, an integrated computational materials engineering approach based on the open source software packages DREAM.3D and DAMASK (Düsseldorf Advanced Materials Simulation Kit) that enables such virtual material development is presented. More specific, our approach consists of the following three steps: (1) acquire statistical quantities that describe a microstructure, (2) build a representative volume element based on these quantities employing DREAM.3D, and (3) evaluate the representative volume using a predictive crystal plasticity material model provided by DAMASK. Exemplarily, these steps are here conducted for a high-manganese steel.
DOCUMENT TYPE: Article
SOURCE: Scopus

Koyama, M., Akiyama, E., Lee, Y.-K., Raabe, D., Tsuzaki, K.
Overview of hydrogen embrittlement in high-Mn steels
(2017) International Journal of Hydrogen Energy, 42 (17), pp. 12706-12723.
Cited 3 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85015726032&doi=10.1016%2fj.ijhydene.2017.02.214&partnerID=40&md5=d3417b2efd36dc05c3a56da5d5838a11

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AFFILIATIONS: Department of Mechanical Engineering, Kyushu University, Motooka 744, Nishi-ku, Fukuoka, Fukuoka, Japan;
Institute for Materials Research, Tohoku University, Katahira 2-1-1, Aoba-ku, Sendai, Japan;
Department of Materials Science and Engineering, Yonsei University, Seoul, South Korea;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straβe 1, Düsseldorf, Germany;
HYDROGENIUS, Kyushu University, Motooka 744, Nishi-ku, Fukuoka, Fukuoka, Japan
ABSTRACT: Hydrogen and fuels derived from it will serve as the energy carriers of the future. The associated rapidly growing demand for hydrogen energy-related infrastructure materials has stimulated multiple engineering and scientific studies on the hydrogen embrittlement resistance of various groups of high performance alloys. Among these, high-Mn steels have received special attention owing to their excellent strength – ductility – cost relationship. However, hydrogen-induced delayed fracture has been reported to occur in deep-drawn cup specimens of some of these alloys. Driven by this challenge we present here an overview of the hydrogen embrittlement research carried out on high-Mn steels. The hydrogen embrittlement susceptibility of high-Mn steels is particularly sensitive to their chemical composition since the various alloying elements simultaneously affect the material's stacking fault energy, phase stability, hydrogen uptake behavior, surface oxide scales and interstitial diffusivity, all of which affect the hydrogen embrittlement susceptibility.

Here, we discuss the contribution of each of these factors to the hydrogen embrittlement susceptibility of these steels and discuss pathways how certain embrittlement mechanisms can be hampered or even inhibited. Examples of positive effects of hydrogen on the tensile ductility are also introduced. © 2017 Hydrogen Energy Publications LLC
AUTHOR KEYWORDS: Austenitic steel; Deformation twinning; Hydrogen embrittlement; Hydrogen segregation; Martensitic transformation
DOCUMENT TYPE: Review
SOURCE: Scopus

Jiang, S., Wang, H., Wu, Y., Liu, X., Chen, H., Yao, M., Gault, B., Ponge, D., Raabe, D., Hirata, A., Chen, M., Wang, Y., Lu, Z.
Ultrastrong steel via minimal lattice misfit and high-density nanoprecipitation
(2017) Nature, 544 (7651), pp. 460-464. Cited 14 times.
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DOI: 10.1038/nature22032
AFFILIATIONS: State Key Laboratory for Advanced Metals and Materials, University of Science and Technology Beijing, Beijing, China;
Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße, Düsseldorf, Germany;
WPI Advanced Institute for Materials Research, Tohoku University, Sendai, Japan;
Mathematics for Advanced Materials-OIL, AIST-Tohoku University, Sendai, Japan;
Department of Materials Science and Engineering, Johns Hopkins University, Baltimore, MD, United States
ABSTRACT: Next-generation high-performance structural materials are required for lightweight design strategies and advanced energy applications. Maraging steels, combining a martensite matrix with nanoprecipitates, are a class of high-strength materials with the potential for matching these demands. Their outstanding strength originates from semi-coherent precipitates, which unavoidably exhibit a heterogeneous distribution that creates large coherency strains, which in turn may promote crack initiation under load. Here we report a counterintuitive strategy for the design of ultrastrong steel alloys by high-density nanoprecipitation with minimal lattice misfit. We found that these highly dispersed, fully coherent precipitates (that is, the crystal lattice of the precipitates is almost the same as that of the surrounding matrix), showing very low lattice misfit with the matrix and high anti-phase boundary energy, strengthen alloys without sacrificing ductility. Such low lattice misfit (0.03 ± 0.04 per cent) decreases the nucleation barrier for precipitation, thus enabling and stabilizing nanoprecipitates with an extremely high number density (more than 10 24 per cubic metre) and small size (about 2.7 ± 0.2 nanometres). The minimized elastic misfit strain around the particles does not contribute much to the dislocation interaction, which is typically needed for strength increase. Instead, our strengthening mechanism exploits the chemical ordering effect that creates backstresses (the forces opposing deformation) when precipitates are cut by dislocations. We create a class of steels, strengthened by Ni(Al,Fe) precipitates, with a strength of up to 2.2 gigapascals and good ductility (about 8.2 per cent). The chemical composition of the precipitates enables a substantial reduction in cost compared to conventional maraging steels owing to the replacement of the essential but high-cost alloying elements cobalt and titanium with inexpensive and lightweight aluminium. Strengthening of this class of steel alloy is based on minimal lattice misfit to achieve maximal precipitate dispersion and high cutting stress (the stress required for dislocations to cut through coherent precipitates and thus produce plastic deformation), and we envisage that this lattice

misfit design concept may be applied to many other metallic alloys.
DOCUMENT TYPE: Article
SOURCE: Scopus

Tarzimoghadam, Z., Ponge, D., Klöwer, J., Raabe, D.
Hydrogen-assisted failure in Ni-based superalloy 718 studied under in situ hydrogen charging: The role of localized deformation in crack propagation
(2017) Acta Materialia, 128, pp. 365-374. Cited 6 times.
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DOI: 10.1016/j.actamat.2017.02.059
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany;
VDM Metals GmbH, Kleffstraße 23, Altena, Germany
ABSTRACT: We investigated hydrogen embrittlement in Ni-based superalloy 718 by tensile testing at slow strain rate (10−4 s−1) under continuous electrochemical hydrogen charging. Hydrogen-assisted cracking mechanisms were studied via electron backscatter diffraction (EBSD) analysis and electron channeling contrast imaging (ECCI). In order to elucidate the effects of stress or strain in the cracking mechanisms, material conditions with different strength levels were investigated, including samples in solution annealed (as water quenched) and 780 °C age-hardened states. The microstructure observations in the vicinity of the cracks enabled us to establish correlations between the microstructure, crack initiation sites, and crack propagation pathways. Fracture in the hydrogen-charged samples was dominated by localized plastic deformation. Strain-controlled transgranular cracking was caused by shear localization due to hydrogen-enhanced localized plasticity (HELP) and void nucleation and coalescence along {111} slip planes in both, the solution annealed and age-hardened materials. Stress-assisted intergranular cracking in the presence of hydrogen was only observed in the high strength age-hardened material, due to slip localization at grain boundaries, grain boundary triple junction cracking, and δ/γ-matrix interface cracking. To investigate the effect of δ-phase in crack propagation along grain boundaries, the over-aged state (aged at 870 °C) with different precipitation conditions for the δ-phase was also investigated. Observations confirmed that presence of δ-phase promotes hydrogen-induced intergranular failure by initializing micro-cracks from δ/γ interfaces. © 2017 Acta Materialia Inc.
AUTHOR KEYWORDS: Alloy 718; Hydrogen embrittlement; Hydrogen-enhanced localized plasticity; Planar slip; Slip localization
DOCUMENT TYPE: Article
SOURCE: Scopus

Peng, Z., Choi, P.-P., Gault, B., Raabe, D.
Evaluation of Analysis Conditions for Laser-Pulsed Atom Probe Tomography: Example of Cemented Tungsten Carbide
(2017) Microscopy and Microanalysis, 23 (2), pp. 431-442. Cited 2 times.
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DOI: 10.1017/S1431927616012654
AFFILIATIONS: Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strae 1, Düsseldorf, Germany;
Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon, South Korea
ABSTRACT: Cemented tungsten carbide has been analyzed using laser-pulsed atom probe tomography (APT). The influence of experimental parameters,

including laser pulse energy, pulse repetition rate, and specimen base temperature, on the acquired data were evaluated from different aspects, such as mass spectrum, chemical composition, noise-to-signal ratio, and multiple events. Within all the applied analysis conditions, only 1 MHz pulse repetition rate led to a strong detector saturation effect, resulting in a largely biased chemical composition. A comparative study of the laser energy settings showed that an ~12 times higher energy was required for the less focused green laser of the LEAPTM 3000X HR system to achieve a similar evaporation field as the finer spot ultraviolet laser of the LEAPTM 5000 XS system.
AUTHOR KEYWORDS: atom probe tomography; data quality; laser-pulsing; tungsten carbide
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Stoffers, A., Barthel, J., Liebscher, C.H., Gault, B., Cojocaru-Mirédin, O., Scheu, C., Raabe, D.
Correlating Atom Probe Tomography with Atomic-Resolved Scanning Transmission Electron Microscopy: Example of Segregation at Silicon Grain Boundaries
(2017) Microscopy and Microanalysis, 23 (2), pp. 291-299.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85013031434&doi=10.1017%2fS1431927617000034&partnerID=40&md5=e3e7aae82b11a589261bd875cf19a0f6

DOI: 10.1017/S1431927617000034
AFFILIATIONS: Institute of Physics (IA), RWTH Aachen University, Otto-Blumenthal-Strae, Aachen, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strae 1, Düsseldorf, Germany;
Central Facility for Electron Microscopy, RWTH Aachen University, Ahornstrae 55, Aachen, Germany;
Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich GmbH, Jülich, Germany
ABSTRACT: In the course of a thorough investigation of the performance-structure-chemistry interdependency at silicon grain boundaries, we successfully developed a method to systematically correlate aberration-corrected scanning transmission electron microscopy and atom probe tomography. The correlative approach is conducted on individual APT and TEM specimens, with the option to perform both investigations on the same specimen in the future. In the present case of a Σ9 grain boundary, joint mapping of the atomistic details of the grain boundary topology, in conjunction with chemical decoration, enables a deeper understanding of the segregation of impurities observed at such grain boundaries.
AUTHOR KEYWORDS: atom probe tomography; correlative microscopy; grain boundary; scanning transmission electron microscopy; silicon
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Dey, P., Nazarov, R., Dutta, B., Yao, M., Herbig, M., Friák, M., Hickel, T., Raabe, D., Neugebauer, J.
Ab initio explanation of disorder and off-stoichiometry in Fe-Mn-Al-C κ carbides
(2017) Physical Review B, 95 (10), art. no. 104108, . Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85016265499&doi=10.1103%2fPhysRevB.95.104108&partnerID=40&md5=ccd43f7d3f0b6bc979680c4da95a0826

DOI: 10.1103/PhysRevB.95.104108
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Lawrence Livermore National Laboratory, Livermore, CA, United States;

Institute of Physics of Materials, V.v.i., Academy of Sciences of the Czech Republic, Brno, Czech Republic;
Central European Institute of Technology, CEITEC MU, Masaryk University, Kamenice 5, Brno, Czech Republic
ABSTRACT: Carbides play a central role for the strength and ductility in many materials. Simulating the impact of these precipitates on the mechanical performance requires knowledge about their atomic configuration. In particular, the C content is often observed to substantially deviate from the ideal stoichiometric composition. In this work, we focus on Fe-Mn-Al-C steels, for which we determined the composition of the nanosized κ carbides (Fe,Mn)3AlC by atom probe tomography in comparison to larger precipitates located in grain boundaries. Combining density functional theory with thermodynamic concepts, we first determine the critical temperatures for the presence of chemical and magnetic disorder in these carbides. Second, the experimentally observed reduction of the C content is explained as a compromise between the gain in chemical energy during partitioning and the elastic strains emerging in coherent microstructures.

DOCUMENT TYPE: Article
SOURCE: Scopus

Li, Z., Raabe, D.
Influence of compositional inhomogeneity on mechanical behavior of an interstitial dual-phase high-entropy alloy
(2017) Materials Chemistry and Physics, . Article in Press. Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85018323834&doi=10.1016%2fj.matchemphys.2017.04.050&partnerID=40&md5=e4fae30ee0051e35d0c5684f87bd93f0

DOI: 10.1016/j.matchemphys.2017.04.050
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237, Düsseldorf, Germany
ABSTRACT: In this study we present and discuss the influence of compositional inhomogeneity on the mechanical behavior of an interstitially alloyed dual-phase non-equiatomic high-entropy alloy (Fe49.5Mn30Co10Cr10C0.5). Various processing routes including hot-rolling, homogenization, cold-rolling and recrystallization annealing were performed on the cast alloys to obtain samples in different compositional homogeneity states. Grain sizes of the alloys were also considered. Tensile testing and microstructural investigations reveal that the deformation behavior of the interstitial dual-phase high-entropy alloy samples varied significantly depending on the compositional homogeneity of the specimens probed. In the case of coarse-grains (~300 μm) obtained for cast alloys without homogenization treatment, ductility and strain-hardening of the material was significantly reduced due to its compositional inhomogeneity. This detrimental effect was attributed to preferred deformation-driven phase transformation occurring in the Fe enriched regions with lower stacking fault energy, promoting early stress-strain localization. The grain-refined alloy (~4 μm) with compositional heterogeneity which was obtained for recrystallization annealed alloys without homogenization treatment was characterized by almost total loss in work-hardening. This effect was attributed to large local shear strains due to the inhomogeneous planar slip. These insights demonstrate the essential role of compositional homogeneity through applying corresponding processing steps for the development of advanced high-entropy alloys.
AUTHOR KEYWORDS: Compositional homogeneity; Dual phase; High-entropy alloy; Mechanical properties; Transformation-induced plasticity
DOCUMENT TYPE: Article in Press

SOURCE: Scopus

Koyama, M., Zhang, Z., Wang, M., Ponge, D., Raabe, D., Tsuzaki, K., Noguchi, H., Tasan, C.C.
Bone-like crack resistance in hierarchical metastable nanolaminate steels
(2017) Science, 355 (6329), pp. 1055-1057. Cited 11 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85014953898&doi=10.1126%2fscience.aal2766&partnerID=40&md5=69e0cd2da82ed0534cb2e25835da5bf5

DOI: 10.1126/science.aal2766
AFFILIATIONS: Kyushu University, Motooka 744, Fukuoka, Japan;
Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA, United States
ABSTRACT: Fatigue failures create enormous risks for all engineered structures, as well as for human lives, motivating large safety factors in design and, thus, inefficient use of resources. Inspired by the excellent fracture toughness of bone, we explored the fatigue resistance in metastability-assisted multiphase steels. We show here that when steel microstructures are hierarchical and laminated, similar to the substructure of bone, superior crack resistance can be realized. Our results reveal that tuning the interface structure, distribution, and phase stability to simultaneously activate multiple micromechanisms that resist crack propagation is key for the observed leap in mechanical response. The exceptional properties enabled by this strategy provide guidance for all fatigue-resistant alloy design efforts.
DOCUMENT TYPE: Article
SOURCE: Scopus

Nagashima, T., Koyama, M., Bashir, A., Rohwerder, M., Tasan, C.C., Akiyama, E., Raabe, D., Tsuzaki, K.
Interfacial hydrogen localization in austenite/martensite dual-phase steel visualized through optimized silver decoration and scanning Kelvin probe force microscopy
(2017) Materials and Corrosion, 68 (3), pp. 306-310. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84985998193&doi=10.1002%2fmaco.201609104&partnerID=40&md5=d774f1ef55f0d5570cb3c5b46f258cf9

DOI: 10.1002/maco.201609104
AFFILIATIONS: Department of Mechanical Engineering, Kyushu University, 744 Motooka, Nishi-ku, Fukuoka, Japan;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straβe 1Düsseldorf, Germany;
Christian Doppler Laboratory for Diffusion and Segregation MechanismsDüsseldorf, Germany;
National Institute for Materials Science, 1-2-1, SengenIbaraki, Japan
ABSTRACT: The hydrogen distribution in an austenite–martensite dual-phase steel was investigated using silver decoration and scanning Kelvin probe force microscopy. The silver decoration technique optimized for spacial resolution reveals interfacial segregation of hydrogen along the plate-type martensite–martensite grain boundaries. In addition, the scanning Kelvin probe force microscopy kinetically elucidates that hydrogen preferentially diffused out from the martensite–martensite grain boundaries. These preferential sites of hydrogen desorption correspond to the regions of hydrogen-assisted damage.
AUTHOR KEYWORDS: hydrogen-assisted damage; scanning Kelvin probe force microscopy; silver decoration; thermal desorption spectroscopy
DOCUMENT TYPE: Article
SOURCE: Scopus

Seol, J.-B., Na, S.-H., Gault, B., Kim, J.-E., Han, J.-C., Park, C.-G., Raabe, D.
Core-shell nanoparticle arrays double the strength of steel
(2017) Scientific Reports, 7, art. no. 42547, . Cited 4 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85013662922&doi=10.1038%2fsrep42547&partnerID=40&md5=a7eef1e6c964b060fc0ad32b6d807698

DOI: 10.1038/srep42547
AFFILIATIONS: National Institute for Nanomaterials Technology, POSTECH, Pohang, South Korea;
Department of Materials Science and Engineering, POSTECH, Pohang, South Korea;
Max-Planck-Institut für Eisenforschung, Max-Planck-Strae 1, Düsseldorf, Germany
ABSTRACT: Manipulating structure, defects and composition of a material at the atomic scale for enhancing its physical or mechanical properties is referred to as nanostructuring. Here, by combining advanced microscopy techniques, we unveil how formation of highly regular nano-arrays of nanoparticles doubles the strength of an Fe-based alloy, doped with Ti, Mo, and V, from 500 MPa to 1 GPa, upon prolonged heat treatment. The nanoparticles form at moving heterophase interfaces during cooling from the high-temperature face-centered cubic austenite to the body-centered cubic ferrite phase. We observe MoC and TiC nanoparticles at early precipitation stages as well as core-shell nanoparticles with a Ti-C rich core and a Mo-V rich shell at later precipitation stages. The core-shell structure hampers particle coarsening, enhancing the material's strength. Designing such highly organized metallic core-shell nanoparticle arrays provides a new pathway for developing a wide range of stable nano-architectured engineering metallic alloys with drastically enhanced properties. ©The Author(s) 2017.
DOCUMENT TYPE: Article
SOURCE: Scopus

Zhang, J., Tasan, C.C., Lai, M.J., Dippel, A.-C., Raabe, D.
Complexion-mediated martensitic phase transformation in Titanium
(2017) Nature Communications, 8, art. no. 14210, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85011589705&doi=10.1038%2fncomms14210&partnerID=40&md5=23f76a887dc71dfda42de90d3c98d1b9

DOI: 10.1038/ncomms14210
AFFILIATIONS: Max-Planck-Institut Für Eisenforschung, Max-Planck-Strasse 1, Düsseldorf, Germany;
State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, China;
Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA, United States;
Deutsches Elektronen-Synchrotron DESY, Notkestrasse 85, Hamburg, Germany
ABSTRACT: The most efficient way to tune microstructures and mechanical properties of metallic alloys lies in designing and using athermal phase transformations. Examples are shape memory alloys and high strength steels, which together stand for 1,500 million tons annual production. In these materials, martensite formation and mechanical twinning are tuned via composition adjustment for realizing complex microstructures and beneficial mechanical properties. Here we report a new phase transformation that has the potential to widen the application window of Ti alloys, the most important structural material in aerospace design, by nanostructuring them via complexion-mediated transformation. This is a reversible martensitic transformation mechanism that leads to a final nanolaminate structure of α″ (orthorhombic) martensite bounded with planar complexions of athermal ω (a-ω hexagonal). Both phases are crystallographically related to the parent β

(BCC) matrix. As expected from a planar complexion, the a-ω is stable only at the hetero-interface. © The Author(s) 2017.
DOCUMENT TYPE: Article
SOURCE: Scopus

Li, Z., Tasan, C.C., Springer, H., Gault, B., Raabe, D.
Interstitial atoms enable joint twinning and transformation induced plasticity in strong and ductile high-entropy alloys
(2017) Scientific Reports, 7, art. no. 40704, . Cited 8 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85009483676&doi=10.1038%2fsrep40704&partnerID=40&md5=b016ca6bed8044c8df40cab9c3c8136d

DOI: 10.1038/srep40704
AFFILIATIONS: Max-Planck-Institut Für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA, United States
ABSTRACT: High-entropy alloys (HEAs) consisting of multiple principle elements provide an avenue for realizing exceptional mechanical, physical and chemical properties. We report a novel strategy for designing a new class of HEAs incorporating the additional interstitial element carbon. This results in joint activation of twinning- and transformation-induced plasticity (TWIP and TRIP) by tuning the matrix phase's instability in a metastable TRIP-assisted dual-phase HEA. Besides TWIP and TRIP, such alloys benefit from massive substitutional and interstitial solid solution strengthening as well as from the composite effect associated with its dual-phase structure. Nanosize particle formation and grain size reduction are also utilized. The new interstitial TWIP-TRIP-HEA thus unifies all metallic strengthening mechanisms in one material, leading to twice the tensile strength compared to a single-phase HEA with similar composition, yet, at identical ductility. © The Author(s) 2017.
DOCUMENT TYPE: Article
SOURCE: Scopus

Svendsen, B., Shanthraj, P., Raabe, D.
Finite-deformation phase-field chemomechanics for multiphase, multicomponent solids
(2017) Journal of the Mechanics and Physics of Solids, . Article in Press.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85031726409&doi=10.1016%2fj.jmps.2017.10.005&partnerID=40&md5=1165327a1c5c3de85a8c25dca8e9465a

DOI: 10.1016/j.jmps.2017.10.005
AFFILIATIONS: Material Mechanics, RWTH Aachen University, Schinkelstr. 2, 52062 Aachen, Germany;
Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: The purpose of this work is the development of a framework for the formulation of geometrically non-linear inelastic chemomechanical models for a mixture of multiple chemical components diffusing among multiple transforming solid phases. The focus here is on general model formulation. No specific model or application is pursued in this work. To this end, basic balance and constitutive relations from non-equilibrium thermodynamics and continuum mixture theory are combined with a phase-field-based description of multicomponent solid phases and their interfaces. Solid phase modeling is based in particular on a chemomechanical free energy and stress relaxation via the evolution of phase-specific concentration fields, order-parameter fields (e.g., related to chemical ordering, structural ordering, or defects), and local internal variables. At the mixture level, differences or contrasts in phase composition and phase local deformation in phase interface regions are treated as mixture internal variables. In this context, various phase

interface models are considered. In the equilibrium limit, phase contrasts in composition and local deformation in the phase interface region are determined via bulk energy minimization. On the chemical side, the equilibrium limit of the current model formulation reduces to a multicomponent, multiphase, generalization of existing two-phase binary alloy interface equilibrium conditions (e.g., KKS). On the mechanical side, the equilibrium limit of one interface model considered represents a multiphase generalization of Reuss-Sachs conditions from mechanical homogenization theory. Analogously, other interface models considered represent generalizations of interface equilibrium conditions consistent with laminate and sharp-interface theory. In the last part of the work, selected existing models are formulated within the current framework as special cases and discussed in detail. © 2017 Elsevier Ltd.
AUTHOR KEYWORDS: Chemical inhomogeneity; Chemomechanics; Continuum thermodynamics; Finite deformation; Mechanical inhomogeneity
DOCUMENT TYPE: Article in Press
SOURCE: Scopus

Aparicio-Fernández, R., Szczepaniak, A., Springer, H., Raabe, D.
Crystallisation of amorphous Fe – Ti – B alloys as a design pathway for nano-structured high modulus steels
(2017) Journal of Alloys and Compounds, 704, pp. 565-573.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85013113155&doi=10.1016%2fj.jallcom.2017.02.077&partnerID=40&md5=0db6491d4aae812657c8fa7a8eef60b4

DOI: 10.1016/j.jallcom.2017.02.077
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: We systematically studied the transformation temperatures, type and growth kinetics of phases formed during annealing of Fe – 10.10 Ti – 3.86 B alloys, initially amorphous after rapid solidification. With increasing the temperature, four distinct crystallisation steps could be determined. At 530 °C α-Fe (partly supersaturated with Ti) appeared, and at 600 °C small amounts of not identified phases formed in the amorphous matrix. The matrix fully crystallised to α-Fe and contained (Fe,Ti)-B rich particles at 730 °C, which transformed to the equilibrium TiB2phase at 755 °C. During annealing at 1000 °C both α-Fe and TiB2exhibited parabolic, apparently diffusion controlled growth at rates of about 2.333 and 0.466 nm s−1/2, respectively. Factors influencing the amorphisation as well as strategies for the fabrication of nano-structured high stiffness low density steels via crystallisation from an amorphous precursor state are outlined and discussed. © 2017 Elsevier B.V.
AUTHOR KEYWORDS: Density; Metal matrix composites; Metallic glass; Steel; Stiffness; Titanium diboride
DOCUMENT TYPE: Article
SOURCE: Scopus

Grilli, N., Janssens, K.G.F., Nellessen, J., Sandlöbes, S., Raabe, D.
Multiple slip dislocation patterning in a dislocation-based crystal plasticity finite element method
(2017) International Journal of Plasticity, . Article in Press.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85031316540&doi=10.1016%2fj.ijplas.2017.09.015&partnerID=40&md5=aa8cc34c7ed19cc4302a2f54eb015c2e

DOI: 10.1016/j.ijplas.2017.09.015
AFFILIATIONS: Laboratory for Nuclear Materials, Nuclear Energy and Safety Department, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland;
NXMM Laboratory, IMX, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland;
Max-Planck-Institut für Eisenforschung GmbH, Department for Microstructure Physics and Alloy Design, 40237 Düsseldorf, Germany;

Institute of Physical Metallurgy and Metal Physics, RWTH, Aachen University, D-52056 Aachen, Germany
ABSTRACT: Dislocation structures forming during cyclic loading of fcc metals are fatigue damage precursors. Their specific structures are caused by the motion and interactions of dislocations. Depending on the load conditions, the grain orientation, the stacking fault energy, a variety of different dislocation structures appear in the material such as labyrinths, cells, veins and persistent slip bands. We present a continuum dislocation-based model for cyclic fatigue and incorporate it into a crystal plasticity finite element solver. A method for the simulation of dislocation junction formation is introduced, which reproduces the behaviour of discrete objects, such as dislocations, in a continuum framework. The formation of dislocation walls after 50 and 100 deformation cycles at 0.95% and 0.65% strain amplitude starting from an initial random dislocation distribution is predicted for ⟨001⟩ and ⟨11-0⟩ oriented crystals. Simulations and cyclic tension-compression experiments of polycrystalline 316L stainless steel are performed to compare our model with another model based on edge and screw dislocation densities. The simulated dislocation structures and experimental results, obtained with the electron channeling contrast imaging technique, are compared using a 2D orientation distribution function of the dislocation structures. The dominant orientation of dislocation walls is predicted by the new model; it turns out to be perpendicular to the intersection line between the two slip planes involved in their formation and at an angle of around 45o from the loading axis. This agrees well with the experimental observations and represents a step forward for understanding the formation mechanism of these dislocation structures. © 2017 Elsevier Ltd.
AUTHOR KEYWORDS: Dislocation-based crystal plasticity; Dislocations; Fatigue; Finite element method
DOCUMENT TYPE: Article in Press
SOURCE: Scopus

Jägle, E.A., Sheng, Z., Kürnsteiner, P., Ocylok, S., Weisheit, A., Raabe, D.
Comparison of maraging steel micro- and nanostructure produced conventionally and by laser additive manufacturing
(2017) Materials, 10 (1), art. no. 8, . Cited 3 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85011650417&doi=10.3390%2fma10010008&partnerID=40&md5=ef218db598e974b3663751a36bf2a9dc

DOI: 10.3390/ma10010008
AFFILIATIONS: Department Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, Düsseldorf, Germany;
Institut für Eisenhüttenkunde, Rheinisch-Westfälische Technische Hochschule Aachen, Intzestrasse 1, Aachen, Germany;
Competence Area Additive Manufacturing and Functional Layers, Fraunhofer Institut für Lasertechnik, Steinbachstrasse 15, Aachen, Germany
ABSTRACT: Maraging steels are used to produce tools by Additive Manufacturing (AM) methods such as Laser Metal Deposition (LMD) and Selective Laser Melting (SLM). Although it is well established that dense parts can be produced by AM, the influence of the AM process on the microstructure-in particular the content of retained and reversed austenite as well as the nanostructure, especially the precipitate density and chemistry, are not yet explored. Here, we study these features using microhardness measurements, Optical Microscopy, Electron Backscatter Diffraction (EBSD), Energy Dispersive Spectroscopy (EDS), and Atom Probe Tomography (APT) in the as-produced state and during ageing heat treatment. We find that due to microsegregation, retained austenite exists in the as-LMD- and as-SLM-produced states but not in the conventionally-produced material. The hardness in the as-LMD-produced state is higher than in the

conventionally and SLM-produced materials, however, not in the uppermost layers. By APT, it is confirmed that this is due to early stages of precipitation induced by the cyclic re-heating upon further deposition- i.e., the intrinsic heat treatment associated with LMD. In the peak-aged state, which is reached after a similar time in all materials, the hardness of SLM- and LMD-produced material is slightly lower than in conventionally-produced material due to the presence of retained austenite and reversed austenite formed during ageing. © 2017 by the authors.
AUTHOR KEYWORDS: Additive manufacturing; Atom probe tomography; Austenite reversion; Intrinsic heat treatment; Laser metal deposition; Maraging steel; Precipitation strengthening
DOCUMENT TYPE: Article
SOURCE: Scopus

Koprek, A., Cojocaru-Miredin, O., Wuerz, R., Freysoldt, C., Gault, B., Raabe, D.
Cd and Impurity Redistribution at the CdS/CIGS Interface after Annealing of CIGS-Based Solar Cells Resolved by Atom Probe Tomography
(2017) IEEE Journal of Photovoltaics, 7 (1), art. no. 7762819, pp. 313-321.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84999114096&doi=10.1109%2fJPHOTOV.2016.2629841&partnerID=40&md5=05c3bdf471662c90c5ebd5dfb1d6d895

DOI: 10.1109/JPHOTOV.2016.2629841
AFFILIATIONS: Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
I. Physikalisches Institut IA, RWTH Aachen University, Aachen, Germany;
Zentrum für Sonnenenergie-und Wasserstoff-Forschung Baden Württemberg, Stuttgart, Germany;
Department of Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: Cd and impurity redistribution in the vicinity of the CdS/C(In,Ga)Se2 (CIGS) interface is studied by means of atom probe tomography. We find an increase of the Cd content in the CIGS layer and redistribution of O (in form of O+ and OH+) at the CdS/CIGS interface after annealing the samples at 200, 250, and 300 °C. About 0.2 at% of Na impurity is observed at the interface, across the range of heat treatments performed here. Simultaneously, the J-V measurements of the treated samples show a drop in the open-circuit voltage and fill factor, and thus of the cell efficiency, compared with the untreated sample. © 2011-2012 IEEE.
AUTHOR KEYWORDS: Atom probe tomography (APT); C(In,Ga)Se2 (CIGS) thin-film solar cells; CdS/CIGS interface; impurity segregation; internal interfaces
DOCUMENT TYPE: Article
SOURCE: Scopus

Luebke, A., Loza, K., Patnaik, R., Enax, J., Raabe, D., Prymak, O., Fabritius, H.-O., Gaengler, P., Epple, M.
Reply to the 'Comments on "dental lessons from past to present: Ultrastructure and composition of teeth from plesiosaurs, dinosaurs, extinct and recent sharks"' by H. Botella: Et al., RSC Adv., 2016, 6, 74384-74388
(2017) RSC Advances, 7 (11), pp. 6215-6222.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85010366286&doi=10.1039%2fc6ra27121a&partnerID=40&md5=35f7b64e8b00d9b83276976eca9ffd62

DOI: 10.1039/c6ra27121a
AFFILIATIONS: Institute of Inorganic Chemistry, Center for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, Universitaetsstr. 5-7, Essen, Germany;
Centre of Advanced Study in Geology, Panjab University, Chandigarh, India;

Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany;
ORMED, Institute for Oral Medicine, University of Witten/Herdecke, Alfred-Herrhausen-Straße 45, Witten, Germany
ABSTRACT: The structure and composition of 13 fossilized tooth and bone samples aged between 3 and 70 million years were analysed. It was found that they all contained high amounts of fluoroapatite. This indicates that originally present hydroxyapatite had been converted to fluoroapatite during the diagenesis. Thus, the chemical analysis allows no conclusion with respect to the original composition of our fossil samples. Our results indicate that the diagenetic transformation of hydroxyapatite into fluoroapatite is at least partially dependent on microstructural characteristics of the original tissue such as the degree of porosity. © 2017 The Royal Society of Chemistry.
DOCUMENT TYPE: Article
SOURCE: Scopus

Baron, C., Springer, H., Raabe, D.
Combinatorial screening of the microstructure–property relationships for Fe–B–X stiff, light, strong and ductile steels
(2016) Materials and Design, 112, pp. 131-139.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84988499970&doi=10.1016%2fj.matdes.2016.09.065&partnerID=40&md5=34bc67890142e5da46ca78e5210f4c71

DOI: 10.1016/j.matdes.2016.09.065
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: We systematically screened the mechanical, physical and microstructural properties of the alloy systems Fe–10 B–5 X (at.%; X = Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W), in order to identify novel metal matrix composite steels as next generation lightweight materials. The alloys were synthesised and processed by bulk liquid metallurgical techniques, and subsequently analysed for their mechanical and physical properties (i.e. Young's modulus, density, tensile strength and ductility) as well their microstructure and constitution. From the wide variety of observed boride phases and microstructures and resultant different properties, Cr and Zr additions were found to be most effective. Cr qualifies well as the high fraction of M2B borides of spherical morphology allows achieving a similar stiffness/density ratio and mechanical performance as the reference Ti alloyed materials, but at substantially reduced alloy costs. Zr blended composites on the other hand are softer and less ductile, but the alignment of spiky ZrB2 particles during swaging led to a much higher – though most probably anisotropic – specific modulus. Consequences and recommendations for future alloy and processing design are outlined and discussed. © 2016 Elsevier Ltd
AUTHOR KEYWORDS: Density; Ductility; Lightweight design; Steel; Stiffness; Strength
DOCUMENT TYPE: Article
SOURCE: Scopus

Baron, C., Springer, H., Raabe, D.
Effects of Mn additions on microstructure and properties of Fe–TiB2 based high modulus steels
(2016) Materials and Design, 111, pp. 185-191. Cited 3 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84985909423&doi=10.1016%2fj.matdes.2016.09.003&partnerID=40&md5=231fdc677865977c4cd4be8ce573b181

DOI: 10.1016/j.matdes.2016.09.003
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

ABSTRACT: We studied the effects of Mn additions from 0 to 30 wt.% on microstructure, mechanical and physical properties of liquid metallurgy synthesised high modulus steels in hypo- and hyper-eutectic TiB2 concentrations. While Mn has little effect on density, both Young's modulus and mechanical properties were strongly affected by the achieved wide spectrum of matrix microstructures, ranging from ferrite to martensite, reverted austenite, ε-martensite and austenite. Mn additions of 20 and 30 wt.% did not translate into enhanced mechanical performance despite the higher inherent ductility of the predominantly austenitic matrix, and instead eliminate the intended weight saving potential by significantly reducing the Young's modulus. Martensitic matrices of Mn concentrations of 10 wt.%, on the other hand, are favourable for improved matrix/particle co-deformation without sacrificing too much of the composites' stiffness. In hypo-eutectic Fe – TiB2 based steels, mechanical properties on the level of high strength dual phase steels could be achieved (~ 900 MPa UTS and 20% tensile elongation) but with an enhanced Young's modulus of 217 GPa and reduced density of 7460 kg m− 3. These significantly improved physical and mechanical properties render Mn alloyed high modulus steels promising candidate materials for next generation lightweight structural applications. © 2016 Elsevier Ltd
AUTHOR KEYWORDS: Alloy design; Density; Mechanical properties; Steel; young's modulus
DOCUMENT TYPE: Article
SOURCE: Scopus

Springer, H., Baron, C., Szczepaniak, A., Jägle, E.A., Wilms, M.B., Weisheit, A., Raabe, D.
Efficient additive manufacturing production of oxide- and nitride-dispersion-strengthened materials through atmospheric reactions in liquid metal deposition
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DOI: 10.1016/j.matdes.2016.08.084
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Fraunhofer Institut für Lasertechnik, Aachen, Germany
ABSTRACT: Despite being extremely attractive compounds for strengthening, oxides and nitride particles have found only limited use in metallic materials design, as obtaining appropriate size and dispersion up to now necessitates production by time- and cost-intensive powder metallurgy processes. Here we present an alternative production method, based on the oxide and nitride formation during liquid-metal-deposition procedures in oxygen and/or nitrogen containing atmospheres. Rapid solidification of the small liquid zone suppresses floatation and agglomeration of particles, while subsequent thermo-mechanical treatments densify the material and aids particle dispersion. The in-situ particle formation coupled to the high deposition rates ensures a drastically shortened production chain. The feasibility of the method is exemplarily demonstrated on austenitic stainless steel and commercially available deposition techniques as used in additive manufacturing, performed without shielding gas but instead at air. Even without substantial optimisation of processes and material, > 2 vol.% of hard and stable Cr2N particles with sizes down to 80 nm could be evenly dispersed, resulting in pronounced strengthening at both room temperature and 700 °C without significant loss in ductility. Future possibilities for creating novel generations of cost effective and lean high strength materials, especially for high temperature applications, are outlined and discussed. © 2016 Elsevier Ltd
AUTHOR KEYWORDS: Additive manufacturing; Dispersion strengthening; ODS steel
DOCUMENT TYPE: Article

SOURCE: Scopus

Shanthraj, P., Sharma, L., Svendsen, B., Roters, F., Raabe, D.
A phase field model for damage in elasto-viscoplastic materials
(2016) Computer Methods in Applied Mechanics and Engineering, 312, pp. 167-185. Cited 5 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85000350902&doi=10.1016%2fj.cma.2016.05.006&partnerID=40&md5=7deb85447f3a665a6e75c5931c1b4f05

DOI: 10.1016/j.cma.2016.05.006
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
AICES, RWTH Aachen University, Schinkelstraße 2, Aachen, Germany;
Department of Mechanical Engineering, Eindhoven University of Technology, P.O. Box 513, Eindhoven, Netherlands;
Material Mechanics, RWTH Aachen University, Schinkelstraße 2, Aachen, Germany
ABSTRACT: A phase field method for brittle fracture is formulated for a finite strain elasto-viscoplastic material using a novel obstacle phase field energy model. The obstacle energy model results in a crack profile with compact support, and thus gives a physically realistic description of the material behaviour at the vicinity of the crack tip. The resulting variational inequality is discretised by a finite element method, and is efficiently solved using a reduced space NEWTON method. The solution accuracy and numerical performance of this method is compared with a conventional phase field energy model for brittle fracture through representative examples, and a significant reduction in the numerical solution cost is demonstrated. © 2016 Elsevier B.V.
AUTHOR KEYWORDS: Finite deformation; Fracture; Phase field; Viscoplasticity
DOCUMENT TYPE: Article
SOURCE: Scopus

Morsdorf, L., Jeannin, O., Barbier, D., Mitsuhara, M., Raabe, D., Tasan, C.C.
Multiple mechanisms of lath martensite plasticity
(2016) Acta Materialia, 121, pp. 202-214. Cited 5 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84987941400&doi=10.1016%2fj.actamat.2016.09.006&partnerID=40&md5=b83e5a3e868c671b0f113a64f95370fb

DOI: 10.1016/j.actamat.2016.09.006
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
ArcelorMittal Research and Development, Voie Romaine-BP30320, Maizières-lès-Metz, Cedex, France;
Department of Engineering Sciences for Electronics and Materials, Kyushu University, 6-1 Kasugakoen, Kasuga, Fukuoka, Japan;
Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA, United States
ABSTRACT: The multi-scale complexity of lath martensitic microstructures requires scale-bridging analyses to better understand the deformation mechanisms activated therein. In this study, plasticity in lath martensite is investigated by multi-field mapping of deformation-induced microstructure, topography, and strain evolution at different spatial resolution vs. field-of-view combinations. These investigations reveal site-specific initiation of dislocation activity within laths, as well as significant plastic accommodation in the vicinity of high angle block and packet boundaries. The observation of interface plasticity raises several questions regarding the role of thin inter-lath austenite films. Thus, accompanying transmission electron microscopy and synchrotron x-ray diffraction experiments are carried out to investigate the stability of

these films to mechanical loading, and to discuss alternative boundary sliding mechanisms to explain the observed interface strain localization. © 2016 Acta Materialia Inc.
AUTHOR KEYWORDS: Austenite; DIC; EBSD; Micro-mechanics; Strain mapping
DOCUMENT TYPE: Article
SOURCE: Scopus

Zhang, H., Springer, H., Aparicio-Fernández, R., Raabe, D.
Improving the mechanical properties of Fe – TiB2 high modulus steels through controlled solidification processes
(2016) Acta Materialia, 118, pp. 187-195. Cited 4 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84980347505&doi=10.1016%2fj.actamat.2016.07.056&partnerID=40&md5=5c0f1c378c09fe4df026f5761ad61251

DOI: 10.1016/j.actamat.2016.07.056
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: We investigated novel pathways to improve the mechanical properties of liquid metallurgy produced Fe – TiB2 based high modulus steels (HMS) by controlled solidification kinetics and subsequent thermo-mechanical treatments. The solidification rate was varied by casting of hyper-eutectic alloys (20 vol% TiB2) into moulds with differing internal thickness. Ingots between 5 and 40 mm thickness exhibited irregular particle microstructure consisting of sharp-edged coarse primary particles (increasingly clustered with slower solidification) and closely spaced irregular lamellae. Casting defects can be alleviated by hot rolling, but the mechanical properties remain unsatisfactory. Increasing the solidification rate results only at mould thicknesses of 4 mm and below in a significant refinement of the particle microstructure, necessitating liquid metal deposition techniques to utilise it for obtained improved mechanical performance of HMS. Decreasing the solidification rate causes density-induced floatation of the primary particles, which can be used in block-casting for the production of alloys consisting of small and spheroidised eutectic particles, exhibiting high ductility and superior toughness. Annealing just above the solidus-temperature allows the eutectic zones to liquefy and sink, leaving only primary TiB2 particles behind in the top zone of the alloy. Despite the increased particle fraction up to 24 vol%, both strength, specific modulus and ductility are improved over standard processed HMS alloys with 20 vol% TiB2. © 2016 Acta Materialia Inc.
AUTHOR KEYWORDS: Density; Ductility; Steel; Strength; Toughness; Young's modulus
DOCUMENT TYPE: Article
SOURCE: Scopus

Wong, S.L., Madivala, M., Prahl, U., Roters, F., Raabe, D.
A crystal plasticity model for twinning- and transformation-induced plasticity
(2016) Acta Materialia, 118, pp. 140-151. Cited 8 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84979517105&doi=10.1016%2fj.actamat.2016.07.032&partnerID=40&md5=678a9ec41c188b8953846987ba31547d

DOI: 10.1016/j.actamat.2016.07.032
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany;
Institut für Eisenhüttenkunde (IEHK), RWTH Aachen University, Aachen, Germany
ABSTRACT: A dislocation density-based crystal plasticity model incorporating both transformation-induced plasticity (TRIP) and twinning-induced plasticity (TWIP) is presented. The approach is a physically-based model which reflects microstructure investigations of ε-martensite, twins

and dislocation structures in high manganese steels. Validation of the model was conducted using experimental data for a TRIP/TWIP Fe-22Mn-0.6C steel. The model is able to predict, based on the difference in the stacking fault energies, the activation of TRIP and/or TWIP deformation mechanisms at different temperatures. © 2016 Acta Materialia Inc.
AUTHOR KEYWORDS: Constitutive modeling; Crystal plasticity; Deformation twinning; Martensitic phase transformation
DOCUMENT TYPE: Article
SOURCE: Scopus

Lemmens, B., Springer, H., Duarte, M.J., De Graeve, I., De Strycker, J., Raabe, D., Verbeken, K.
Atom probe tomography of intermetallic phases and interfaces formed in dissimilar joining between Al alloys and steel
(2016) Materials Characterization, 120, pp. 268-272. Cited 2 times.
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DOI: 10.1016/j.matchar.2016.09.008
AFFILIATIONS: Department of Materials Science and Engineering, Ghent University (UGent), Technologiepark 903, Zwijnaarde, Belgium;
Research group of Electrochemical and Surface Engineering (SURF), Vrije Universiteit Brussel (VUB), Pleinlaan 2, Brussels, Belgium;
Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
ArcelorMittal Global R&D Gent, J.F. Kennedylaan 3, Zelzate, Belgium
ABSTRACT: While Si additions to Al are widely used to reduce the thickness of the brittle intermetallic seam formed at the interface during joining of Al alloys to steel, the underlying mechanisms are not clarified yet. The developed approach for the site specific atom probe tomography analysis revealed Si enrichments at grain and phase boundaries between the θ (Fe_4Al_{13}) and η (Fe_2Al_5) phase, up to about ten times that of the concentration in Al. The increase in Si concentration could play an important role for the growth kinetics of the intermetallic phases formed for example in hot-dip aluminizing of steel. © 2016 Elsevier Inc.
AUTHOR KEYWORDS: Aluminium; Hot dip aluminizing; Intermetallics; Steel; Welding
DOCUMENT TYPE: Article
SOURCE: Scopus

Zhang, S., Fang, H., Gramsma, M.E., Kwakernaak, C., Sloof, W.G., Tichelaar, F.D., Kuzmina, M., Herbig, M., Raabe, D., Brück, E., van der Zwaag, S., van Dijk, N.H.
Autonomous Filling of Grain-Boundary Cavities during Creep Loading in Fe-Mo Alloys
(2016) Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 47 (10), pp. 4831-4844. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84979666707&doi=10.1007%2fs11661-016-3642-0&partnerID=40&md5=ddf0cea27498d31891962c87ba282ba4

DOI: 10.1007/s11661-016-3642-0
AFFILIATIONS: Fundamental Aspects of Materials and Energy, Faculty of Applied Sciences, Delft University of Technology, Mekelweg 15, Delft, Netherlands;
Novel Aerospace Materials Group, Faculty of Aerospace Engineering, Delft University of Technology, Kluyverweg 1, Delft, Netherlands;
Department of Materials Science and Engineering, Delft University of Technology, Mekelweg 2, Delft, Netherlands;
Kavli Institute of Nanoscience, National Centre for HREM, Delft University of Technology, Lorentzweg 1, Delft, Netherlands;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany

ABSTRACT: We have investigated the autonomous repair of creep damage by site-selective precipitation in a binary Fe-Mo alloy (6.2 wt pct Mo) during constant-stress creep tests at temperatures of 813 K, 823 K, and 838 K (540 °C, 550 °C, and 565 °C). Scanning electron microscopy studies on the morphology of the creep-failed samples reveal irregularly formed deposits that show a close spatial correlation with the creep cavities, indicating the filling of creep cavities at grain boundaries by precipitation of the Fe2Mo Laves phase. Complementary transmission electron microscopy and atom probe tomography have been used to characterize the precipitation mechanism and the segregation at grain boundaries in detail. © 2016, The Author(s).
DOCUMENT TYPE: Article
SOURCE: Scopus

Hohenwarter, A., Völker, B., Kapp, M.W., Li, Y., Goto, S., Raabe, D., Pippan, R.
Ultra-strong and damage tolerant metallic bulk materials: A lesson from nanostructured pearlitic steel wires
(2016) Scientific Reports, 6, art. no. 33228, . Cited 7 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84987757894&doi=10.1038%2fsrep33228&partnerID=40&md5=a013dc534f04b326131adc05731c7523

DOI: 10.1038/srep33228
AFFILIATIONS: Department of Materials Physics, Montanuniversität Leoben, Jahnstrasse 12, Leoben, Austria;
Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstrasse 12, Leoben, Austria;
Max-Planck Institut für Eisenforschung, Max-Planck-Strasse 1, Düsseldorf, Germany;
Akita University, Tegata Gakuencho, Akita, Japan
ABSTRACT: Structural materials used for safety critical applications require high strength and simultaneously high resistance against crack growth, referred to as damage tolerance. However, the two properties typically exclude each other and research efforts towards ever stronger materials are hampered by drastic loss of fracture resistance. Therefore, future development of novel ultra-strong bulk materials requires a fundamental understanding of the toughness determining mechanisms. As model material we use today's strongest metallic bulk material, namely, a nanostructured pearlitic steel wire, and measured the fracture toughness on micron-sized specimens in different crack growth directions and found an unexpected strong anisotropy in the fracture resistance. Along the wire axis the material reveals ultra-high strength combined with so far unprecedented damage tolerance. We attribute this excellent property combination to the anisotropy in the fracture toughness inducing a high propensity for micro-crack formation parallel to the wire axis. This effect causes a local crack tip stress relaxation and enables the high fracture toughness without being detrimental to the material's strength. © 2016 The Author(s).
DOCUMENT TYPE: Article
SOURCE: Scopus

Fabritius, H.-O., Ziegler, A., Friák, M., Nikolov, S., Huber, J., Seidl, B.H.M., Ruangchai, S., Alagboso, F.I., Karsten, S., Lu, J., Janus, A.M., Petrov, M., Zhu, L.-F., Hemzalová, P., Hild, S., Raabe, D., Neugebauer, J.
Functional adaptation of crustacean exoskeletal elements through structural and compositional diversity: A combined experimental and theoretical study
(2016) Bioinspiration and Biomimetics, 11 (5), art. no. 055006, . Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84992092181&doi=10.1088%2f1748-3190%2f11%2f5%2f055006&partnerID=40&md5=55615e6f48ca1409b7421eb83584fd51

DOI: 10.1088/1748-3190/11/5/055006

AFFILIATIONS: Department Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Central Facility for Electron Microscopy, University of Ulm, Ulm, Germany;
Department Computational Materials Design, Max-Planck-Institut Für Eisenforschung GmbH, Düsseldorf, Germany;
Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic;
Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic;
Institute of Mechanics, Bulgarian Academy of Sciences, Sofia, Bulgaria;
Institut Für Werkstoffforschung, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany;
Department of Polymer Science, Johannes Kepler University Linz, Linz, Austria
ABSTRACT: The crustacean cuticle is a composite material that covers the whole animal and forms the continuous exoskeleton. Nano-fibers composed of chitin and protein molecules form most of the organic matrix of the cuticle that, at the macroscale, is organized in up to eight hierarchical levels. At least two of them, the exo- and endocuticle, contain a mineral phase of mainly Mg-calcite, amorphous calcium carbonate and phosphate. The high number of hierarchical levels and the compositional diversity provide a high degree of freedom for varying the physical, in particular mechanical, properties of the material. This makes the cuticle a versatile material ideally suited to form a variety of skeletal elements that are adapted to different functions and the eco-physiological strains of individual species. This review presents our recent analytical, experimental and theoretical studies on the cuticle, summarising at which hierarchical levels structure and composition are modified to achieve the required physical properties. We describe our multi-scale hierarchical modeling approach based on the results from these studies, aiming at systematically predicting the structure-composition-property relations of cuticle composites from the molecular level to the macro-scale. This modeling approach provides a tool to facilitate the development of optimized biomimetic materials within a knowledge-based design approach. © 2016 IOP Publishing Ltd.
AUTHOR KEYWORDS: amorphous calcium carbonate; amorphous calcium phosphate; Crustacea; cuticle; Decapoda; Isopoda; multi-scale modeling
DOCUMENT TYPE: Article
SOURCE: Scopus

Oh, H.S., Ma, D., Leyson, G.P., Grabowski, B., Park, E.S., Kormann, F., Raabe, D.
Lattice distortions in the FeCoNiCrMn high entropy alloy studied by theory and experiment
(2016) Entropy, 18 (9), art. no. 321, . Cited 7 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85013859479&doi=10.3390%2fe18090321&partnerID=40&md5=c2383b3a46baeafc622c8016ae04c52e

DOI: 10.3390/e18090321
AFFILIATIONS: Department of Materials Science and Engineering, Seoul National University, Seoul, South Korea;
Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Department of Materials Science and Engineering, Delft University of Technology, Mekelweg 2, Delft, Netherlands
ABSTRACT: Lattice distortions constitute one of the main features characterizing high entropy alloys. Local lattice distortions have, however, only rarely been investigated in these multi-component alloys. We, therefore, employ a combined theoretical electronic structure and experimental approach to study the atomistic distortions in the FeCoNiCrMn high entropy (Cantor) alloy by means of density-functional theory and extended X-ray absorption fine structure spectroscopy. Particular attention is paid to element-resolved distortions for each constituent. The

individual mean distortions are small on average, <1%, but their fluctuations (i.e., standard deviations) are an order of magnitude larger, in particular for Cr andMn. Good agreement between theory and experiment is found. © 2016 by the authors.
AUTHOR KEYWORDS: Density functional theory; Extended X-ray absorption fine-structure spectroscopy; High entropy alloy; Lattice distortions
DOCUMENT TYPE: Article
SOURCE: Scopus

Toji, Y., Matsuda, H., Raabe, D.
Effect of Si on the acceleration of bainite transformation by pre-existing martensite
(2016) Acta Materialia, 116, pp. 250-262. Cited 4 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84976632764&doi=10.1016%2fj.actamat.2016.06.044&partnerID=40&md5=6697ce1c4b10c5fc3d5e0ffe42266dc4

DOI: 10.1016/j.actamat.2016.06.044
AFFILIATIONS: Steel Research Laboratory, JFE Steel Corporation, 1 Kawasaki-cho, Chuo-ku, Chiba, Japan;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: Bainite transformation was investigated focusing on the influence of pre-existing martensite on the transformation kinetics, morphology and crystallographic orientation of subsequently formed bainite using EBSD and atom probe tomography. Two 1.1 wt% C-3wt.%Mn steels with and without 2 wt% Si were used to clarify the effect of Si. Steels were rapidly cooled from 900 °C to 300 °C and held at this temperature, or quenched from 900 °C once in water to generate approximately 30 vol% martensite followed by holding at 300 °C. Bainite transformation was clearly accelerated by pre-existing martensite in both Si-containing and Si-free steels. Bainite surrounds the pre-existing martensite in the Si-free steel, whereas it grows to the interior of the austenite grains in the steel containing 2 wt% Si. The major orientation relationship between bainite and adjacent austenite was changed by the presence of martensite from Nishiyama-Wassermann (N-W) to Greninger-Troiano (G-T) regardless of Si content. Clear carbon partitioning from martensite into austenite was observed prior to the bainite transformation in the 2 wt% Si steel, which was not observed in the Si-free steel. We suggest that the dislocations introduced by the martensite transformation act as a primary factor accelerating the bainite transformation when martensite is introduced prior to the bainite transformation. © 2016 Acta Materialia Inc.
AUTHOR KEYWORDS: Atom probe tomography; Austenite; Bainite; Martensite; Quenching & partitioning
DOCUMENT TYPE: Article
SOURCE: Scopus

Welsch, E., Ponge, D., Hafez Haghighat, S.M., Sandlöbes, S., Choi, P., Herbig, M., Zaefferer, S., Raabe, D.
Strain hardening by dynamic slip band refinement in a high-Mn lightweight steel
(2016) Acta Materialia, 116, pp. 188-199. Cited 16 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84975894296&doi=10.1016%2fj.actamat.2016.06.037&partnerID=40&md5=c4fee53a729661a90631aa9ca2701ddb

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AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany;
Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Aachen, Germany;
Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon, South Korea

ABSTRACT: The strain hardening mechanism of a high-Mn lightweight steel (Fe-30.4Mn-8Al-1.2C (wt%)) is investigated by electron channeling contrast imaging (ECCI) and transmission electron microscopy (TEM). The alloy is characterized by a constant high strain hardening rate accompanied by high strength and high ductility (ultimate tensile strength: 900 MPa, elongation to fracture: 68%). Deformation microstructures at different strain levels are studied in order to reveal and quantify the governing structural parameters at micro- and nanometer scales. As the material deforms mainly by planar dislocation slip causing the formation of slip bands, we quantitatively study the evolution of the slip band spacing during straining. The flow stress is calculated from the slip band spacing on the basis of the passing stress. The good agreement between the calculated values and the tensile test data shows dynamic slip band refinement as the main strain hardening mechanism, enabling the excellent mechanical properties. This novel strain hardening mechanism is based on the passing stress acting between co-planar slip bands in contrast to earlier attempts to explain the strain hardening in high-Mn lightweight steels that are based on grain subdivision by microbands. We discuss in detail the formation of the finely distributed slip bands and the gradual reduction of the spacing between them, leading to constantly high strain hardening. TEM investigations of the precipitation state in the as-quenched state show finely dispersed atomically ordered clusters (size < 2 nm). The influence of these zones on planar slip is discussed. © 2016 Acta Materialia Inc.
AUTHOR KEYWORDS: Dynamic slip band refinement; ECCI; High-manganese light weight steel; Strain hardening
DOCUMENT TYPE: Article
SOURCE: Scopus

Hassani, M., Engels, P., Raabe, D., Varnik, F.
Localized plastic deformation in a model metallic glass: A survey of free volume and local force distributions
(2016) Journal of Statistical Mechanics: Theory and Experiment, 2016 (8), art. no. 084006, . Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84986000903&doi=10.1088%2f1742-5468%2f2016%2f08%2f084006&partnerID=40&md5=b079c3e1557a4aa34df15dbac62e7ea1

DOI: 10.1088/1742-5468/2016/08/084006
AFFILIATIONS: Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Universitätsstraße 150, Bochum, Germany; Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: Plastic deformation of a model glass is investigated via large scale molecular dynamics simulations. The role of microscopic fluctuations of the structure for the deformation behavior is highlighted by demonstrating that statistically independent samples prepared via an identical protocol develop qualitatively distinct deformation paths. As a quantitative measure, the spatial distribution of the particle based excess volume is monitored via Voronoi tesselation. While the fluctuations of the thus defined single-particle based excess volume do not seem to show any signature of the strain field, a non-local definition of the excess volume clearly correlates with the observed shear deformation field. The distribution of the force acting on individual particles also shows a pattern strongly similar to that of the strain. In line with other studies, these results underline the importance of both the structural heterogeneities as well as the fluctuations of the locally acting forces and stresses for plastic deformation in amorphous solids. © 2016 IOP Publishing Ltd and SISSA Medialab srl.
AUTHOR KEYWORDS: aging; glasses (structural); glassy dynamics; heterogeneous materials; slow relaxation; transport properties
DOCUMENT TYPE: Review
SOURCE: Scopus

Li, Y.J., Herbig, M., Goto, S., Raabe, D.
Formation of nanosized grain structure in martensitic 100Cr6 bearing steels upon rolling contact loading studied by atom probe tomography
(2016) Materials Science and Technology (United Kingdom), 32 (11), pp. 1100-1105. Cited 4 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84981709586&doi=10.1080%2f02670836.2015.1120458&partnerID=40&md5=ebd00a78f8d915097c4fc3271d1521b8

DOI: 10.1080/02670836.2015.1120458
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: To understand the origin of white etching cracks (WECs), a systematic microstructural characterisation in the regions affected from the near-surface region down to the subsurface layers where WECs occur is necessary. As a starting point, we focus on the near-surface region of an axial thrust bearing, made of martensitic 100Cr6 steel, to study the influence of rolling contact loading on the microstructure and the resulting distributions of the major alloying elements C and Cr using atom probe tomography. We find that upon rolling contact loading the original plate-like martensitic structure evolves into a nanosized equiaxed grain structure with C segregation up to 5 at.-% at the grain boundaries. Cementite particles, located at grain boundaries and triple junctions, undergo spheroidisation. The originally homogeneously distributed Cr becomes enriched in spheroidised cementite particles. The microstructural changes give strong hints that rolling contact loading induces plastic deformation and an increased temperature on the near-surface region. This paper is part of a Themed Issue on Recent developments in bearing steels.
AUTHOR KEYWORDS: Atom probe tomography; Carbide precipitation; Grain boundary segregation; Matensitic 100Cr6 bearing steels; Nanocrystalline steels; Rolling contact fatigue; White etching cracks
DOCUMENT TYPE: Article
SOURCE: Scopus

Pristovsek, M., Han, Y., Zhu, T., Oehler, F., Tang, F., Oliver, R.A., Humphreys, C.J., Tytko, D., Choi, P.-P., Raabe, D., Brunner, F., Weyers, M.
Structural and optical properties of (1122) InGaN quantum wells compared to (0001) and (1120)
(2016) Semiconductor Science and Technology, 31 (8), art. no. 085007, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84979633331&doi=10.1088%2f0268-1242%2f31%2f8%2f085007&partnerID=40&md5=eebeeab33945a16026c2b34895edc00a

DOI: 10.1088/0268-1242/31/8/085007
AFFILIATIONS: Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge, United Kingdom; Max-Planck-Institut für Eisenforschung GmbH, Department of Microstructure Physics and Alloy Design, Max-Planck-Straße 1, Düsseldorf, Germany; Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Str. 4, Berlin, Germany
ABSTRACT: We benchmarked growth, microstructure and photo luminescence (PL) of (112-2) InGaN quantum wells (QWs) against (0001) and (112-0). In incorporation, growth rate and the critical thickness of (112-2) QWs are slightly lower than (0001) QWs, while the In incorporation on (112-0) is reduced by a factor of three. A small step-bunching causes slight fluctuations of the emission wavelength. Transmission electron microscopy as well as atom probe tomography (APT) found very flat interfaces with little In segregation even for 20% In content. APT frequency distribution analysis revealed some deviation from a random InGaN alloy, but not as severe as for (112-0). The slight deviation of (112-2) QWs from an ideal random alloy did not broaden the 300 K PL, the line widths were similar for (112-2) and (0001) while (112-0) QWs were broader. Despite the high

structural quality and narrow PL, the integrated PL signal at 300 K was about 4 lower on (112-2) and more than 10 lower on (112-0). © 2016 IOP Publishing Ltd.
AUTHOR KEYWORDS: atom probe tomography; InGaN; optical properties; quantum well; semi-polar; step-bunching
DOCUMENT TYPE: Article
SOURCE: Scopus

Belde, M., Springer, H., Raabe, D.
Vessel microstructure design: A new approach for site-specific core-shell micromechanical tailoring of TRIP-assisted ultra-high strength steels
(2016) Acta Materialia, 113, pp. 19-31. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84966292318&doi=10.1016%2fj.actamat.2016.04.051&partnerID=40&md5=c1c4dcdae2fbdcda576b88a61cf782ce

DOI: 10.1016/j.actamat.2016.04.051
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: The mechanical performance of multi-phase steel microstructures critically depends on the constituents' chemical and morphological constitutions, which in combination determine the composite hardness, the onset of plasticity, internal load and strain-partitioning, as well as the stability and transformation kinetics of retained austenite in case of TRIP steels. The novel approach of utilising temporary vessel phases, hence termed vessel microstructure design, enables the tuning of constituent phase properties by linking their formation to a controllable landscape of chemical gradients. This approach hinges on the introduction of alloy carbides as a temporary container, or 'vessel' phase, deliberately producing localised enrichment of alloying elements in a structure predetermined by preliminary heat treatments, referred to as conditioning and accumulation stages. These vessel carbides, which act as reservoirs for specific alloying elements, are then partially dissolved through flash heating, leading to a self-organising landscape of alloying elements in the vicinity of the dissolving particles. The resulting three- or multiple phase microstructures then consist of confined laminates incorporating retained carbides, enveloped by retained austenite shells, embedded within a martensitic matrix. Such complex yet entirely self-organized microstructures offer unique opportunities for strain and load partitioning which we refer to as core-shell micromechanics. Different variants of these core-shell composite structures are produced and examined together with reference microstructures by tensile testing, hardness mappings, impact toughness, X-ray measurements, as well as by electron microscopy. It is found that these novel microstructures, when tempered, exhibit ultra-high strength and delayed necking, enabled by a combination of gradual strain-hardening and transformation-induced plasticity that is tuneable via control of the initial carbide structure.
AUTHOR KEYWORDS: Composite; Microstructure design; Strength; TRIP-Assisted steel; Uniform elongation
DOCUMENT TYPE: Article
SOURCE: Scopus

Gross, M., Steinbach, I., Raabe, D., Varnik, F.
Response to 'Comment on 'Viscous coalescence of droplets: A lattice Boltzmann study'' [Phys. Fluids 28, 079101 (2016)]
(2016) Physics of Fluids, 28 (7), art. no. 079102, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84979752320&partnerID=40&md5=babd91aeb9a762aaa3bc78bc7ca4c748

AFFILIATIONS: Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Universitaetsstr. 90a, Bochum, Germany;

Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, Düsseldorf, Germany;
Max-Planck-Institute for Intelligent Systems, Stuttgart, Germany
DOCUMENT TYPE: Note
SOURCE: Scopus

Huang, L.-F., Grabowski, B., Zhang, J., Lai, M.-J., Tasan, C.C., Sandlöbes, S., Raabe, D., Neugebauer, J.
From electronic structure to phase diagrams: A bottom-up approach to understand the stability of titanium–transition metal alloys
(2016) Acta Materialia, 113, pp. 311-319. Cited 4 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84967202985&doi=10.1016%2fj.actamat.2016.04.059&partnerID=40&md5=891b5ce7d93066237fbc2f5516a1f17e

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AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Department of Materials Science and Engineering, Northwestern University, Evanston, IL, United States;
State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, China;
Department of Materials Science and Engineering, MIT, Cambridge, MA, United States;
Institut für Metallkunde und Metallphysik, RWTH Aachen, Kopernikusstr. 14, Aachen, Germany
ABSTRACT: We have computed formation energies for all technologically relevant transition metal solutes in the α, β, and ω phases of Ti, employing ab initio simulations. We analyze and explain their periodic-table trends, and from their differences we derive stabilization energies which provide direct insight into phase stabilization effects of the various solutes with respect to α, β, and ω. This allows us to identify strong β stabilizers in the middle of each electronic d shell in consistency with experimental knowledge. Based on an extension of the stabilization energies to free energies we derive a wide range of Ti-transition metal phase diagrams. A detailed comparison to available experimental martensitic transformation temperatures and to measurements performed in this study shows that, despite some quantitative discrepancies, the qualitative trends can be expected to be correct. An important feature that is displayed by a limited range of the computed phase diagrams is a triple point at which the three phases, α, β, and ω, meet. This insight provides a plausible explanation for the complexity observed in gum metals, a class of Ti alloys with very special materials properties. © 2016 Acta Materialia Inc.
AUTHOR KEYWORDS: Density functional theory; Phase diagram; Stability; Titanium alloys; Transition metal
DOCUMENT TYPE: Article
SOURCE: Scopus

Stechmann, G., Zaefferer, S., Konijnenberg, P., Raabe, D., Gretener, C., Kranz, L., Perrenoud, J., Buecheler, S., Tiwari, A.N.
3-Dimensional microstructural characterization of CdTe absorber layers from CdTe/CdS thin film solar cells
(2016) Solar Energy Materials and Solar Cells, 151, pp. 66-80. Cited 6 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84962311035&doi=10.1016%2fj.solmat.2016.02.023&partnerID=40&md5=3fdae66ffafe571d21f822275b8c0ca8

DOI: 10.1016/j.solmat.2016.02.023
AFFILIATIONS: Max-Planck-Institut Für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany;

Empa - Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, Dübendorf, Switzerland
ABSTRACT: The present work reports on a study on the microstructure and its evolution during processing of CdTe absorber layers from CdTe/CdS thin film solar cells grown by low-temperature processes in substrate configuration. Investigations were performed at different stages of the cell manufacturing, from deposition to the final functional solar cell, with the aim to understand the microstructure formation of the photoactive layer. To this end 3-dimensional microstructure characterization was performed using focused ion beam/electron backscatter diffraction tomography ("3D-EBSD") together with conventional 2D-EBSD. The analyses revealed strong microstructural and textural changes developing across the thickness of the absorber material, between the back contact and the p-n junction interfaces. Based on the 3-dimensional reconstruction of the CdTe thin film, a coherent growth model was proposed, emphasizing the microstructural continuity before and after a typical CdCl2-annealing activation treatment. One of the principal results is that the absorber layer is created by two concomitant processes, deposition and recrystallization, which led to different textures and microstructures. Further changes are the result of subsequent annealing treatments, favoring twinning and promoting well-defined texture components. The results open the possibility for a grain boundary engineering approach applied to the design of such cells. © 2016 Elsevier B.V.
AUTHOR KEYWORDS: CdTe; EBSD; Grain boundary; Growth; Microstructure; Thin film
DOCUMENT TYPE: Article
SOURCE: Scopus

Nellessen, J., Sandlöbes, S., Raabe, D.
Low cycle fatigue in aluminum single and bi-crystals: On the influence of crystal orientation
(2016) Materials Science and Engineering A, 668, pp. 166-179. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84969287141&doi=10.1016%2fj.msea.2016.05.054&partnerID=40&md5=c6ce9503f383be5ca521abe94c287c9c

DOI: 10.1016/j.msea.2016.05.054
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Department for Microstructure Physics and Alloy Design, Düsseldorf, Germany;
Institut für Metallkunde und Metallphysik, RWTH Aachen University, Aachen, Germany
ABSTRACT: Aluminum single crystals with three different double-slip orientations and two aluminum bi-crystals - one with a high-angle grain boundary and one with a low-angle grain boundary - were cyclically deformed up to 100 cycles under constant displacement control. The distribution of the local strain and the local strain amplitudes was captured by in-situ digital image correlation (DIC). Dislocation structure analysis was performed by electron channeling contrast imaging (ECCI) and the evolution of local misorientations was recorded by high resolution electron backscatter diffraction (EBSD). The DIC results show a homogeneous strain amplitude distribution in the single crystals while the measured strain amplitude in the low-angle grain boundary bi-crystal sample differs significantly. ECCI observations reveal the presence of dislocation cells elongated along the trace of the primary {111} slip plane in all investigated crystals and the formation of deformation bands parallel to the trace of {110} planes. Deformation bands (DB) were observed in all samples but their frequency and misorientation with respect to the matrix was found to sensitively depend on the crystal orientation and the local strain amplitude. Our results on the bi-crystals show that the grain orientation mainly determines the local stresses and therefore also the formation of the associated dislocation structures rather than the grain boundary character. © 2016 Elsevier B.V.

AUTHOR KEYWORDS: Aluminum single and bi-crystals; Dislocation structure formations; Electron channeling contrast imaging (ECCI); Low cycle fatigue (LCF)
DOCUMENT TYPE: Article
SOURCE: Scopus

Otto, F., Dlouhý, A., Pradeep, K.G., Kuběnová, M., Raabe, D., Eggeler, G., George, E.P.
Decomposition of the single-phase high-entropy alloy CrMnFeCoNi after prolonged anneals at intermediate temperatures
(2016) Acta Materialia, 112, pp. 40-52. Cited 54 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84963615057&doi=10.1016%2fj.actamat.2016.04.005&partnerID=40&md5=ad447ee0b09fd2ed1a8fe6f8fa7404fe

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AFFILIATIONS: Institute for Materials, Ruhr University Bochum, Bochum, Germany;
Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic;
Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: Among the vast number of multi-principal-element alloys that are referred to as high-entropy alloys (HEAs) in the literature, only a limited number solidify as single-phase solid solutions. The equiatomic HEA, CrMnFeCoNi, is a face-centered cubic (FCC) prototype of this class and has attracted much attention recently because of its interesting mechanical properties. Here we evaluate its phase stability after very long anneals of 500 days at 500-900 °C during which it is reasonable to expect thermodynamic equilibrium to have been established. Microstructural analyses were performed using complementary analysis techniques including scanning and transmission electron microscopy (SEM/TEM/STEM), energy dispersive X-ray (EDX) spectroscopy, selected area electron diffraction (SAD), and atom probe tomography (APT). We show that the alloy is a single-phase solid solution after homogenization for 2 days at 1200 °C and remains in this state after a subsequent anneal at 900 °C for 500 days. However, it is unstable and forms second-phase precipitates at 700 and 500 °C. A Cr-rich σ phase forms at 700 °C, whereas three different phases (L10-NiMn, B2-FeCo and a Cr-rich body-centered cubic, BCC, phase) precipitate at 500 °C. These precipitates are located mostly at grain boundaries, but also form at intragranular inclusions/pores, indicative of heterogeneous nucleation. Since there is limited entropic stabilization of the solid solution state even in the extensively investigated CrMnFeCoNi alloy, the stability of other HEAs currently thought to be solid solutions should be carefully evaluated, especially if they are being considered for applications in vulnerable temperature ranges.
AUTHOR KEYWORDS: Aging; High-entropy alloy; Phase stability; Phase transformations; Solid solution
DOCUMENT TYPE: Article
SOURCE: Scopus

Kim, J.-K., Ko, W.-S., Sandlöbes, S., Heidelmann, M., Grabowski, B., Raabe, D.
The role of metastable LPSO building block clusters in phase transformations of an Mg-Y-Zn alloy
(2016) Acta Materialia, 112, pp. 171-183. Cited 9 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84963744391&doi=10.1016%2fj.actamat.2016.04.016&partnerID=40&md5=ec1959b4c2348f649e183c9a5b75b9e0

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AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Aachen, Germany;
Ernst Ruska-Centre (ER-C) for Microscopy and Spectroscopy with Electrons, Jülich Research Center, Jülich, Germany;
School of Materials Science and Engineering, University of Ulsan, Ulsan, South Korea;
Interdisciplinary Center for Analytics on the Nanoscale, Universität Duisburg-Essen, Duisburg, Germany
ABSTRACT: We present a systematic atomic scale analysis of the structural evolution of long-period-stacking-ordered (LPSO) structures in the (i) α-Mg matrix and in the (ii) interdendritic LPSO phase of an Mg97Y2Zn1 (at. %) alloy annealed at 500°C, using high resolution high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM). Various types of metastable LPSO building block clusters have been observed in both regions. The thermodynamic phase stabilities computed by density-functional-theory calculations explain the diversity of the LPSO structures which are distinguished by their different arrangements of the Y/Zn enriched LPSO building blocks that have a local fcc stacking sequence on the close packed planes. A direct evidence of the transformation from 18R to 14H is presented. This finding suggests that LPSO structures can change their separation distance - quantified by the number of α-Mg layers between them - at a low energy penalty by generating the necessary Shockley partial dislocation on a specific glide plane. Based on our results the most probable transformation sequence of LPSO precipitate plates in the α-Mg matrix is: single building block → various metastable LPSO building block clusters → 14H, and the most probable transformation sequence in the interdendritic LPSO phase is: 18R→ various metastable LPSO building block clusters → 14H. The thermodynamically most stable structures in both the α-Mg matrix and the interdendritic LPSO phase are a mixture of 14H and α-Mg.

AUTHOR KEYWORDS: Density functional theory (DFT); Long period stacking ordered structure; Magnesium alloy; Phase transformation; Transmission electron microscopy (TEM)
DOCUMENT TYPE: Article
SOURCE: Scopus

Wu, X., Ma, D., Eisenlohr, P., Raabe, D., Fabritius, H.-O.
From insect scales to sensor design: Modelling the mechanochromic properties of bicontinuous cubic structures
(2016) Bioinspiration and Biomimetics, 11 (4), art. no. 045001, . Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84984684929&doi=10.1088%2f1748-3190%2f11%2f4%2f045001&partnerID=40&md5=8918c4624532ff643ac50f215f29bf04

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AFFILIATIONS: Department of Chemistry, Paderborn University, Warburger Straße 100, Paderborn, Germany;
Department Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany;
Department Chemical Engineering and Materials Science, Michigan State University, 428 S. Shaw Lane, East Lansing, MI, United States
ABSTRACT: Many of the three-dimensional photonic crystals occurring in the scales of insects have bicontinuous cubic structures. Their optical properties have been studied extensively, however little is known about their mechanical properties and their optical response under deformation. We demonstrated a mechanochromic effect by deforming the scales of a weevil and calculated the elastic, optical and mechanochromic (assuming homogeneous deformation) properties of the three types of bicontinuous cubic structures occurring in nature: P-structure (primitive), G-structure (gyroid) and D-structure (diamond). The results show that all investigated

properties of these three structure types strongly depend on their geometry, structural parameters such as volume fractions of the two constituting phases and the directions of the incident light or applied stress, respectively. Interestingly, the mechanochromic simulation results predict that these structures may show blue-shift or even red-shift under compression along certain directions. Our results provide design guidelines for mechanochromic sensing materials operating in the elastic regime, including parameters such as sensitivity and direction of spectral shift. © 2016 IOP Publishing Ltd.
AUTHOR KEYWORDS: bicontinuous cubic structures; insects; mechanochromic material; photonic crystals
DOCUMENT TYPE: Article
SOURCE: Scopus

Lapauw, T., Tytko, D., Vanmeensel, K., Huang, S., Choi, P.-P., Raabe, D., Caspi, E.N., Ozeri, O., To Baben, M., Schneider, J.M., Lambrinou, K., Vleugels, J.
(Nbx, Zr1-x)4AlC3 MAX Phase Solid Solutions: Processing, Mechanical Properties, and Density Functional Theory Calculations
(2016) Inorganic Chemistry, 55 (11), pp. 5445-5452. Cited 9 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84973326018&doi=10.1021%2facs.inorgchem.6b00484&partnerID=40&md5=d305bcaf4e3a7beb8bb2e6dc4c27af66

DOI: 10.1021/acs.inorgchem.6b00484
AFFILIATIONS: KU Leuven, Department of Materials Engineering, Kasteelpark Arenberg 44, Leuven, Belgium;
SCKCEN, Boeretang 200, Mol, Belgium;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck Strasse 1, Düsseldorf, Germany;
Physics Department, Nuclear Research Centre-Negev, PO Box 9001, Beer-Sheva, Israel;
Reactor Department, Nuclear Research Center-Soreq, Yavne, Israel;
Materials Chemistry, RWTH Aachen University, Kopernikusstrasse 10, Aachen, Germany
ABSTRACT: The solubility of zirconium (Zr) in the Nb4AlC3 host lattice was investigated by combining the experimental synthesis of (Nbx, Zr1-x)4AlC3 solid solutions with density functional theory calculations. High-purity solid solutions were prepared by reactive hot pressing of NbH0.89, ZrH2, Al, and C starting powder mixtures. The crystal structure of the produced solid solutions was determined using X-ray and neutron diffraction. The limited Zr solubility (maximum of 18.5% of the Nb content in the host lattice) in Nb4AlC3 observed experimentally is consistent with the calculated minimum in the energy of mixing. The lattice parameters and microstructure were evaluated over the entire solubility range, while the chemical composition of (Nb0.85, Zr0.15)4AlC3 was mapped using atom probe tomography. The hardness, Young's modulus, and fracture toughness at room temperature as well as the high-temperature flexural strength and E-modulus of (Nb0.85, Zr0.15)4AlC3 were investigated and compared to those of pure Nb4AlC3. Quite remarkably, an appreciable increase in fracture toughness was observed from 6.6 ± 0.1 MPa/m1/2 for pure Nb4AlC3 to 10.1 ± 0.3 MPa/m1/2 for the (Nb0.85, Zr0.15)4AlC3 solid solution. © 2016 American Chemical Society.
DOCUMENT TYPE: Article
SOURCE: Scopus

Lai, M.J., Tasan, C.C., Raabe, D.
On the mechanism of {332} twinning in metastable β titanium alloys
(2016) Acta Materialia, 111, pp. 173-186. Cited 10 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84962007067&doi=10.1016%2fj.actamat.2016.03.040&partnerID=40&md5=97bac9326be317d1061efdacad0945f1

DOI: 10.1016/j.actamat.2016.03.040
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: {332} twinning, an unusual twinning mode in other body-centered cubic (bcc) metals and alloys, has been demonstrated to be a fundamental deformation mode in bcc metastable β titanium alloys. Recent studies suggest that this twinning mode plays an important role in enhancing the work hardening and thus improving the mechanical properties. Here, we studied the mechanism of this twinning mode in a metastable β Ti-36Nb-2Ta-3Zr (wt.%) alloy. Tensile tests were performed to induce the formation of {332} twins. By using electron backscatter diffraction, transmission electron microscopy and in situ scanning electron microscopy, the surface-to-bulk microstructures and the initiation and propagation of {332} twins were investigated. In addition to the previously reported high densities of straight dislocations within the twin, we have observed that an α″ martensite band is present near the surface adjacent to the twin. During annealing at 900°C, the α″ martensite band transforms into the adjacent twin rather than into the matrix, indicating that {332} twin nucleates within α″ martensite. Further evidence for this is the constitution of the twin in the initial stage of its formation, where the first portion formed consists of α″ martensite. During propagation, the twins propagating to the opposite directions can merge together when their lateral boundaries impinge on each other. Based on the experimental observations, an α″-assisted twinning mechanism is proposed and the origin of the dislocations within {332} twin is discussed accordingly. © 2016 Published by Elsevier Ltd on behalf of Acta Materialia Inc.
AUTHOR KEYWORDS: Deformation twinning; Electron backscatter diffraction; Martensitic transformation; Transmission electron microscopy; β titanium
DOCUMENT TYPE: Article
SOURCE: Scopus

Wang, M.-M., Tasan, C.C., Ponge, D., Raabe, D.
Spectral TRIP enables ductile 1.1 GPa martensite
(2016) Acta Materialia, 111, pp. 262-272. Cited 10 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84962915547&doi=10.1016%2fj.actamat.2016.03.070&partnerID=40&md5=fca0ddb24c2cc0c7814b8c58c9c8c961

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AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA, United States
ABSTRACT: Introduction of interlath reverted austenite is an effective method to design ductile lath martensitic steels. The challenge in this concept is that all reverted austenite films have similar mechanical stability, hence, they all undergo transformation-induced plasticity (TRIP) at the same strain level. Here we propose a new thermo-mechanical treatment route to activate the TRIP effect over a broad strain regime and refer to it as 'spectral TRIP effect'. It aims at spreading the micro-mechanical stability of reverted austenite grains by widening the austenite nucleation barrier in martensite. To validate the proposed thermo-mechanical treatment route, an as-quenched medium-Mn martensitic steel was cold rolled prior to the reversion treatment at 600 °C. Microstructure characterization was carried out by electron backscatter diffraction (EBSD) and electron channeling contrast imaging (ECCI). Mechanical tests show that the approach is effective. The spectral TRIP effect improves both, the strength and the ductility due to the well dispersed size distribution and the associated size-dependent deformation and phase transformation behavior of the reverted austenite grains, extending TRIP-related work hardening over a broad strain range. © 2016 Acta Materialia Inc.
AUTHOR KEYWORDS: ECCI; Grain size; Martensitic transformation; Medium manganese steel; Twinning

DOCUMENT TYPE: Article
SOURCE: Scopus

Jia, N., Raabe, D., Zhao, X.
Crystal plasticity modeling of size effects in rolled multilayered Cu-Nb composites
(2016) Acta Materialia, 111, pp. 116-128.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84961875056&doi=10.1016%2fj.actamat.2016.03.055&partnerID=40&md5=18170a35a0a3095dab98438b1dfa7e72

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AFFILIATIONS: Key Laboratory for Anisotropy and Texture of Materials, Ministry of Education, School of Material Science and Engineering, Northeastern University, Shenyang, China;
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
ABSTRACT: We present size-dependent crystal plasticity finite element simulations of the deformation microstructure, plastic flow and texture evolution in multilayered Cu-Nb composites during cold rolling. The model is based on a constitutive framework incorporating thermally activated dislocation slip, mechanical twinning and non-crystallographic shear banding. It also accounts for the dislocation density evolution and its dependence on initial grain size. By performing a series of quadricrystal simulations considering characteristic heterophase microstructures, the underlying micromechanics and texture of the composites are explored. Significant shear banding occurs in both phases, primarily determined by their initial orientations. For each phase, the activation of shear banding is also affected by the mechanical properties and orientations of the adjacent phase. For composites with an initial single layer thickness of 35 μm or 4 μm, the layer thickness reduction after rolling is non-uniform and the typical rolling textures for bulk pure metals develop in the respective phases. For the 75 nm initial single layer thickness composite, both phases are reduced uniformly in thickness and the initial orientations prevail. The predictions agree well with experimental observations in cold-rolled Cu-Nb thin films. The simulations reveal that for the composites with initial single layer thickness of micrometer scale, dislocation slip is the dominant deformation mechanism although shear banding increasingly carries the deformation at larger strains. For the samples with initial single layer thickness of a few tens of nanometers, shear banding and dislocation slip are the dominant mechanisms. This transition in deformation characteristics leads to different textures in micrometer- and nanometer-scaled multilayers.
AUTHOR KEYWORDS: Crystal plasticity finite element model; Multilayered composite; Shear band; Texture
DOCUMENT TYPE: Article
SOURCE: Scopus

Nematollahi, Gh.A., Grabowski, B., Raabe, D., Neugebauer, J.
Multiscale description of carbon-supersaturated ferrite in severely drawn pearlitic wires
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https://www.scopus.com/inward/record.uri?eid=2-s2.0-84962798224&doi=10.1016%2fj.actamat.2016.03.052&partnerID=40&md5=a0b3ecfcbf6826f1a6c952f6f8c009a4

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AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
ABSTRACT: A multiscale simulation approach based on atomistic calculations and a discrete diffusion model is developed and applied to carbon-supersaturated ferrite, as experimentally observed in severely deformed pearlitic steel. We employ the embedded atom method and the nudged elastic band technique to determine the energetic profile of a carbon atom around a

screw dislocation in bcc iron. The results clearly indicate a special region in the proximity of the dislocation core where C atoms are strongly bound, but where they can nevertheless diffuse easily due to low barriers. Our analysis suggests that the previously proposed pipe mechanism for the case of a screw dislocation is unlikely. Instead, our atomistic as well as the diffusion model results support the so-called drag mechanism, by which a mobile screw dislocation is able to transport C atoms along its glide plane. Combining the C-dislocation interaction energies with density-functional-theory calculations of the strain dependent C formation energy allows us to investigate the C supersaturation of the ferrite phase under wire drawing conditions. Corresponding results for local and total C concentrations agree well with previous atom probe tomography measurements indicating that a significant contribution to the supersaturation during wire drawing is due to dislocations. © 2016 Acta Materialia Inc.
AUTHOR KEYWORDS: Carbon; Dislocations; Drag mechanism; Multiscale; Pearlite; Supersaturation; Wire drawing
DOCUMENT TYPE: Article
SOURCE: Scopus

Li, Z., Pradeep, K.G., Deng, Y., Raabe, D., Tasan, C.C.
Metastable high-entropy dual-phase alloys overcome the strength-ductility trade-off
(2016) Nature, 534 (7606), pp. 227-230. Cited 127 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84963602237&doi=10.1038%2fnature17981&partnerID=40&md5=26630db47da0ef863694331eab3adf88

DOI: 10.1038/nature17981
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA, United States
ABSTRACT: Metals have been mankind's most essential materials for thousands of years; however, their use is affected by ecological and economical concerns. Alloys with higher strength and ductility could alleviate some of these concerns by reducing weight and improving energy efficiency. However, most metallurgical mechanisms for increasing strength lead to ductility loss, an effect referred to as the strength-ductility trade-off. Here we present a metastability-engineering strategy in which we design nanostructured, bulk high-entropy alloys with multiple compositionally equivalent high-entropy phases. High-entropy alloys were originally proposed to benefit from phase stabilization through entropy maximization. Yet here, motivated by recent work that relaxes the strict restrictions on high-entropy alloy compositions by demonstrating the weakness of this connection, the concept is overturned. We decrease phase stability to achieve two key benefits: interface hardening due to a dual-phase microstructure (resulting from reduced thermal stability of the high-temperature phase); and transformation-induced hardening (resulting from the reduced mechanical stability of the room-temperature phase). This combines the best of two worlds: extensive hardening due to the decreased phase stability known from advanced steels and massive solid-solution strengthening of high-entropy alloys. In our transformation-induced plasticity-assisted, dual-phase high-entropy alloy (TRIP-DP-HEA), these two contributions lead respectively to enhanced trans-grain and inter-grain slip resistance, and hence, increased strength. Moreover, the increased strain hardening capacity that is enabled by dislocation hardening of the stable phase and transformation-induced hardening of the metastable phase produces increased ductility. This combined increase in strength and ductility distinguishes the TRIP-DP-HEA alloy from other recently developed structural materials. This metastability-engineering strategy should thus usefully guide design in the near-infinite compositional space of high-entropy alloys.
DOCUMENT TYPE: Article

SOURCE: Scopus

Lübke, A., Enax, J., Wey, K., Fabritius, H.-O., Raabe, D., Epple, M.
Composites of fluoroapatite and methylmethacrylate-based polymers (PMMA) for biomimetic tooth replacement
(2016) Bioinspiration and Biomimetics, 11 (3), art. no. 035001, . Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84984698407&doi=10.1088%2f1748-3190%2f11%2f3%2f035001&partnerID=40&md5=d1b1776bc982a4c9847da8a041dabdff

DOI: 10.1088/1748-3190/11/3/035001
AFFILIATIONS: Institute of Inorganic Chemistry, Centre for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, Universitaetsstr. 5-7, Essen, Germany;
Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: Synthetic composite materials that mimic the structure and composition of mammalian tooth enamel were prepared by mixing fluoroapatite rods (diameter 2-3 µm, thickness about 0.5 µm) and methylmethacrylate (MMA), followed by polymerization either during or immediately after ultracentrifugation, using either a tertiary amine/radical initiator for polymerization at room temperature or a radical initiator for thermal polymerization. This led to mineral-rich composites (mineral content between 50 and 75 wt%). To enhance the mechanical stability and the interaction between fluoroapatite and polymer matrix, small amounts of differently functionalized MMA monomers were added to the co-monomer mixture. Another approach was the coating of the fluoroapatite rods with silica and the polymerization in the presence of a siloxane-functionalized MMA monomer. The hardness of the composites was about 0.2-0.4 GPa as determined by Vickers indentation tests, about 2 times higher than the polymer matrix alone. The composites had a good resistance against acids (60 min at pH 3, 37 °C).
AUTHOR KEYWORDS: biomimetics; ceramics; polymers; teeth
DOCUMENT TYPE: Article
SOURCE: Scopus

Baron, C., Springer, H., Raabe, D.
Efficient liquid metallurgy synthesis of Fe-TiB2 high modulus steels via in-situ reduction of titanium oxides
(2016) Materials and Design, 97, pp. 357-363. Cited 4 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84961793530&doi=10.1016%2fj.matdes.2016.02.076&partnerID=40&md5=7dbb700f59648a668e9dd90c1e5f2b3f

DOI: 10.1016/j.matdes.2016.02.076
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: We studied the in-situ reduction of Ti oxides by Al as an alternative and cost effective route for the liquid metallurgical synthesis of low density, high stiffness steels (high modulus steels) containing about 10 vol.% TiB2. TiO2, TiO1.83 and TiO were inserted via iron tubes into Fe-B melts, with Al either premixed with the oxide powders or liquid in the melt. Depending on Ti oxide type and location of the redox partner Al, greatly differing reaction kinetics, slag formation and corresponding microstructures of the high modulus steels were observed. TiO1.83 and TiO premixed with Al showed the highest TiB2 yield in the cast steel and are thus favourable candidates for the cost effective production of high modulus steels. Based on our findings, a novel synthesis process is proposed, based on filling wire injection into a continuous casting process, allowing the utilisation of the additionally formed oxide particles for the further improvement of the property profile of high modulus steels.

AUTHOR KEYWORDS: Aluminothermic reduction; Density; Liquid metallurgy; Metal-matrix-composites; Steel; Young's modulus
DOCUMENT TYPE: Article
SOURCE: Scopus

Zhang, H., Diehl, M., Roters, F., Raabe, D.
A virtual laboratory using high resolution crystal plasticity simulations to determine the initial yield surface for sheet metal forming operations
(2016) International Journal of Plasticity, 80, pp. 111-138. Cited 13 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84959318095&doi=10.1016%2fj.ijplas.2016.01.002&partnerID=40&md5=ecd595ee4bc587d6341d7325374c8709

DOI: 10.1016/j.ijplas.2016.01.002
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany;
Institute of Forming Technology and Equipment, Shanghai Jiao Tong University, 1954 Hua Shan Road, Shanghai, China
ABSTRACT: We present a virtual laboratory to investigate the anisotropic yield behavior of polycrystalline materials by using high resolution crystal plasticity simulations. Employing a fast spectral method solver enables us to conduct a large number of full-field virtual experiments with different stress states to accurately identify the yield surface of the probed materials. Based on the simulated yield stress points, the parameters for many commonly used yield functions are acquired simultaneously with a nonlinear least square fitting procedure. Exemplarily, the parameters of four yield functions frequently used in sheet metal forming, namely Yld91, Yld2000-2D, Yld2004-18p, and Yld2004-27p are adjusted to accurately describe the yield behavior of an AA3014 aluminum alloy at two material states, namely with a recrystallization texture and a cold rolling texture. The comparison to experimental results proves that the methodology presented, combining accuracy with efficiency, is a promising micromechanics-based tool for probing the mechanical anisotropy of polycrystalline metals and for identifying the parameters of advanced yield functions.
AUTHOR KEYWORDS: A. Cutting and forming; A. Yield condition; B. Anisotropic material; B. Crystal plasticity; Spectral methods
DOCUMENT TYPE: Article
SOURCE: Scopus

Ram, F., Li, Z., Zaefferer, S., Hafez Haghighat, S.M., Zhu, Z., Raabe, D., Reed, R.C.
On the origin of creep dislocations in a Ni-base, single-crystal superalloy: An ECCI, EBSD, and dislocation dynamics-based study
(2016) Acta Materialia, 109, pp. 151-161. Cited 5 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84959574638&doi=10.1016%2fj.actamat.2016.02.038&partnerID=40&md5=1ddee5d0c9645dad4b34e1cf1b2c31f1

DOI: 10.1016/j.actamat.2016.02.038
AFFILIATIONS: Max-Planck Institut für Eisenforschung GmbH, Max-Planck-str. 1, Düsseldorf, Germany;
Department of Materials, University of Oxford, Parks Road, Oxford, United Kingdom
ABSTRACT: This work investigates the origin of creep dislocations in a Ni-base, single crystal superalloy subject to creep at an intermediate stress and temperature. Employing high angular resolution electron backscatter diffraction (HR-EBSD), electron channeling contrast imaging under controlled diffraction conditions (cECCI) and discrete dislocation dynamics (DDD) modelling, it is shown that low-angle boundaries - which correspond to dendrite boundaries or their residues after annealing - are not the major sources of creep dislocations. At the onset of creep deformation,

they are the only active sources. Creep dislocations are emitted from them and percolate into the dislocation-depleted crystal. However, the percolation is very slow. As creep deformation proceeds, before the boundary-originated dislocations move further than a few micrometers away from their source boundary, individual dislocations that are spread throughout the undeformed microstructure become active and emit avalanches of creep dislocations in boundary-free regions, i.e. regions farther than a few micrometer away from boundaries. Upon their activation, the density of creep dislocations in boundary-free regions soars by two orders of magnitude; and the entire microstructure becomes deluged with creep dislocations. The total area of boundary-free regions is several times the total area of regions covered by boundary-originated creep dislocations. Therefore, the main sources of creep dislocations are not low-angle boundaries but individual, isolated dislocations in boundary-free regions.

AUTHOR KEYWORDS: Creep dislocations; Dislocation dynamics; Low-angle grain boundaries; Single-crystal Ni-base supperalloys
DOCUMENT TYPE: Article
SOURCE: Scopus

Tarzimoghadam, Z., Rohwerder, M., Merzlikin, S.V., Bashir, A., Yedra, L., Eswara, S., Ponge, D., Raabe, D.
Multi-scale and spatially resolved hydrogen mapping in a Ni-Nb model alloy reveals the role of the δ phase in hydrogen embrittlement of alloy 718
(2016) Acta Materialia, 109, pp. 69-81. Cited 19 times.
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DOI: 10.1016/j.actamat.2016.02.053
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany;
Advanced Instrumentation for Ion-Nano-Analytics (AINA), MRT Department, Luxembourg Institute of Science and Technology (LIST), 41 rue du Brill, Belvaux, Luxembourg
ABSTRACT: We investigated the hydrogen distribution and desorption behavior in an electrochemically hydrogen-charged binary Ni-Nb model alloy to study the role of δ phase in hydrogen embrittlement of alloy 718. We focus on two aspects, namely, (1) mapping the hydrogen distribution with spatial resolution enabling the observation of the relations between desorption profiles and desorption sites; and (2) correlating these observations with mechanical testing results to reveal the degradation mechanisms. The trapping states of hydrogen in the alloy were globally analyzed by Thermal Desorption Spectroscopy (TDS). Additionally, spatially resolved hydrogen mapping was conducted using silver decoration, Scanning Kelvin Probe Force Microscopy (SKPFM) and Secondary Ion Mass Spectrometry (SIMS): The Ag decoration method revealed rapid effusion of hydrogen at room temperature from the γ-matrix. The corresponding kinetics was resolved in both, space and time by the SKPFM measurements. At room temperature the hydrogen release from the γ-matrix steadily decreased until about 100 h and then was taken over by the δ phase from which the hydrogen was released much slower. For avoiding misinterpretation of hydrogen signals stemming from environmental effects we also charged specimens with deuterium. The deuterium distribution in the microstructure was studied by SIMS. The combined results reveal that hydrogen dissolves more preferably inside the γ-matrix and is diffusible at room temperature while the δ phase acts as a deeper trapping site for hydrogen. With this joint and spatially resolving approach we observed the microstructure- and time-dependent distribution and release rate of hydrogen with high spatial and temporal resolution. Correlating the obtained results with mechanical testing of the hydrogen-charged samples shows that hydrogen enhanced decohesion (HEDE) occurring at the δ/matrix interfaces promotes the embrittlement.

AUTHOR KEYWORDS: Alloy 718; Delta phase; HEDE; Hydrogen embrittlement; Hydrogen mapping
DOCUMENT TYPE: Article
SOURCE: Scopus

Souza, F.M., Padilha, A.F., Gutierrez-Urrutia, I., Raabe, D.
Microstructural analysis in the Fe-30.5Mn-8.0Al-1.2C and Fe-30.5Mn-2.1Al-1.2C steels upon cold rolling
(2016) Revista Escola de Minas, 69 (2), pp. 167-173.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84971632083&doi=10.1590%2f0370-44672015690097&partnerID=40&md5=a077d4a94057925a15a4f13a75a603be

DOI: 10.1590/0370-44672015690097
AFFILIATIONS: Secretaria de Estado de Educação de Minas Gerais, Belo Horizonte, Minas Gerais, Brazil;
Universidade de São Paulo – USP, Escola Politécnica, Departamento de Engenharia Metalúrgica e de Materiais, São Paulo, São Paulo, Brazil;
National Institute for Materials Science, Research Center for Strategic Materials, Microstructure Design Group, Tsukuba, Japan;
Max-Planck-Institut fur Eisenforschung GmbH, Department of Microstructure Physics and Alloy Design, Dusseldorf, Germany
ABSTRACT: Electron backscatter diffraction (EBSD) and electron channeling contrast imaging (ECCI) were used to examine microstructural changes of the austenitic low-density Fe-30.5Mn-8.0Al-1.2C (8Al) and Fe-30.5Mn-2.1Al-1.2C (2Al) (wt.%) steels during cold rolling. As the strain increased, deformation mechanisms, such as stacking faults, slip, mechanical twinning, and shear banding were activated in both steels cold rolled up to strain of 0.69. Only slip was noted in these steels at low strain (ε=0.11) and slip dominance was detected in the 8Al steel at higher strains. Shear banding became active at higher strain (ε~0.7) in these materials. An inhomogeneous microstructure formed in both alloys at such strain level. More extensive mechanical twinning in the 2Al alloy than that in the 8Al alloy was observed. Fish bone-like structure patterns were revealed in the 8Al steel and a river-like structure in the 2Al steel. Detailed microstructure features as elongated and fragmented grains along the rolling direction (RD) were found for both steels, as already observed in other high-Mn steels. These deformed structures are composed by lamellar packets which can contain mechanical twins or slip lines and shear bands.
AUTHOR KEYWORDS: Austenitic steels; EBSD; ECCI; Fe-Mn-Al-C alloys; Fe-Mn-C alloys; Microstructure; TWIP steels
DOCUMENT TYPE: Article
SOURCE: Scopus

Aparicio-Fernández, R., Springer, H., Szczepaniak, A., Zhang, H., Raabe, D.
In-situ metal matrix composite steels: Effect of alloying and annealing on morphology, structure and mechanical properties of TiB2 particle containing high modulus steels
(2016) Acta Materialia, 107, pp. 38-48. Cited 7 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84957002245&doi=10.1016%2fj.actamat.2016.01.048&partnerID=40&md5=18c21900edbd6300ed13447728ad5fc0

DOI: 10.1016/j.actamat.2016.01.048
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: We systematically study the morphology, size and dispersion of TiB2 particles formed in-situ from Fe-Ti-B based melts, as well as their chemical composition, crystal structure and mechanical properties. The effects of 5 wt.% additions of Cr, Ni, Co, Mo, W, Mn, Al, Si, V, Ta, Nb and Zr, respectively, as well as additional annealing treatments, were investigated in order to derive guidelines for the knowledge based alloy

design of steels with an increased stiffness/density ratio and sufficiently high ductility. All alloying elements were found to increase the size of the coarse primary TiB2 particles, while Co led to the most homogeneous size distribution. The size of the eutectic TiB2 constituents was decreased by all alloying additions except Ni, while their aspect ratio was little affected. No clear relation between chemical composition, crystal structure and mechanical properties of the particles could be observed. Annealing of the as-cast alloys slightly increased the size of the primary particles, but at the same time strongly spheroidised the eutectics. Additions of Co and Cr appear thus as the best starting point for designing novel in-situ high modulus metal matrix composite steels, while using Mn in concert with thermo-mechanical processing is most suited to adapt the matrix' microstructure and optimise the particle/matrix co-deformation processes.
AUTHOR KEYWORDS: Density; Liquid metallurgy; Metal-matrix-composites; Steels; Young's modulus
DOCUMENT TYPE: Article
SOURCE: Scopus

Schnabel, V., Köhler, M., Evertz, S., Gamcova, J., Bednarcik, J., Music, D., Raabe, D., Schneider, J.M.
Revealing the relationships between chemistry, topology and stiffness of ultrastrong Co-based metallic glass thin films: A combinatorial approach (2016) Acta Materialia, 107, pp. 213-219. Cited 5 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84957922511&doi=10.1016%2fj.actamat.2016.01.060&partnerID=40&md5=7d3f113a43d1e42e6c633dbb55822b00

DOI: 10.1016/j.actamat.2016.01.060
AFFILIATIONS: Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, Aachen, Germany;
Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
Deutsches Elektronen Synchrotron DESY, FS-PE Group, Notkestrasse 85, Hamburg, Germany;
Pavol Jozef Šafárik University, Department of Condensed Matter Physics, Park Angelinum 9, Košice, Slovakia
ABSTRACT: An efficient way to study the relationship between chemical composition and mechanical properties of thin films is to utilize the combinatorial approach, where spatially resolved mechanical property measurements are conducted along a concentration gradient. However, for thin film glasses many properties including the mechanical response are affected by chemical topology. Here a novel method is introduced which enables spatially resolved short range order analysis along concentration gradients of combinatorially synthesized metallic glass thin films. For this purpose a CoZrTaB metallic glass film of 3 μm thickness is deposited on a polyimide foil, which is investigated by high energy X-ray diffraction in transmission mode. Through the correlative chemistry-topology-stiffness investigation, we observe that an increase in metalloid concentration from 26.4 to 32.7 at% and the associated formation of localized (hybridized) metal - metalloid bonds induce a 10% increase in stiffness. Concomitantly, along the same composition gradient, a metalloid-concentration-induced increase in first order metal - metal bond distances of 1% is observed, which infers itinerant (metallic) bond weakening. Hence, the metalloid concentration induced increase in hybridized bonding dominates the corresponding weakening of metallic bonds.
AUTHOR KEYWORDS: Combinatorics; Hybridization; Metallic glass; Topology
DOCUMENT TYPE: Article
SOURCE: Scopus

Raabe, D., Roters, F., Neugebauer, J., Gutierrez-Urrutia, I., Hickel, T., Bleck, W., Schneider, J.M., Wittig, J.E., Mayer, J.

Ab initio-guided design of twinning-induced plasticity steels
(2016) MRS Bulletin, 41 (4), pp. 320-325. Cited 9 times.
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DOI: 10.1557/mrs.2016.63
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, RWTCH Aachen University, Germany;
Max-Planck-Institut für Eisenforschung, Germany;
National Institute for Materials Science, Japan;
Department of Computational Materials Design, Max-Planck-Institut für Eisenforschung, Germany;
Steel Institute, RWTH Aachen University, Germany;
RWTH Aachen University, Germany;
Vanderbilt University, United States;
Central Facility for Electron Microscopy, RWTH Aachen University, Ernst Ruska-Centre, Forschungszentrum Jülich, Germany
ABSTRACT: The twinning-induced plasticity effect enables designing austenitic Fe-Mn-C-based steels with >70% elongation with an ultimate tensile strength >1 GPa. These steels are characterized by high strain hardening due to the formation of twins and complex dislocation substructures that dynamically reduce the dislocation mean free path. Both mechanisms are governed by the stacking-fault energy (SFE) that depends on composition. This connection between composition and substructure renders these steels ideal model materials for theory-based alloy design: Ab initio-guided composition adjustment is used to tune the SFE, and thus, the strain-hardening behavior for promoting the onset of twinning at intermediate deformation levels where the strain-hardening capacity provided by the dislocation substructure is exhausted. We present thermodynamic simulations and their use in constitutive models, as well as electron microscopy and combinatorial methods that enable validation of the strain-hardening mechanisms. Copyright © 2016 Materials Research Society.
AUTHOR KEYWORDS: ductility; microstructure; simulation; steel; strength
DOCUMENT TYPE: Article
SOURCE: Scopus

Morsdorf, L., Pradeep, K.G., Herzer, G., Kovács, A., Dunin-Borkowski, R.E., Povstugar, I., Konygin, G., Choi, P., Raabe, D.
Phase selection and nanocrystallization in Cu-free soft magnetic FeSiNbB amorphous alloy upon rapid annealing
(2016) Journal of Applied Physics, 119 (12), art. no. 124903, . Cited 1 time.
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DOI: 10.1063/1.4944595
AFFILIATIONS: Department for Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, Düsseldorf, Germany;
Materials Chemistry, RWTH Aachen University, Kopernikusstrasse 10, Aachen, Germany;
Vacuumschmelze GmbH and Co KG, Grüner Weg 37, Hanau, Germany;
Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Peter Grünberg Institute 5, Forschungszentrum Jülich, Jülich, Germany;
Physical-Technical Institute UrB RAS, Kirov str. 132, Izhevsk, Russian Federation;
Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology, Daejeon, South Korea
ABSTRACT: Nucleation of soft magnetic Fe3Si nanocrystals in Cu-free Fe74.5Si15.5Nb3B7 alloy, upon rapid (10 s) and conventional (30 min) annealing, was investigated using x-ray diffraction, transmission electron

microscopy, Mössbauer spectroscopy, and atom probe tomography. By employing rapid annealing, preferential nucleation of Fe3Si nanocrystals was achieved, whereas otherwise there is simultaneous nucleation of both Fe3Si and undesired Fe-B compound phases. Analysis revealed that the enhanced Nb diffusivity, achieved during rapid annealing, facilitates homogeneous nucleation of Fe3Si nanocrystals while shifting the secondary Fe-B crystallization to higher temperatures resulting in pure soft magnetic nanocrystallization with very low coercivities of ~10 A/m.
DOCUMENT TYPE: Article
SOURCE: Scopus

Brands, D., Balzani, D., Scheunemann, L., Schröder, J., Richter, H., Raabe, D.
Computational modeling of dual-phase steels based on representative three-dimensional microstructures obtained from EBSD data
(2016) Archive of Applied Mechanics, 86 (3), pp. 575-598. Cited 6 times.
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DOI: 10.1007/s00419-015-1044-1
AFFILIATIONS: Abteilung Bauwissenschaften, Fakultät für Ingenieurwissenschaften, Institut für Mechanik, Universität Duisburg-Essen, Universitätsstraße 15, Essen, Germany;
Fakultät für Bauingenieurwesen, Institut für Mechanik und Flächentragwerke, TU Dresden, Dresden, Germany;
ThyssenKrupp Steel Europe AG, Technologie and Innovation, TIS-AT-UT Umformtechnik, Dortmund, Germany;
Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
ABSTRACT: The microstructure of dual-phase steels consisting of a ferrite matrix with embedded martensite inclusions is the main contributor to the mechanical properties such as high ultimate tensile strength, high work hardening rate, and good ductility. Due to the composite structure and the wide field of applications of this steel type, a wide interest exists in corresponding virtual computational experiments. For a reliable modeling, the microstructure should be included. For that reason, in this paper we follow a computational strategy based on the definition of a representative volume element (RVE). These RVEs will be constructed by a set of tomographic measurements and mechanical tests. In order to arrive at more efficient numerical schemes, we also construct statistically similar RVEs, which are characterized by a lower complexity compared with the real microstructure but which represent the overall material behavior accurately. In addition to the morphology of the microstructure, the austenite–martensite transformation during the steel production has a relevant influence on the mechanical properties and is considered in this contribution. This transformation induces a volume expansion of the martensite phase. A further effect is determined in nanoindentation test, where it turns out that the hardness in the ferrite phase increases exponentially when approaching the martensitic inclusion. To capture these gradient properties in the computational model, the volumetric expansion is applied to the martensite phase, and the arising equivalent plastic strain distribution in the ferrite phase serves as basis for a locally graded modification of the ferritic yield curve. Good accordance of the model considering the gradient yield behavior in the ferrite phase is observed in the numerical simulations with experimental data.
AUTHOR KEYWORDS: Dual-phase steel; EBSD–FIB; Microheterogeneous materials; Multiscale simulations; Reconstruction of microstructure; RVE; SSRVE; Volume expansion of martensite
DOCUMENT TYPE: Article

SOURCE: Scopus

Jägle, E.A., Sheng, Z., Wu, L., Lu, L., Risse, J., Weisheit, A., Raabe, D.
Precipitation Reactions in Age-Hardenable Alloys During Laser Additive Manufacturing
(2016) JOM, 68 (3), pp. 943-949. Cited 4 times.
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DOI: 10.1007/s11837-015-1764-2
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, Düsseldorf, Germany;
Institut für Eisenhüttenkunde, Rheinisch-Westfälische Technische Hochschule Aachen, Intzestrasse 1, Aachen, Germany;
Fraunhofer Institut für Lasertechnik, Steinbachstrasse 15, Aachen, Germany
ABSTRACT: We describe and study the thermal profiles experienced by various age-hardenable alloys during laser additive manufacturing (LAM), employing two different manufacturing techniques: selective laser melting and laser metal deposition. Using scanning electron microscopy and atom probe tomography, we reveal at which stages during the manufacturing process desired and undesired precipitation reactions can occur in age-hardenable alloys. Using examples from a maraging steel, a nickel-base superalloy and a scandium-containing aluminium alloy, we demonstrate that precipitation can already occur during the production of the powders used as starting material, during the deposition of material (i.e. during solidification and subsequent cooling), during the intrinsic heat treatment effected by LAM (i.e. in the heat affected zones) and, naturally, during an ageing post-heat treatment. These examples demonstrate the importance of understanding and controlling the thermal profile during the entire additive manufacturing cycle of age-hardenable materials including powder synthesis.

DOCUMENT TYPE: Article
SOURCE: Scopus

Cereceda, D., Diehl, M., Roters, F., Raabe, D., Perlado, J.M., Marian, J.
Unraveling the temperature dependence of the yield strength in single-crystal tungsten using atomistically-informed crystal plasticity calculations
(2016) International Journal of Plasticity, 78, pp. 242-265. Cited 17 times.
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DOI: 10.1016/j.ijplas.2015.09.002
AFFILIATIONS: Department of Materials Science and Engineering, University of California Los Angeles, Los Angeles, CA, United States;
Physical and Life Sciences Dirct., Lawrence Livermore National Laboratory, LivermoreCA, United States;
Instituto de Fusión Nuclear, Universidad Politécnica de Madrid, Madrid, Spain;
Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: We use a physically-based crystal plasticity model to predict the yield strength of body-centered cubic (bcc) tungsten single crystals subjected to uniaxial loading. Our model captures the thermally-activated character of screw dislocation motion and full non-Schmid effects, both of which are known to play critical roles in bcc plasticity. The model uses atomistic calculations as the sole source of constitutive information, with no parameter fitting of any kind to experimental data. Our results are in excellent agreement with experimental measurements of the yield stress as a function of temperature for a number of loading orientations. The validated

methodology is employed to calculate the temperature and strain-rate dependence of the yield strength for 231 crystallographic orientations within the standard stereographic triangle. We extract the strain-rate sensitivity of W crystals at different temperatures, and finish with the calculation of yield surfaces under biaxial loading conditions that can be used to define effective yield criteria for engineering design models. © 2015 Elsevier Ltd.
AUTHOR KEYWORDS: Bcc crystal plasticity; Non-Schmid effects; Screw dislocations; Single crystal tungsten; Yield stress
DOCUMENT TYPE: Article
SOURCE: Scopus

Yao, M.J., Dey, P., Seol, J.-B., Choi, P., Herbig, M., Marceau, R.K.W., Hickel, T., Neugebauer, J., Raabe, D.
Combined atom probe tomography and density functional theory investigation of the Al off-stoichiometry of κ-carbides in an austenitic Fe-Mn-Al-C low density steel
(2016) Acta Materialia, 106, pp. 229-238. Cited 19 times.
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AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
National Institute for Nanomaterials Technology, POSTECH, Pohang, South Korea;
Deakin University, Institute for Frontier Materials, Geelong, VIC, Australia
ABSTRACT: We report on the investigation of the off-stoichiometry and site-occupancy of κ-carbide precipitates within an austenitic (γ), Fe-29.8Mn-7.7Al-1.3C (wt.%) alloy using a combination of atom probe tomography and density functional theory. The chemical composition of the κ-carbides as measured by atom probe tomography indicates depletion of both interstitial C and substitutional Al, in comparison to the ideal stoichiometric L′12 bulk perovskite. In this work we demonstrate that both these effects are coupled. The off-stoichiometric concentration of Al can, to a certain extent, be explained by strain caused by the κ/γ mismatch, which facilitates occupation of Al sites in κ-carbide by Mn atoms (Mnγ Al anti-site defects). The large anti-site concentrations observed by our experiments, however, can only be stabilized if there are C vacancies in the vicinity of the anti-site. © 2016 Acta Materialia Inc.
AUTHOR KEYWORDS: Atom probe tomography (APT); Austenitic low density steel; Coherent precipitates; Density functional theory (DFT); Off-stoichiometry
DOCUMENT TYPE: Article
SOURCE: Scopus

Tan, X.-D., Xu, Y.-B., Ponge, D., Yang, X.-L., Hu, Z.-P., Peng, F., Ju, X.-W., Wu, D., Raabe, D.
Effect of intercritical deformation on microstructure and mechanical properties of a low-silicon aluminum-added hot-rolled directly quenched and partitioned steel
(2016) Materials Science and Engineering A, 656, pp. 200-215. Cited 3 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84961316892&doi=10.1016%2fj.msea.2016.01.040&partnerID=40&md5=a333876764f3268056c3b954799bc84c

DOI: 10.1016/j.msea.2016.01.040
AFFILIATIONS: State Key Laboratory of Rolling and Automation, Northeastern University, Shenyang, China;

Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, Düsseldorf, Germany;
CERI LONG PRODUCT CO., LTD., Beijing, China
ABSTRACT: Here, we applied hot-rolling in conjunction with direct quenching and partitioning (HDQ&P) processes with different rolling schedules to a low-C low-Si Al-added steel. Ferrite was introduced into the steel by intercritical rolling and air cooling after hot-rolling. The effect of intercritcal deformation on the microstructure evolution and mechanical properties was investigated. The promotion of austenite stabilization and the optimization of the TRIP effect due to a moderate degree of intercritical deformation were systematically explored. The results show that the addition of 1.46 wt% of Al can effectively promote ferrite formation. An intercritical deformation above 800 °C can result in a pronounced bimodal grain size distribution of ferrite and some elongated ferrite grains containing sub-grains. The residual strain states of both austenite and ferrite and the occurrence of bainite transformation jointly increase the retained austenite fraction due to its mechanical stabilization and the enhanced carbon partitioning into austenite from its surrounding phases. An intercritical deformation below 800 °C can profoundly increase the ferrite fraction and promote the recrystallization of deformed ferrite. The formation of this large fraction of ferrite enhances the carbon enrichment in the untransformed austenite and retards the bainite transformation during the partitioning process and finally enhances martensite transformation and decreases the retained austenite fraction. The efficient TRIP effect of retained austenite and the possible strain partitioning of bainite jointly improve the work hardening and formability of the steel and lead to the excellent mechanical properties with relatively high tensile strength (905 MPa), low yield ratio (0.60) and high total elongation (25.2%). © 2016 Elsevier B.V.
AUTHOR KEYWORDS: Austenite stabilization; Hot-rolled directly quenched and partitioned steel; Intercritical deformation; Mechanical properties; Quenching and partitioning; TRIP effect
DOCUMENT TYPE: Article
SOURCE: Scopus

Ma, D., Eisenlohr, P., Epler, E., Volkert, C.A., Shanthraj, P., Diehl, M., Roters, F., Raabe, D.
Crystal plasticity study of monocrystalline stochastic honeycombs under in-plane compression
(2016) Acta Materialia, 103, pp. 796-808. Cited 4 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84948127972&doi=10.1016%2fj.actamat.2015.11.016&partnerID=40&md5=e062497bad632e1a2f3214dc1996ef60

DOI: 10.1016/j.actamat.2015.11.016
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI, United States;
Institute for Materials Physics, University of Göttingen, Friedrich-Hund-Platz 1, Göttingen, Germany;
Aachen Institute for Advanced Study in Computational Engineering Science, RWTH Aachen University, Schinkelstraße 2, Aachen, Germany
ABSTRACT: We present a study on the plastic deformation of single crystalline stochastic honeycombs under in-plane compression using a crystal plasticity constitutive description for face-centered cubic (fcc) materials, focusing on the very early stage of plastic deformation, and identifying the interplay between the crystallographic orientation and the cellular structure during plastic deformation. We observe that despite the stochastic structure, surprisingly, the slip system activations in the honeycombs are almost identical to their corresponding bulk single crystals at the early stage of the plastic deformation. On the other hand, however, the yield stresses of the honeycombs are nearly independent of their

crystallographic orientations. Similar mechanical response is found in compression testing of nanoporous gold micro-pillars aligned with various crystallographic orientations. The macroscopic stress tensors of the honeycombs show the same anisotropy as their respective bulk single crystals. Locally, however, there is an appreciable fluctuation in the local stresses, which are even larger than for polycrystals. This explains why the Taylor/Schmid factor associated with the crystallographic orientation is less useful to estimate the yield stresses of the honeycombs than the bulk single crystals and polycrystals, and why the plastic deformation occurs at smaller strains in the honeycombs than their corresponding bulk single crystals. Besides these findings, the observations of the crystallographic reorientation suggest that conventional orientation analysis tools, such as inverse pole figure and related tools, would in general fail to study the plastic deformation mechanism of monocrystalline cellular materials. © 2015 Acta Materialia Inc.
AUTHOR KEYWORDS: Cellular material; Crystal plasticity; Crystallographic orientation; Honeycomb; Nanoporous gold
DOCUMENT TYPE: Article
SOURCE: Scopus

Hono, K., Raabe, D., Ringer, S.P., Seidman, D.N.
Atom probe tomography of metallic nanostructures
(2016) MRS Bulletin, 41 (1), pp. 23-29. Cited 5 times.
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DOI: 10.1557/mrs.2015.314
AFFILIATIONS: Magnetic Materials Unit, National Institute for Materials Science, Japan;
Department of Microstructure Physics and Alloy Design, Max Planck Institute for Iron Research, Germany;
Australian Institute for Nanoscale Science and Technology, School of Aerospace Mechanical and Mechatronic Engineering, University of Sydney, Australia;
Dept. of Mat. Sci. and Engineering and the Northwestern University Center for Atom Probe Tomography, Northwestern University, United States
ABSTRACT: This article focuses on four topics that demonstrate the importance of atom probe tomography for obtaining nanostructural information that provides deep insights into the structures of metallic alloys, leading to a better understanding of their properties. First, we discuss the microstructure-coercivity relationship of Nd-Fe-B permanent magnets, essential for developing a higher coercivity magnet. Second, we address equilibrium segregation at grain boundaries with the aim of manipulating their interfacial structure, energies, compositions, and properties, thereby enabling beneficial material behavior. Third, recent progress in the search to extend the performance and practicality of the next generation of advanced high-strength steels is discussed. Finally, a study of the temporal evolution of a Ni-Al-Cr alloy through the stages of nucleation, growth, and coarsening (Ostwald ripening) and its relationship with the predictions of a model for quasi-stationary coarsening is described. This information is critical for understanding high-Temperature mechanical properties of the material. © Copyright Materials Research Society 2016Â.
AUTHOR KEYWORDS: atom probe microscopy (APM); atom probe tomography (APT); field ion microscopy (FIM); microstructure; steel; strength
DOCUMENT TYPE: Article
SOURCE: Scopus

Koyama, M., Tasan, C.C., Nagashima, T., Akiyama, E., Raabe, D., Tsuzaki, K.
Hydrogen-assisted damage in austenite/martensite dual-phase steel
(2016) Philosophical Magazine Letters, 96 (1), pp. 9-18. Cited 7 times.

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AFFILIATIONS: Department of Mechanical Engineering, Kyushu University, 744 Motooka, Nishi-ku, Fukuoka, Japan;
Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strae 1, Düsseldorf, Germany;
Research Center for Strategic Materials, National Institute for Materials Science, 1-2-1, Sengen, Ibaraki, Japan
ABSTRACT: For understanding the underlying hydrogen embrittlement mechanism in transformation-induced plasticity steels, the process of damage evolution in a model austenite/martensite dual-phase microstructure following hydrogenation was investigated through multi-scale electron channelling contrast imaging and in situ optical microscopy. Localized diffusible hydrogen in martensite causes cracking through two mechanisms: (1) interaction between {1 1 0}M localized slip and {1 1 2}M twin and (2) cracking of martensite-martensite grain interfaces. The former resulted in nanovoids along the {1 1 2}M twin. The coalescence of the nanovoids generated plate-like microvoids. The latter caused shear localization on the specific plane where the crack along the martensite/martensite boundary exists, which led to additional martensite/martensite boundary cracking. © 2015 Taylor & Francis.
AUTHOR KEYWORDS: damage; electron channeling; Embrittlement; Fe-based alloys; hydrogen in metals; silver decoration
DOCUMENT TYPE: Article
SOURCE: Scopus

Springer, H., Belde, M., Raabe, D.
Combinatorial design of transitory constitution steels: Coupling high strength with inherent formability and weldability through sequenced austenite stability
(2016) Materials and Design, 90, pp. 1100-1109. Cited 7 times.
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DOI: 10.1016/j.matdes.2015.11.050
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: We introduce a novel alloying and processing scheme for high strength steels, which allows for precise and cost-effective cold forming due to high fractions of metastable austenite, and a subsequent low-distortion, coating-preserving strengthening through martensitic transformation induced by low temperature treatments. As the constitution is thus synchronised with the processing requirements, we refer to these materials as Transitory Constitution Steels. Suitable alloy compositions were identified by high throughput screenings through the exemplarily material systems Fe-5Ni-0.3C-(3-15)Mn and Fe-13.5Cr-6Mn-2Cu-0.2C-(0-2)Ni (wt.%) using combinatorial bulk metallurgical methods. The transformation behaviour, mechanical properties and underlying microstructural phenomena were studied in more detail after upscaling of selected compositions. The steel Fe-13.5Cr-6Mn-1.5Cu-0.2C (wt.%) exhibited an increase in yield strength from 300 to 1050. MPa after immersion into liquid nitrogen, as well as an ultimate tensile strength of more than 1700. MPa at a total elongation of more than 9%. Despite the ultra high strength, no embrittlement induced by Laser beam welding was observed, highlighting the inherent weldability of steels synthesised by the alloying and processing scheme presented here. Possibilities for flexible alloy design and processing variations are discussed. © 2015 Elsevier Ltd.
AUTHOR KEYWORDS: Austenite stability; Automotive; High throughput alloy design; Steels; Welding

DOCUMENT TYPE: Article
SOURCE: Scopus

Souza, F.M., Padilha, A.F., Gutierrez-Urruti, I., Raabe, D.
Texture evolution in the Fe-30.5Mn-8.0Al-1.2C and Fe-30.5Mn-2.1Al-1.2C steels upon cold rolling
(2016) Revista Escola de Minas, 69 (1), pp. 59-65. Cited 1 time.
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DOI: 10.1590/0370-44672015690122
AFFILIATIONS: PEB - Secretaria de Estado de Educação de Minas Gerais, Belo Horizonte, Minas Gerais, Brazil;
Universidade de São Paulo - USP, Escola Politécnica da Universidade de São Paulo, Departamento de Engenharia, Metalúrgica e de Materiais, São Paulo, São Paulo, Brazil;
National Institute for Materials Science, Research Center for Strategic Materials, Microstructure Design Group, Tsukuba, Japan;
Max-Planck-Institut fur Eisenforschung GmbH, Department of Microstructure Physics and Alloy Design, Dusseldorf, Germany
ABSTRACT: Crystallographic textures of the austenitic low-density Fe-30.5Mn-8.0Al-1.2C (8Al) and Fe-30.5Mn-2.1Al-1.2C (2Al) (wt.%) steels were examined during cold rolling by means of electron backscatter diffraction (EBSD) and electron channeling contrast imaging (ECCI). Random oriented grains orient towards Goss- and brass-components along the α-fiber as the strain increased, with activation of slip, mechanical twinning, and shear banding, for both steels. S- and copper-orientations were also observed in the 8Al steel at 50% reduction. The route of Cu-CuT-Gossbrass texture evolution was found in the 2Al alloy. Cu, Goss, and brass textures occur as a dominant texture in the deformed 8Al alloy. Copper-type texture accompanied with slip at low reduction (20%), as well as Cu-type shear bands, and shear banding inside Goss-oriented grains at higher reduction (50%), were observed in the 8Al steel. It is suggested that this copper-type rolling texture may be attributed to the Al addition, which contributes to its low twinning activity compared to that in the 2Al alloy. Cu-CuT-brass f.c.c. rolling texture transition to form the Brass-type texture was observed at higher reduction in the 2Al alloy with strong similarity to that found in other Fe-Mn-C system TWIP steels.
AUTHOR KEYWORDS: Austenitic steels; EBSD; Fe-Mn-Al-C alloys; Fe-Mn-C alloys; Texture; TWIP steel
DOCUMENT TYPE: Article
SOURCE: Scopus

Tarzimoghadam, Z., Ponge, D., Kloewer, J., Raabe, D.
Hydrogen-Assisted failure in nickel base alloy UNS N07718
(2016) NACE - International Corrosion Conference Series, 3, pp. 2401-2410. Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84991619672&partnerID=40&md5=661772964e292d661102caeaa443d539

AFFILIATIONS: Max-Planck-lnstitut fuer Eisenforschung GmbH, Max-Planck-Strasse 1, Duesseldorf, Germany;
Max-Planck-lnstitut fuer Eisenforschung, Max-Planck-Strasse 1, Duesseldorf, Germany;
VDM Metals GmbH, Kleffstrasse 23, Altena, Germany
ABSTRACT: Hydrogen embrittlement (HE) of nickel base alloy UNS N07718 was studied by tensile testing at low strain rate (10-4 s-1) under hydrogen charging. Hydrogen-Assisted cracking mechanisms were studied via the joint use of Electron BackScatter Diffraction (EBSD) analysis and orientation-optimized Electron Channeling Contrast (ECC) imaging. Both intergranular and transgranular cracking were observed when hydrogen was introduced.

Embrittlement occurred by strong hydrogen-deformation interactions and several mechanisms were found to contribute to hydrogen-Assisted cracking in this alloy. Transgranular cracking was caused by Hydrogen Enhanced Localized Plasticity (HELP)-Assisted shear localization along slip planes. Intergranular cracking was more specifically categorized into three parts: grain boundary triple junction cracking, slip-localization on the grain boundaries and matrix/o1 phase interface cracking. Observations on distinct metallurgical states of alloy UNS N07718, with different precipitation conditions for y" phase and 01 phase confirmed that the 01 phase promotes HE by initializing micro-cracks. © 2016 by NACE.
AUTHOR KEYWORDS: Delta phase; Hydrogen embrittlement; Tensile test; UNS N07718
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Kovács, A., Pradeep, K.G., Herzer, G., Raabe, D., Dunin-Borkowski, R.E.
Magnetic microstructure in a stress-annealed Fe73.5Si15.5B7Nb3Cu1 soft magnetic alloy observed using off-axis electron holography and Lorentz microscopy
(2016) AIP Advances, 6 (5), art. no. 056501, . Cited 2 times.
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DOI: 10.1063/1.4942954
AFFILIATIONS: Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Peter Grünberg Institute, Forschungszentrum Jülich, Jülich, Germany;
Materials Chemistry, RWTH Aachen University, Aachen, Germany;
Department for Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Vacuumschmelze GmbH and Co KG, Hanau, Germany
ABSTRACT: Fe-Si-B-Nb-Cu alloys are attractive for high frequency applications due to their low coercivity and high saturation magnetization. Here, we study the effect of stress annealing on magnetic microstructure in Fe73.5Si15.5B7Nb3Cu1 using off-axis electron holography and the Fresnel mode of Lorentz transmission electron microscopy. A stress of 50 MPa was applied to selected samples during rapid annealing for 4 s, resulting in uniaxial anisotropy perpendicular to the stress direction. The examination of focused ion beam milled lamellae prepared from each sample revealed a random magnetic domain pattern in the sample that had been rapidly annealed in the absence of stress, whereas a highly regular domain pattern was observed in the stress-annealed sample. We also measured a decrease in domain wall width from ~ 94 nm in the sample annealed without stress to ~ 80 nm in the stress-annealed sample. © 2016 Author(s).
DOCUMENT TYPE: Article
SOURCE: Scopus

Guo, W., Gan, B., Molina-Aldareguia, J.M., Poplawsky, J.D., Raabe, D.
Structure and dynamics of shear bands in amorphous-crystalline nanolaminates
(2016) Scripta Materialia, 110, pp. 28-32. Cited 4 times.
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DOI: 10.1016/j.scriptamat.2015.07.038
AFFILIATIONS: Department of Microstructure Physics and Alloy Design, Max-Planck Institut für Eisenforschung, Düsseldorf, Germany;
IMDEA Materials Institute, Getafe, C/Eric Kandel 2, Madrid, Spain;
Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, United States

ABSTRACT: The velocities of shear bands in amorphous CuZr/crystalline Cu nanolaminates were quantified as a function of strain rate and crystalline volume fraction. A rate-dependent transition in flow response was found in a 100 nm CuZr/10 nm Cu nanolaminates. When increasing the Cu layer thickness from 10 nm to 100 nm, the instantaneous velocity of the shear band in these nanolaminates decreases from 11.2 μm/s to <~500 nm/s. Atom probe tomography and transmission election microcopy observation revealed that in post-deformed pillars both grain rotation in the crystalline portion and non-diffusive crystallization in the amorphous layer affect the viscosity of shear bands. © 2015 Acta Materialia Inc.
AUTHOR KEYWORDS: Atom probe tomography; Metallic glass; Nanocrystallization; Nanolaminates; Shear band
DOCUMENT TYPE: Article
SOURCE: Scopus

Gutierrez-Urrutia, I., Archie, F., Raabe, D., Yan, F.-K., Tao, N.-R., Lu, K.
Plastic accommodation at homophase interfaces between nanotwinned and recrystallized grains in an austenitic duplex-microstructured steel
(2016) Science and Technology of Advanced Materials, 17 (1), pp. 29-36. Cited 1 time.
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DOI: 10.1080/14686996.2016.1140302
AFFILIATIONS: Microstructure Physics and Alloy Design, Max-Planck-Institut fűr Eisenforschung, Max-Planck Str. 1, Dűsseldorf, Germany;
Structural Materials Unit, Research Center for Strategic Materials, National Institute for Materials Science, Tsukuba, Ibaraki, Japan;
Institute of Metal Research, Chinese Academy of Sciences, Shenyang National Laboratory for Materials Science, Shenyang, China;
Herbert Gleiter Institute of Nanoscience, Nanjing University of Science & Technology, Nanjing, China
ABSTRACT: The plastic co-deformation behavior at the homophase interfaces between the hard nanotwinned grain inclusions and the soft recrystallized matrix grains in a duplex-microstructured AISI 316L austenitic stainless steel is examined through the analysis of long-range orientation gradients within the matrix grains by electron backscatter diffraction and transmission electron microcopy. Our analysis reveals that the mechanical accommodation of homophase interfaces until a macroscopic strain of 22% is realized within a small area of soft grains (about four grains) adjacent to the homophase interface. The activation of deformation twinning in the first two grain layers results in the occurrence of a ‘hump’ in the orientation gradient profile. We ascribe this effect to the role of deformation twinning on the generation of geometrically necessary dislocations. The smooth profile of the orientation gradient amplitude within the first 10 grain layers indicates a gradual plastic accommodation of the homophase interfaces upon straining. As a consequence, damage nucleation at such interfaces is impeded, resulting in an enhanced ductility of the single phase duplex-microstructured steel. © 2016 The Author(s).
DOCUMENT TYPE: Article
SOURCE: Scopus

Timokhina, I.B., Liss, K.D., Raabe, D., Rakha, K., Beladi, H., Xiong, X.Y., Hodgson, P.D.
Growth of bainitic ferrite and carbon partitioning during the early stages of bainite transformation in a 2 mass% silicon steel studied by in situ neutron diffraction, TEM and APT
(2016) Journal of Applied Crystallography, 49, pp. 399-414. Cited 4 times.

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DOI: 10.1107/S1600576716000418
AFFILIATIONS: Institute for Frontier Materials, Deakin University, Geelong Waurn Ponds Campus, Geelong, VIC, Australia;
Australian Nuclear Science and Technology Organisation, New Illawarra Road, Lucas Heights, NSW, Australia;
Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, Düsseldorf, Germany;
Monash Centre for Electron Microscopy, Monash UniversityVIC, Australia
ABSTRACT: In situ neutron diffraction, transmission electron microscopy (TEM) and atom probe tomography (APT) have been used to study the early stages of bainite transformation in a 2 mass% Si nano-bainitic steel. It was observed that carbon redistribution between the bainitic ferrite and retained austenite at the early stages of the bainite transformation at low isothermal holding occurred in the following sequence: (i) formation of bainitic ferrite nuclei within carbon-depleted regions immediately after the beginning of isothermal treatment; (ii) carbon partitioning immediately after the formation of bainitic ferrite nuclei but substantial carbon diffusion only after 33 min of bainite isothermal holding; (iii) formation of the carbon-enriched remaining austenite in the vicinity of bainitic laths at the beginning of the transformation; (iv) segregation of carbon to the dislocations near the austenite/ferrite interface; and (v) homogeneous redistribution of carbon within the remaining austenite with the progress of the transformation and with the formation of bainitic ferrite colonies. Bainitic ferrite nucleated at internal defects or bainite/austenite interfaces as well as at the prior austenite grain boundary. Bainitic ferrite has been observed in the form of an individual layer, a colony of layers and a layer with sideplates at the early stages of transformation. © 2016 International Union of Crystallography.
AUTHOR KEYWORDS: atom probe tomography; bainite transformation; bainitic ferrite; carbon content; neutron diffraction; retained austenite; transmission electron microscopy
DOCUMENT TYPE: Article
SOURCE: Scopus

Povstugar, I., Zenk, C.H., Li, R., Choi, P.-P., Neumeier, S., Dolotko, O., Hoelzel, M., Göken, M., Raabe, D.
Elemental partitioning, lattice misfit and creep behaviour of Cr containing gammaprime strengthened Co base superalloys
(2016) Materials Science and Technology (United Kingdom), 32 (3), pp. 220-225. Cited 7 times.
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DOI: 10.1179/1743284715Y.0000000112
AFFILIATIONS: Department of Microstructure Physics and Alloy Design, Max-Planck- Institut Fü R Eisenforschung GmbH, Max-Planck-Str. 1, Dusseldorf, Germany;
Institute I, Materials Science and Engineering, Friedrich-Alexander-Universitat Erlangen-Nurnberg (FAU), Erlangen, Germany;
Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universitat Munchen, Lichtenbergstr. 1, Garching, Germany
ABSTRACT: Novel Cr containing Co-Al-W base superalloys were studied by atom probe tomography and neutron diffraction. Cr is found to predominantly partition to the gamma matrix and decrease partitioning of W to gammaprime. Furthermore, Cr significantly enhances the gammaprime volume fraction, decreases the gamma/gammaprime lattice misfit and deteriorates the creep resistance. Addition of Ni to the Cr containing alloys affects partitioning of W and Al, further decreases the lattice misfit and results in the

formation of irregularly shaped precipitates. Al, W and Cr tend to occupy the ‘B'sublattice in the gammaprime-A3B phase (L12 type), while Co and Ni reside in the ‘A' sublattice. © 2016 Institute of Materials.
AUTHOR KEYWORDS: Atom probe tomography; Cobalt base superalloys; Creep; Lattice misfit; Neutron diffraction; Partitioning
DOCUMENT TYPE: Article
SOURCE: Scopus

Zenk, C.H., Neumeier, S., Kolb, M., Volz, N., Fries, S.G., Dolotko, O., Povstugar, I., Raabe, D., Göken, M.
The role of the base element in γ strengthened cobalt/nickel-base superalloys
(2016) Proceedings of the International Symposium on Superalloys, 2016-January, pp. 971-980.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85008204234&partnerID=40&md5=534bcd1fce9acf551a2f78d621def74b

AFFILIATIONS: Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Materials Science and Engineering, Institute I, Martensstr. 5, Erlangen, Germany;
ICAMS, Ruhr-Universität Bochum (RUB), Universitätsstr. 150, Bochum, Germany;
Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, Garching, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Department of Microstructure Physics and Alloy Design, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: Two series of polycrystalline model superalloys - one without and one containing Cr - with varying Ni/Co ratios and otherwise constant element contents were produced and are characterized by a variety of methods. All alloys form a γ/γ′ microstructure after a standard aging treatment at 900 ° C for 100 h. Upon long term aging for 1100 h, the Cr containing Co-base alloy forms undesired intermetallic phases. Liquidus and solidus temperatures are hardly influenced by the Ni/Co content, but the γ′ solvus temperature is strongly decreasing with increasing Co content. Addition of Cr to the alloy series lowers liquidus and solidus, but does not influence the solvus temperature substantially. Neutron diffraction experiments conducted on the Cr containing alloys show that the misfit is negative for alloys rich in Ni, but linearly increases to positive values with increasing Co content. 3D atom probe tomography shows that W preferentially partitions to the γ phase for the Ni-base alloys, whereas it is enriched in γ′ for the Co-base alloys. The partitioning of Co (γ), Cr (γ) and Al (γ′) to their respective phases is much more pronounced in Ni rich alloys, i.e. all elements distribute more equally in the Co-base alloys. Nanoindentation on the Cr free alloy variants reveals that the hardness of the Co-base alloy is higher than the one for the Ni-base alloy. However when Cr is present in the alloy, the hardness of the Ni-base alloy is superior. The same behavior is observed in compressive creep experiments at 900 ° C. The addition of Cr strongly improves the creep resistance of the Ni-base alloy, whereas it slightly worsens the performance of the Co-base alloy.
AUTHOR KEYWORDS: Atom probe tomography; Co-base superalloys; Creep; Lattice misfit; Partitioning behavior
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Djaziri, S., Li, Y., Nematollahi, G.A., Grabowski, B., Goto, S., Kirchlechner, C., Kostka, A., Doyle, S., Neugebauer, J., Raabe, D., Dehm, G.
Deformation-Induced Martensite: A New Paradigm for Exceptional Steels
(2016) Advanced Materials, 28 (35), pp. 7753-7757. Cited 8 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84978049900&doi=10.1002%2fadma.201601526&partnerID=40&md5=995665071f800e81a69e32a0c4467690

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AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany;
Department of Materials Science and Engineering, Faculty of Engineering and Resource Science, Akita University, Tegata Gakuencho, Akita, Japan;
Synchrotronstrahlungsquelle ANKA, Karlsruher Institut für Technologie (KIT), Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen, Germany;
Lehrstuhl Werkstoffdesign Institut für Werkstoffe Fakultät für Maschinenbau Ruhr-Universität Bochum, Universitätsstr. 150, Bochum, Germany
ABSTRACT: Atom-probe tomography (APT) and synchrotron X-ray diffraction (XRD) were combined to study the carbon supersaturation of ferrite for two pearlitic steel-wire compositions, eutectoid and hypereutectoid. The samples were cold-drawn at different strains up to true drawing strains for the eutectoid steel and the hypereutectoid steel, respectively. The wire diameters range from 1.7 mm down to 0.058 mm for the eutectoid steel and from 0.54 mm down to 0.02 mm for the hypereutectoid steel. The findings reveal that cold-drawing of pearlitic steel wires leads to a carbon-supersaturated ferrite causing a spontaneous tetragonal distortion of the ferrite unit cell through a strain-induced deformation driven martensitic transformation. We fi nd that the drawing process induced a significant increase in the carbon content inside the originally nearcarbon-free ferrite until a steady state is approached at drawing strains larger than ca. 4 for the wires. The change of carbon concentration in the ferrite grains during the drawing process is closely related to the tetragonal distortion of the ferrite unit cell.
AUTHOR KEYWORDS: ab initio modelling; atom-probe tomography; cold-drawn pearlitic steel wires; deformation-induced martensite; X-ray diffraction
DOCUMENT TYPE: Article
SOURCE: Scopus

Koprek, A., Cojocaru-Miredin, O., Wuerz, R., Freysoldt, C., Raabe, D.
Cd and impurity redistribution at the p-n junction of CIGS based solar cells resolved by atom-probe tomography
(2015) 2015 IEEE 42nd Photovoltaic Specialist Conference, PVSC 2015, art. no. 7355651, . Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84961659701&doi=10.1109%2fPVSC.2015.7355651&partnerID=40&md5=14a53fa9667f97bea1140851fb3acd03

DOI: 10.1109/PVSC.2015.7355651
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1/ North Rhine-Westphalia, Düsseldorf, Germany;
Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, Industriestrasse 6, Stuttgart, Germany
ABSTRACT: Cd and impurity redistribution in the vicinity of CdS/CIGS interface is studied by means of atom probe tomography (APT). We find an increase of the Cd content in the CIGS layer and redistribution of O at the CdS/CIGS interface after annealing the samples at 200 °C, 250 °C, or 300 °C. Very small amounts (~0.1 at. %) of Na impurity where observed at the p-n junction independent on the heat treatment. Simultaneously, the I-V measurements of the treated samples show a drop in the open circuit voltage and thus of the efficiency compared to the untreated sample. The effect of Cd diffusion in CIGS and of O and Na segregation at the CdS/CIGS interface on the cell performance is discussed. © 2015 IEEE.
AUTHOR KEYWORDS: atom probe tomography; Cu(In,Ga)Se2; impurity segregation; internal interfaces; p-n junction; thin-film solar cells
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Raabe, D., Herbig, M., Kuzmina, M., Sandlöbes, S., Tarzimoghadam, Z., Ponge, D.

Atom probe tomography reveals options for microstructural design of steels and titanium alloys by segregation engineering
(2015) MATEC Web of Conferences, 33, art. no. 01001, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84976488512&doi=10.1051%2fmatecconf%2f20153301001&partnerID=40&md5=2d0dea5398ea63aaef8c3e1385e4f9c7

DOI: 10.1051/matecconf/20153301001
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: Here we discuss approaches for designing microstructures in steels and titanium alloys by manipulating the segregation content and the structural state of lattice defects. Different mechanisms can be utilized in that context, such as for instance site specific segregation as described by the Gibbs isotherm and the generalized defectant concept, confined phase transformation phenomena and the formation of complexions, i.e. confined chemical and structural states at lattice defects. © Owned by the authors, published by EDP Sciences, 2015.
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Pradeep, K.G., Herzer, G., Raabe, D.
Atomic scale study of CU clustering and pseudo-homogeneous Fe-Si nanocrystallization in soft magnetic FeSiNbB(CU) alloys
(2015) Ultramicroscopy, 159, pp. 285-291. Cited 3 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84949624860&doi=10.1016%2fj.ultramic.2015.04.006&partnerID=40&md5=f1879caa386d8ad3b0dfac76d6b33463

DOI: 10.1016/j.ultramic.2015.04.006
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, Düsseldorf, Germany;
Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, Aachen, Germany;
Vacuumschmelze GmbH and Co. KG, Grüner Weg 37, Hanau, Germany
ABSTRACT: A local electrode atom probe has been employed to trace the onset of Cu clustering followed by their coarsening and subsequent growth upon rapid (10s) annealing of an amorphous Fe73.5Si15.5Cu1Nb3B7 alloy. It has been found that the clustering of Cu atoms introduces heterogeneities in the amorphous matrix, leading to the formation of Fe rich regions which crystallizes pseudo-homogeneously into Fe-Si nanocrystals upon annealing. In this paper, we present the data treatment method that allows for the visualization of these different phases and to understand their morphology while still quantifying them in terms of their size, number density and volume fraction. The crystallite size of Fe-Si nanocrystals as estimated from the atom probe data are found to be in good agreement with other complementary techniques like XRD and TEM, emphasizing the importance of this approach towards accurate structural analysis. In addition, a composition driven data segmentation approach has been attempted to determine and distinguish nanocrystalline regions from the remaining amorphous matrix. Such an analysis introduces the possibility of retrieving crystallographic information from extremely fine (2-4nm sized) nanocrystalline regions of very low volume fraction (< 5Vol%) thereby providing crucial in-sights into the chemical heterogeneity induced crystallization process of amorphous materials. © 2015 Elsevier B.V.
AUTHOR KEYWORDS: Atom probe tomography; Clustering; Crystallization; Nanocrystalline microstructure; Soft magnets
DOCUMENT TYPE: Article
SOURCE: Scopus

Haley, D., Choi, P., Raabe, D.
Guided mass spectrum labelling in atom probe tomography
(2015) Ultramicroscopy, 159, pp. 338-345. Cited 3 times.

https://www.scopus.com/inward/record.uri?eid=2-s2.0-84949627750&doi=10.1016%2fj.ultramic.2015.03.005&partnerID=40&md5=e38d22b494d83fc14670dfe5631e7976

DOI: 10.1016/j.ultramic.2015.03.005
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Plack Straße 1, Düsseldorf, Germany;
Department of Materials, University of Oxford, Parks Road, Oxford, United Kingdom
ABSTRACT: Atom probe tomography (APT) is a valuable near-atomic scale imaging technique, which yields mass spectrographic data. Experimental correctness can often pivot on the identification of peaks within a dataset, this is a manual process where subjectivity and errors can arise. The limitations of manual procedures complicate APT experiments for the operator and furthermore are a barrier to technique standardisation. In this work we explore the capabilities of computer-guided ranging to aid identification and analysis of mass spectra. We propose a fully robust algorithm for enumeration of the possible identities of detected peak positions, which assists labelling. Furthermore, a simple ranking scheme is developed to allow for evaluation of the likelihood of each possible identity being the likely assignment from the enumerated set. We demonstrate a simple, yet complete work-chain that allows for the conversion of mass-spectra to fully identified APT spectra, with the goal of minimising identification errors, and the inter-operator variance within APT experiments. This work chain is compared to current procedures via experimental trials with different APT operators, to determine the relative effectiveness and precision of the two approaches. It is found that there is little loss of precision (and occasionally gain) when participants are given computer assistance. We find that in either case, inter-operator precision for ranging varies between 0 and 2 "significant figures" (2 σ confidence in the first n digits of the reported value) when reporting compositions. Intra-operator precision is weakly tested and found to vary between 1 and 3 significant figures, depending upon species composition levels. Finally it is suggested that inconsistencies in inter-operator peak labelling may be the largest source of scatter when reporting composition data in APT.
AUTHOR KEYWORDS: Atom Probe; Data analysis; Standardisation
DOCUMENT TYPE: Article
SOURCE: Scopus

Li, Y.J., Ponge, D., Choi, P., Raabe, D.
Atomic scale investigation of non-equilibrium segregation of boron in a quenched Mo-free martensitic steel
(2015) Ultramicroscopy, 159, pp. 240-247. Cited 4 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84949533820&doi=10.1016%2fj.ultramic.2015.03.009&partnerID=40&md5=53cadf6498c489f6fd4f4b461760d078

DOI: 10.1016/j.ultramic.2015.03.009
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: B-added low carbon steels exhibit excellent hardenability. The reason has been frequently attributed to B segregation at prior austenite grain boundaries, which prevents the austenite to ferrite transformation and favors the formation of martensite. The segregation behavior of B at prior austenite grain boundaries is strongly influenced by processing conditions such as austenitization temperatures and cooling rates and by alloying elements such as Mo, Cr, and Nb. Here an local electrode atom probe was employed to investigate the segregation behavior of B and other alloying elements (C, Mn, Si, and Cr) in a Cr-added Mo-free martensitic steel. Similar to our previous results on a Mo-added steel, we found that in both steels B is segregated at prior austenite grain boundaries with similar excess values, whereas B is neither detected in the martensitic

matrix nor at martensite-martensite boundaries at the given cooling rate of 30 K/s. These results are in agreement with the literature reporting that Cr has the same effect on hardenability of steels as Mo in the case of high cooling rates. The absence of B at martensite-martensite boundaries suggests that B segregates to prior austenite grain boundaries via a non-equilibrium mechanism. Segregation of C at all boundaries such as prior austenite grain boundaries and martensite-martensite boundaries may occur by an equilibrium mechanism. © 2015 Elsevier B.V.
AUTHOR KEYWORDS: Atom probe tomography; Boron segregation; Martensitic steels; Non-equilibrium segregation; Prior austenite grain boundaries; Site-specific sample preparation
DOCUMENT TYPE: Article
SOURCE: Scopus

Stoffers, A., Cojocaru-Mirédin, O., Seifert, W., Zaefferer, S., Riepe, S., Raabe, D.
Grain boundary segregation in multicrystalline silicon: Correlative characterization by EBSD, EBIC, and atom probe tomography
(2015) Progress in Photovoltaics: Research and Applications, 23 (12), pp. 1742-1753. Cited 9 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84957963875&doi=10.1002%2fpip.2614&partnerID=40&md5=39fa3b2efed15366cf5def11645bf59e

DOI: 10.1002/pip.2614
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany;
Brandenburgische Technische Universität Cottbus, Joint Lab IHP, BTU, Platz der Deutschen Einheit 1, Cottbus, Germany;
IHP, Im Technologiepark 25, Frankfurt (Oder), Germany;
Fraunhofer-Institut für Solare Energiesysteme, Heidenhofstraße 2, Freiburg, Germany
ABSTRACT: This study aims to better understand the influence of crystallographic structure and impurity decoration on the recombination activity at grain boundaries in multicrystalline silicon. A sample of the upper part of a multicrystalline silicon ingot with intentional addition of iron and copper has been investigated. Correlative electron-beam-induced current, electron backscatter diffraction, and atom probe tomography data for different types of grain boundaries are presented. For a symmetric coherent Σ3 twin boundary, with very low recombination activity, no impurities are detected. In case of a non-coherent (random) high-angle grain boundary and higher order twins with pronounced recombination activity, carbon and oxygen impurities are observed to decorate the interface. Copper contamination is detected for the boundary with the highest recombination activity in this study, a random high-angle grain boundary located in the vicinity of a triple junction. The 3D atom probe tomography study presented here is the first direct atomic scale identification and quantification of impurities decorating grain boundaries in multicrystalline silicon. The observed deviations in chemical decoration and induced current could be directly linked with different crystallographic structures of silicon grain boundaries. Hence, the current work establishes a direct correlation between grain boundary structure, atomic scale segregation information, and electrical activity. It can help to identify interface-property relationships for silicon interfaces that enable grain boundary engineering in multicrystalline silicon. Copyright © 2015 John Wiley & Sons, Ltd.
AUTHOR KEYWORDS: atom probe tomography; electron backscatter diffraction; electron beam induced current; grain boundaries; multicrystalline silicon solar cells
DOCUMENT TYPE: Article
SOURCE: Scopus

Pei, Z., Ma, D., Friák, M., Svendsen, B., Raabe, D., Neugebauer, J.

Errautm: From generalized stacking fault energies to dislocation properties: Five-energy-point approach and solid solution effects in magnesium (Physical Review B - Condensed Matter and Materials Physics (2015) 92 (064107))
(2015) Physical Review B - Condensed Matter and Materials Physics, 92 (17), art. no. 179901, . Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84948416381&doi=10.1103%2fPhysRevB.92.179901&partnerID=40&md5=9c78c4f59d2819ba57fd544b21ca9ba8

DOI: 10.1103/PhysRevB.92.179901
DOCUMENT TYPE: Erratum
SOURCE: Scopus

Pradeep, K.G., Tasan, C.C., Yao, M.J., Deng, Y., Springer, H., Raabe, D.
Non-equiatomic high entropy alloys: Approach towards rapid alloy screening and property-oriented design
(2015) Materials Science and Engineering A, 648, pp. 183-192. Cited 26 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84942248791&doi=10.1016%2fj.msea.2015.09.010&partnerID=40&md5=45ba4a2c9214e96b96e99223cf6441be

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AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-str.1, Düsseldorf, Germany;
Materials Chemistry, RWTH Aachen University, Kopernikusstr.10, Aachen, Germany;
Department of Engineering Design and Materials, Norwegian University of Science and Technology, Trondheim, Norway
ABSTRACT: The high entropy alloy (HEA) concept has triggered a renewed interest in alloy design, even though some aspects of the underlying thermodynamic concepts are still under debate. This study addresses the short-comings of this alloy design strategy with the aim to open up new directions of HEA research targeting specifically non-equiatomic yet massively alloyed compositions. We propose that a wide range of massive single phase solid solutions could be designed by including non-equiatomic variants. It is demonstrated by introducing a set of novel non-equiatomic multi-component CoCrFeMnNi alloys produced by metallurgical rapid alloy prototyping. Despite the reduced configurational entropy, detailed characterization of these materials reveals a strong resemblance to the well-studied equiatomic single phase HEA: The microstructure of these novel alloys exhibits a random distribution of alloying elements (confirmed by Energy-Dispersive Spectroscopy and Atom Probe Tomography) in a single face-centered-cubic phase (confirmed by X-ray Diffraction and Electron Backscatter Diffraction), which deforms through planar slip (confirmed by Electron-Channeling Contrast Imaging) and leads to excellent ductility (confirmed by uniaxial tensile tests). This approach widens the field of HEAs to non-equiatomic multi-component alloys since the concept enables to tailor the stacking fault energy and associated transformation phenomena which act as main mechanisms to design useful strain hardening behavior. © 2015 Elsevier B.V.
AUTHOR KEYWORDS: Alloy design; CoCrFeMnNi; Non-equiatomic; Single phase; Solid solution
DOCUMENT TYPE: Article
SOURCE: Scopus

Lai, M.J., Tasan, C.C., Raabe, D.
Deformation mechanism of ω-enriched Ti-Nb-based gum metal: Dislocation channeling and deformation induced ω-β transformation
(2015) Acta Materialia, 100, art. no. 12375, pp. 290-300. Cited 17 times.

https://www.scopus.com/inward/record.uri?eid=2-s2.0-84940982023&doi=10.1016%2fj.actamat.2015.08.047&partnerID=40&md5=20e5ac5214fb3d6abf3e7febc2f89dc6

DOI: 10.1016/j.actamat.2015.08.047
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: Gum metal, a class of multifunctional β titanium alloys, has attracted much attention in the past decade due to its initially-proposed dislocation-free deformation mechanism based on giant faults, i.e., macroscopic planar defects carrying significant plastic strain. Special deformation features were observed in these alloys, such as plastic flow localization, pronounced surface steps, low work hardening, and large elongation. These were all proposed to arise from the special giant fault mechanism activated in the β-Ti matrix, while the initial presence or mechanically-induced formation of other phases was debated in several follow-up studies. Here, we set off with Ti-Nb-based gum metal samples with confirmed presence of large amounts of nanometer-sized hexagonal ω particles. Deformation experiments demonstrate all the features observed in the original reports, mentioned above. However, careful characterization reveals that the deformation bands (similar to giant faults) where plastic flow localized are "dislocation channels" that are depleted of ω phase. These channels are proposed to form by a {1 1 2}<1 1 1> dislocation dissociation mechanism, promoting reverse transformation of the ω phase into the β phase. The deformation induced ω-β transformation and the associated dislocation channeling process can explain the presence of the aforementioned special deformation features in the current gum metal. © 2015 Acta Materialia Inc.
AUTHOR KEYWORDS: Dislocation channeling; Gum metal; Synchrotron X-ray diffraction; Transmission electron microscopy; ω phase
DOCUMENT TYPE: Article
SOURCE: Scopus

Pierce, D.T., Jiménez, J.A., Bentley, J., Raabe, D., Wittig, J.E.
The influence of stacking fault energy on the microstructural and strain-hardening evolution of Fe-Mn-Al-Si steels during tensile deformation
(2015) Acta Materialia, 100, pp. 178-190. Cited 40 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84941565768&doi=10.1016%2fj.actamat.2015.08.030&partnerID=40&md5=7ad8577a7510e8a7513ae4c5e6f2e51b

DOI: 10.1016/j.actamat.2015.08.030
AFFILIATIONS: Advanced Steel Processing and Products Research Center, Colorado School of Mines, 1500 Illinois St., Golden, CO, United States;
Centro Nacional de Investigaciones Metalurgicas (CSIC), Avda. Gregorio del Amo, 8, Madrid, Spain;
Microscopy and Microanalytical Sciences, P.O. Box 7103, Oak Ridge, TN, United States;
Max-Planck-Institut für Eisenforschung, Max-Planck Str. 1, Düsseldorf, Germany;
Vanderbilt University, 2301 Vanderbilt Place, Nashville, TN, United States
ABSTRACT: Understanding the relationship between the stacking-fault energy (SFE), deformation mechanisms, and strain-hardening behavior is important for alloying and design of high-Mn austenitic transformation- and twinning-induced plasticity (TRIP/TWIP) steels. The present study investigates the influence of SFE on the microstructural and strain-hardening evolution of three TRIP/TWIP alloys (Fe-22/25/28Mn-3Al-3Si wt.%). The SFE is increased by systemically increasing the Mn content from 22 to 28 wt.%. The Fe-22Mn-3Al-3Si alloy, with a SFE of 15 mJ m-2, deforms by planar dislocation glide and strain-induced ε<inf>hcp</inf>-/α<inf>bcc</inf>-martensite formation which occurs from the onset of plastic deformation, resulting in improved work-hardening at low strains but lower total elongation. With an increased SFE of 21 mJ m-2 in the Fe-25Mn-3Al-3Si alloy, both mechanical twinning and

ε<inf>hcp</inf>-martensite formation are activated during deformation, and result in the largest elongation of the three alloys. A SFE of 39 mJ m-2 enables significant dislocation cross slip and suppresses ε<inf>hcp</inf>-martensite formation, causing reduced work-hardening during the early stages of deformation in the Fe-28Mn-3Al-3Si alloy while mechanical twinning begins to enhance the strain-hardening after approximately 10% strain. The increase in SFE from 15 to 39 mJ m-2 results in significant changes in the deformation mechanisms and, at low strains, decreased work-hardening, but has a relatively small influence on strength and ductility. © 2015 Acta Materialia Inc.
AUTHOR KEYWORDS: Plasticity mechanisms; Stacking-fault energy; TRIP steel; Twinning; TWIP steel
DOCUMENT TYPE: Article
SOURCE: Scopus

Ma, D., Grabowski, B., Körmann, F., Neugebauer, J., Raabe, D.
Ab initio thermodynamics of the CoCrFeMnNi high entropy alloy: Importance of entropy contributions beyond the configurational one
(2015) Acta Materialia, 100, pp. 90-97. Cited 41 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84941360368&doi=10.1016%2fj.actamat.2015.08.050&partnerID=40&md5=4d6192bfe84205abb6a9ff7b4df77973

DOI: 10.1016/j.actamat.2015.08.050
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany;
Department of Materials Science and Engineering, Delft University of Technology, Mekelweg 2, CD Delft, Netherlands
ABSTRACT: We investigate the thermodynamic properties of the prototype equi-atomic high entropy alloy (HEA) CoCrFeMnNi by using finite-temperature ab initio methods. All relevant free energy contributions are considered for the hcp, fcc, and bcc structures, including electronic, vibrational, and magnetic excitations. We predict the paramagnetic fcc phase to be most stable above room temperature in agreement with experiment. The corresponding thermal expansion and bulk modulus agree likewise well with experimental measurements. A careful analysis of the underlying entropy contributions allows us to identify that the originally postulated dominance of the configurational entropy is questionable. We show that vibrational, electronic, and magnetic entropy contributions must be considered on an equal footing to reliably predict phase stabilities in HEA systems. © 2015 Acta Materialia Inc.
AUTHOR KEYWORDS: Ab initio; High entropy alloys; Magnetism; Phase stability; Thermodynamics
DOCUMENT TYPE: Article
SOURCE: Scopus

Wen, Y., Xiao, H., Peng, H., Li, N., Raabe, D.
Relationship Between Damping Capacity and Variations of Vacancies Concentration and Segregation of Carbon Atom in an Fe-Mn Alloy
(2015) Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 46 (11), pp. 4828-4833. Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84942983104&doi=10.1007%2fs11661-015-3111-1&partnerID=40&md5=102a5bd8fa8379dab2d2bd3738567842

DOI: 10.1007/s11661-015-3111-1
AFFILIATIONS: College of Manufacturing Science and Engineering, Sichuan University, Chengdu, China;
Max-Planck Institut für Eisenforschung, Düsseldorf, Germany;
National Key Laboratory for Reactor Fuel and Materials, Nuclear Power Institute of China, Chengdu, China
ABSTRACT: We investigated effects of quenching temperature and ageing on variations of vacancies concentration and segregation of solute atoms and

their relationship with damping capacity in an Fe-Mn alloy. The damping capacity can be remarkably improved by lowering vacancies concentration but deteriorated by segregation of carbon atoms. A higher damping capacity can be obtained by furnace cooling or quenching and then ageing in Fe-Mn alloy with lower carbon content or addition of Ti or Nb. © 2015, The Minerals, Metals & Materials Society and ASM International.
DOCUMENT TYPE: Article
SOURCE: Scopus

Zhang, J.-L., Tasan, C.C., Lai, M.L., Zhang, J., Raabe, D.
Damage resistance in gum metal through cold work-induced microstructural heterogeneity
(2015) Journal of Materials Science, 50 (17), pp. 5694-5708. Cited 3 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84930759715&doi=10.1007%2fs10853-015-9105-y&partnerID=40&md5=f37411a100499ac2063819023291cf6c

DOI: 10.1007/s10853-015-9105-y
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: Cold-worked alloys exhibit high strength, but suffer from limited ductility. In contrast, Ti-based gum metal was reported to exhibit high strength combined with good ductility upon severe pre-straining. Motivated by this anomaly, we systematically studied the evolution of gum metal microstructure during severe cold working (swaging and rolling) and the resulting deformation and damage micro-mechanical mechanisms during follow-up tensile deformation. To this end, various experimental in situ and post-mortem methodologies are employed, including scanning electron microscopy imaging, high-resolution electron backscatter diffraction mapping and transmission electron microscopy. These observations reveal that intense grain refinement takes place through dislocation plasticity-dominated deformation banding upon cold working. The observed enhancement in crack blunting and failure resistance which prolongs the post-necking ductility of gum metal during follow-up tensile straining can be attributed to the deformation-induced development of local heterogeneities in texture and grain size. © 2015, Springer Science+Business Media New York.
DOCUMENT TYPE: Article
SOURCE: Scopus

Pei, Z., Friák, M., Sandlöbes, S., Nazarov, R., Svendsen, B., Raabe, D., Neugebauer, J.
Rapid theory-guided prototyping of ductile Mg alloys: From binary to multi-component materials
(2015) New Journal of Physics, 17 (9), art. no. 093009, . Cited 7 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84943559624&doi=10.1088%2f1367-2630%2f17%2f9%2f093009&partnerID=40&md5=c4f5d643d3a6755174ab74cdfcfb8ede

DOI: 10.1088/1367-2630/17/9/093009
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH-Aachen University, Aachen, Germany;
Institute of Physics of Materials, Academy of Sciences of the Czech Republic, V.V.I., Žižkova 22, Brno, Czech Republic;
Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Aachen, Germany;
Material Mechanics, Faculty of Georesources and Materials Engineering, RWTH Aachen University, Aachen, Germany
ABSTRACT: In order to identify a method allowing for a fast solute assessment without lengthy ab initio calculations, we analyze correlations and anti-correlation between the stacking fault energies (SFEs), which were shown to be related to the macroscopic ductility in Mg alloys, and five

material parameters of 18 different elemental solutes. Our analysis reveals that the atomic volume V of pure solutes, their electronegativity ν and bulk modulus B are either linearly or logarithmically related to the SFE. Comparing the impact of solutes with that of yttrium (that increases the ductility in Mg) we propose a single numerical quantity (called yttrium similarity index, YSI) that is based on these inter-relations. Subsequently, we evaluate this new figure of merit for 76 elements from the periodic table of elements in search for solutes reducing the SFE. Limiting ourselves first to binary Mg alloys, we hardly find any alternative solutes providing similar reduction as that due to rare-earth (RE) additions. Therefore, we extended our search to ternary Mg alloys. Assuming that the physical properties of solute combinations can be represented by their average values, 2850 solute combinations were checked and 133 solute pairs (not including any RE elements) have been found to have a YSI larger than 0.85. Quantum-mechanical calculations have been subsequently performed for 11 solute pairs with YSIs higher than 0.95 and they were all found to reduce the in excellent agreement with the predictions based on the YSI.
AUTHOR KEYWORDS: ab initio; alloys; ductile; magnesium; rare-earth; ternary
DOCUMENT TYPE: Article
SOURCE: Scopus

Wang, M., Tasan, C.C., Koyama, M., Ponge, D., Raabe, D.
Enhancing Hydrogen Embrittlement Resistance of Lath Martensite by Introducing Nano-Films of Interlath Austenite
(2015) Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 46 (9), pp. 3797-3802. Cited 17 times.
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DOI: 10.1007/s11661-015-3009-y
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
Department of Mechanical Engineering, Kyushu University, 744 Motooka, Nishi-ku, Fukuoka, Japan
ABSTRACT: Partial reversion of interlath austenite nano-films is investigated as a potential remedy for hydrogen embrittlement susceptibility of martensitic steels. We conducted uniaxial tensile tests on hydrogen-free and pre-charged medium-Mn transformation-induced plasticity-maraging steels with different austenite film thicknesses. Mechanisms of crack propagation and microstructure interaction are quantitatively analyzed using electron channelling contrast imaging and electron backscatter diffraction, revealing a promising strategy to utilize austenite reversion for hydrogen-resistant martensitic steel design.
DOCUMENT TYPE: Article
SOURCE: Scopus

Kuzmina, M., Herbig, M., Ponge, D., Sandlöbes, S., Raabe, D.
Linear complexions: Confined chemical and structural states at dislocations
(2015) Science, 349 (6252), pp. 1080-1083. Cited 47 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84941308663&doi=10.1126%2fscience.aab2633&partnerID=40&md5=c31c170ee5a0805ab29dc82975feca63

DOI: 10.1126/science.aab2633
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: For 5000 years, metals have been mankind's most essential materials owing to their ductility and strength. Linear defects called dislocations carry atomic shear steps, enabling their formability. We

report chemical and structural states confined at dislocations. In a body-centered cubic Fe-9 atomic percent Mn alloy, we found Mn segregation at dislocation cores during heating, followed by formation of face-centered cubic regions but no further growth. The regions are in equilibrium with the matrix and remain confined to the dislocation cores with coherent interfaces. The phenomenon resembles interface-stabilized structural states called complexions. A cubic meter of strained alloy contains up to a light year of dislocation length, suggesting that linear complexions could provide opportunities to nanostructure alloys via segregation and confined structural states.
DOCUMENT TYPE: Article
SOURCE: Scopus

Renner, F.U., Ankah, G.N., Bashir, A., Ma, D., Biedermann, P.U., Shrestha, B.R., Nellessen, M., Khorashadizadeh, A., Losada-Pérez, P., Duarte, M.J., Raabe, D., Valtiner, M.
Self-Assembled Monolayers: Star-Shaped Crystallographic Cracking of Localized Nanoporous Defects (Adv. Mater. 33/2015)
(2015) Advanced materials (Deerfield Beach, Fla.), 27 (33), p. 4947.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84973446508&doi=10.1002%2fadma.201570223&partnerID=40&md5=075cd0f23cbed5d03bc0c706fecaf845

DOI: 10.1002/adma.201570223
AFFILIATIONS: Institute for Materials Research (IMO), Hasselt University and Associated Lab IMEC Division IMOMEC, Wetenschapspark 1, 3590, Diepenbeek, Belgium;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237, Düsseldorf, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237, Düsseldorf, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237, Düsseldorf, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237, Düsseldorf, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237, Düsseldorf, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237, Düsseldorf, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237, Düsseldorf, Germany;
Institute for Materials Research (IMO), Hasselt University and Associated Lab IMEC Division IMOMEC, Wetenschapspark 1, 3590, Diepenbeek, Belgium;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237, Düsseldorf, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237, Düsseldorf, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237, Düsseldorf, Germany
ABSTRACT: On page 4877, F. U. Renner, A. Bashir, M. Valtiner, and co-workers describe a star-like dealloying corrosion morphology that appears during the localized attack of smooth well-prepared Cu-Au surfaces. The surfaces are initially protected by thiol or selenol inhibitior films. Localized dealloying of Cu-Au produces nanoporous gold under stress and crystallographic cracks - thereby opening a new approach combining surface science with nanoscale mechanical testing.
AUTHOR KEYWORDS: cracking; dealloying; inhibition; localized corrosion; self-assembled monolayers
DOCUMENT TYPE: Article
SOURCE: Scopus

Renner, F.U., Ankah, G.N., Bashir, A., Ma, D., Biedermann, P.U., Shrestha, B.R., Nellessen, M., Khorashadizadeh, A., Losada-Pérez, P., Duarte, M.J., Raabe, D., Valtiner, M.
Star-Shaped Crystallographic Cracking of Localized Nanoporous Defects
(2015) Advanced Materials, 27 (33), pp. 4877-4882. Cited 4 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84940725601&doi=10.1002%2fadma.201405565&partnerID=40&md5=2f8d1ac3665a08d33dcc177bd8435890

DOI: 10.1002/adma.201405565
AFFILIATIONS: Institute for Materials Research (IMO), HUAL IMEC Division IMOMEC, Wetenschapspark 1, Diepenbeek, Belgium;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: On self-assembled monolayer-covered Cu-Au substrates, localized volume shrinkage at initial dealloying sites leads to cracks within the attacked regions. It is started from well-controlled surface structures to gain fundamental insights in the driving mechanisms of localized corrosion and crack formation. Both the crack density and the crack morphology are critically dependent on surface orientation, crystallography, and inhibitor molecule species. © 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
AUTHOR KEYWORDS: cracking; dealloying; inhibition; localized corrosion; self-assembled monolayers
DOCUMENT TYPE: Article
SOURCE: Scopus

Choi, W.S., De Cooman, B.C., Sandlöbes, S., Raabe, D.
Size and orientation effects in partial dislocation-mediated deformation of twinning-induced plasticity steel micro-pillars
(2015) Acta Materialia, 98, art. no. 12304, pp. 391-404. Cited 20 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84938803755&doi=10.1016%2fj.actamat.2015.06.065&partnerID=40&md5=b485fb8e1c6071b53bcf810c6a4e63da

DOI: 10.1016/j.actamat.2015.06.065
AFFILIATIONS: Graduate Institute of Ferrous Technology, Pohang University of Science and Technology, Pohang, South Korea;
Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: Abstract Bulk and micro-pillar single crystals were used to investigate the twinning-induced plasticity mechanism in austenitic Fe-22 wt%Mn-0.6 wt%C TWIP steel. Compression of micro-pillars oriented either for deformation-induced twinning or for perfect dislocation glide was carried out for pillars with diameters in the range of 600 nm to 4 μm. The same size dependence of the critical resolved shear stress was observed for both orientations. The critical micro-pillar diameter for size-independent plasticity was approximately 7.6 μm. Partial dislocation-mediated formation of twins and ε-martensite was observed in micro-pillars oriented for twinning by transmission electron microscopy. The elastic-plastic transition in micro-pillars oriented for deformation twinning did not involve twinning, and dislocation-dislocation interactions were a necessary precondition for twin formation. © 2015 Acta Materialia Inc.
AUTHOR KEYWORDS: Micro-compression; Micro-pillar; Twin nucleation; Twinning; TWIP steel
DOCUMENT TYPE: Article
SOURCE: Scopus

Ma, D., Friák, M., Von Pezold, J., Neugebauer, J., Raabe, D.
Ab initio study of compositional trends in solid solution strengthening in metals with low Peierls stresses
(2015) Acta Materialia, 98, art. no. 12303, pp. 367-376. Cited 3 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84938830781&doi=10.1016%2fj.actamat.2015.07.054&partnerID=40&md5=aef2eaa4725810fbf244f03d7d245377

DOI: 10.1016/j.actamat.2015.07.054
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany;
Institute of Physics of Materials, Academy of Sciences of the Czech Republic, v.v.i, Žižkova 22, Brno, Czech Republic
ABSTRACT: Abstract We identify and analyze general trends governing solid solution strengthening in binary alloys containing solutes across the Periodic table using quantum-mechanical calculations. Here we present calculations for the model system of Al binary solid solutions. The identified trends originate from an approximately parabolic dependence of two strengthening parameters to quantitatively predict the solid solution strengthening effect, i.e. the volume and slip misfit parameters. The volume misfit parameter shows a minimum (concave-up behavior) as a function of the solute element group number in the periodic table, whereas the slip misfit parameter shows a maximum (concave-down behavior). By analyzing reported data, a similar trend is also found in Ni and Mg (basal slip) binary systems. Hence, these two strengthening parameters are strongly anti-correlated, which can be understood in terms of the Fermi level shift in the framework of free electron model. The chemical trends identified in this study enable a rapid and efficient identification of the solutes that provide optimum solid-solution strengthening. The approach described here may thus serve as basis for ab initio guided metallurgical materials design. © 2015 Acta Materialia Inc.
AUTHOR KEYWORDS: Ab-initio; Al alloys; DFT; Mg alloys; Mg basal slip; Ni alloys; Solid solution strengthening
DOCUMENT TYPE: Article
SOURCE: Scopus

Pei, Z., Ma, D., Friák, M., Svendsen, B., Raabe, D., Neugebauer, J.
From generalized stacking fault energies to dislocation properties: Five-energy-point approach and solid solution effects in magnesium
(2015) Physical Review B - Condensed Matter and Materials Physics, 92 (6), art. no. 064107, . Cited 5 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84939832336&doi=10.1103%2fPhysRevB.92.064107&partnerID=40&md5=c54d7e691a11d590aae5ed36d496604f

DOI: 10.1103/PhysRevB.92.064107
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Institute of Physics of Materials, Academy of Sciences of the Czech Republic, V.v.i., Žižkova 22, Brno, Czech Republic;
Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH-Aachen University, Aachen, Germany
ABSTRACT: Using ab initio calculations and symmetrized plane waves, we analyze the basal-plane generalized stacking fault energies in pure Mg and Mg-Y alloys and show that the knowledge of energies of only five specific points is sufficient to accurately predict the core structures and Peierls stresses of (a)-type edge dislocations in these alloys. Our five-point approach substantially reduces the computational cost related to the Peierls-Nabarro (PN) model and allows for a high-throughput application of the PN model to study Peierls stress changes in Mg upon alloying. We employ our approach to study Mg binary alloys containing nine rare-earth (RE) and 11 other solutes. Based on the Peierls stresses of these 20 Mg alloys calculated from the Peierls-Nabarro model, the solutes are divided into three groups: (i) the first group, consisting of Be, Zn, Tl, Tc, Os, Ru, Re, and Co, when added as solutes into Mg, lead to more compact dislocation core structures and larger Peierls stresses than found for pure Mg. (ii) Elements in the second group, including Ti, Nd, Lu, Zr, Hf, La, and Pr change the core widths and Peierls stresses moderately. (iii) The solutes in the third group containing Y, Er, Tm, Ho, and Sc extend the stacking fault width, and the resulting Peierls stresses are generally very low.

Based on an error analysis, we conclude that the first group has a clear solute strengthening effect and the third group has a clear solute softening effect, while the effects of the elements in the second group are too small to be resolved by the present approach. © 2015 American Physical Society. ©2015 American Physical Society.
DOCUMENT TYPE: Article
SOURCE: Scopus

Schwan, M., Naikade, M., Raabe, D., Ratke, L.
From hard to rubber-like: mechanical properties of resorcinol–formaldehyde aerogels
(2015) Journal of Materials Science, 50 (16), pp. 5482-5493. Cited 5 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84930271644&doi=10.1007%2fs10853-015-9094-x&partnerID=40&md5=82f9145a316e35ace0fdd020d51637a0

DOI: 10.1007/s10853-015-9094-x
AFFILIATIONS: Institute of Materials Research, German Aerospace Center, Linder Hoehe, Cologne, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: Four types of resorcinol–formaldehyde (RF) aerogels, stiff, brittle, low-flexible, and super-flexible are studied in this work. Despite several studies on mechanical properties on RF aerogels their response when exposed to compressive loading and their fracture behavior are not well investigated. Here, we cover aerogels with a very broad density range of 0.08–0.3 g cm−3 and compressive moduli from 0.12 to 28 MPa. We relate the microstructure of the synthesized aerogels and their behavior under uniaxial compression. Additionally, this work is the first, to our knowledge, to implement the usage of digital image correlation for characterizing the deformation of RF aerogels. The comparison of surface strain distribution of four types of aerogels provides an insight to their reaction on compressive loading. © 2015, Springer Science+Business Media New York.
DOCUMENT TYPE: Article
SOURCE: Scopus

Ma, D., Eisenlohr, P., Shanthraj, P., Diehl, M., Roters, F., Raabe, D.
Analytical bounds of in-plane Young's modulus and full-field simulations of two-dimensional monocrystalline stochastic honeycomb structures
(2015) Computational Materials Science, 109, art. no. 6642, pp. 323-329. Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84938518551&doi=10.1016%2fj.commatsci.2015.07.041&partnerID=40&md5=3da29344591b103d45cca0bb7fd5722b

DOI: 10.1016/j.commatsci.2015.07.041
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany;
Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI, United States;
Aachen Institute for Advanced Study in Computational Engineering Science, RWTH Aachen University, Schinkelstraße 2, Aachen, Germany
ABSTRACT: Abstract In this study, we focus on the interplay between the honeycomb structure and the crystallographic orientation. Specifically, the in-plane Young's moduli of monocrystalline stochastic honeycombs are calculated by a numerical and an analytical approach. The in-plane Young's moduli of the honeycombs were calculated numerically using a solution scheme for the full-field mechanical equilibrium based on spectral methods and anisotropic crystal elasticity. The analytical approach formulates two alternative assumptions, i.e. uniform force and uniform strain per strut, considers the elastic anisotropy of the base material, and depends on the two-variable distribution of the strut length and inclination angle as the

structural parameters characterizing the stochastic honeycombs. The uniform strain assumption agrees closely with the numerical simulation results and constitutes an improvement compared to analytical solutions proposed in previous studies. © 2015 Elsevier B.V.
AUTHOR KEYWORDS: Anisotropic elasticity; Cellular material; Crystallographic orientation; Honeycomb
DOCUMENT TYPE: Article
SOURCE: Scopus

Siboni, N.H., Raabe, D., Varnik, F.
Aging in amorphous solids: A study of the first-passage time and persistence time distributions
(2015) EPL, 111 (4), art. no. 48004, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84941584969&doi=10.1209%2f0295-5075%2f111%2f48004&partnerID=40&md5=a013e0aa1a6a391bfa9b250ff8ca9750

DOI: 10.1209/0295-5075/111/48004
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck Straße 1, Düsseldorf, Germany;
Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität, Bochum Universitätsstraße 150, Bochum, Germany
ABSTRACT: The time distribution of relaxation events in an aging system is investigated via molecular-dynamics simulations. The focus is on the distribution functions of the first-passage time, p1(δt), and the persistence time, p(τ). In contrast to previous reports, both p1 and p are found to evolve with time upon aging. The age dependence of the persistence time distribution is shown to be sensitive to the details of the algorithm used to extract it from particle trajectories. By updating the reference point in event detection algorithm and accounting for the event specific aging time, we uncover the age dependence of p(τ), hidden to previous studies. Moreover, the apparent age dependence of p1 in continuous time random walk with an age-independent p(τ) is shown to result from an implicit synchronization of all the random walkers at the starting time.
DOCUMENT TYPE: Article
SOURCE: Scopus

Ma, D., Yao, M., Pradeep, K.G., Tasan, C.C., Springer, H., Raabe, D.
Phase stability of non-equiatomic CoCrFeMnNi high entropy alloys
(2015) Acta Materialia, 98, art. no. 12279, pp. 288-296. Cited 36 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84937876590&doi=10.1016%2fj.actamat.2015.07.030&partnerID=40&md5=5a283dcde72bcee0c2b86d14bd782541

DOI: 10.1016/j.actamat.2015.07.030
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany;
Materials Chemistry, RWTH Aachen University, Kopernikusstraße 10, Aachen, Germany
ABSTRACT: Abstract The objective of this study is to experimentally and theoretically investigate the phase stability of non-equiatomic Fe<inf>x</inf>Mn<inf>62-x</inf>Ni<inf>30</inf>Co<inf>6</inf>Cr<inf>2</inf> based high entropy alloys, where x ranges from 22 to 42 at.%. Another aim is to systematically and critically assess the predictive capability of the CALPHAD approach for such high entropy alloy systems. We find that the CALPHAD simulations provide a very consistent assessment of phase stability yielding good agreement with experimental observations. These include the equilibrium phase formation at high temperatures, the constituent phases after non-equilibrium solidification processes, unfavorable segregation profiles inherited from solidification together with the associated nucleation and growth of low temperature phases, and undesired martensitic transformation effects. Encouraged by these consistent theoretical and experimental results, we extend our simulations to other alloy systems with

equiatomic compositions reported in the literature. Using these other equiatomic model systems we demonstrate how systematic CALPHAD simulations can improve and accelerate the design of multicomponent alloy systems. © 2015 Acta Materialia Inc.
AUTHOR KEYWORDS: CALPHAD; High entropy alloy; Phase stability; Thermodynamics
DOCUMENT TYPE: Article
SOURCE: Scopus

Tarzimoghadam, Z., Sandlöbes, S., Pradeep, K.G., Raabe, D.
Microstructure design and mechanical properties in a near-α Ti-4Mo alloy
(2015) Acta Materialia, 97, art. no. 12228, pp. 291-304. Cited 18 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84937540438&doi=10.1016%2fj.actamat.2015.06.043&partnerID=40&md5=51f7930aee72642f30b0d3ea5c5e8224

DOI: 10.1016/j.actamat.2015.06.043
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: Abstract We study the effects of different heat treatment routes on microstructure engineering and the resulting mechanical response in a plain binary Ti-4Mo (wt%) model alloy. We observe a broad variety of microstructure formation mechanisms including diffusion driven allotropic phase transformations as well as shear and/or diffusion dominated modes of martensitic transformations, enabling a wealth of effective microstructure design options even in such a simple binary Ti alloy. This wide variety of microstructures allows tailoring the mechanical properties ranging from low yield strength (350 MPa) and high ductility (30-35% tensile elongation) to very high yield strength (1100 MPa) and medium ductility (10-15% tensile elongation) as well as a variety of intermediate states. Mechanical testing and microstructure characterization using optical microscopy, scanning electron microscopy based techniques, transmission electron microscopy and atom probe tomography were performed revealing that minor variations in the heat treatment cause significant changes in the resulting microstructures (e.g. structural refinement, transition between diffusive and martensitic transformations). The experimental results on microstructure evolution during the applied different heat treatment routes are discussed with respect to the mechanical properties. © 2015 Acta Materialia Inc.
AUTHOR KEYWORDS: Atom probe tomography; Electron microscopy; Mechanical properties; Microstructure characterization; Microstructure engineering; Ti alloy
DOCUMENT TYPE: Article
SOURCE: Scopus

Shen, Y.F., Jia, N., Wang, Y.D., Sun, X., Zuo, L., Raabe, D.
Suppression of twinning and phase transformation in an ultrafine grained 2 GPa strong metastable austenitic steel: Experiment and simulation
(2015) Acta Materialia, 97, art. no. 12238, pp. 305-315. Cited 12 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84937562271&doi=10.1016%2fj.actamat.2015.06.053&partnerID=40&md5=8796c13425feca941eb38af1a3ba9890

DOI: 10.1016/j.actamat.2015.06.053
AFFILIATIONS: Key Laboratory for Anisotropy and Texture of Materials, MOE, Northeastern University, Shenyang, China;
Computational Science and Mathematics Division, Pacific Northwest National Laboratory, Richland, WA, United States;
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
ABSTRACT: Abstract An ultrafine-grained 304 austenitic 18 wt.% Cr-8 wt.% Ni stainless steel with a grain size of ~270 nm was synthesized by accumulative rolling (67% total reduction) and annealing (550°C, 150 s). Uniaxial tensile testing at room temperature reveals an extremely high

yield strength of 1890 ± 50 MPa and a tensile strength of 2050 ± 30 MPa, while the elongation reaches 6 ± 1%. Experimental characterization on samples with different grain sizes between 270 nm and 35 μm indicates that both, deformation twinning and martensitic phase transformation are significantly retarded with increasing grain refinement. A crystal plasticity finite element model incorporating a constitutive law reflecting the grain size-controlled dislocation slip and deformation twinning captures the micromechanical behavior of the steels with different grain sizes. Comparison of simulation and experiment shows that the deformation of ultrafine-grained 304 steels is dominated by the slip of partial dislocations, whereas for coarse-grained steels dislocation slip, twinning and martensite formation jointly contribute to the shape change. © 2015 Acta Materialia Inc.
AUTHOR KEYWORDS: Deformation; Twin; Ultrafine grain; Ultrahigh strength
DOCUMENT TYPE: Article
SOURCE: Scopus

Yan, D., Tasan, C.C., Raabe, D.
High resolution in situ mapping of microstrain and microstructure evolution reveals damage resistance criteria in dual phase steels
(2015) Acta Materialia, 96, pp. 399-409. Cited 28 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84933575509&doi=10.1016%2fj.actamat.2015.05.038&partnerID=40&md5=3bc9227d7682555c35df8170ebf6dbbd

DOI: 10.1016/j.actamat.2015.05.038
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: Microstructures of multi-phase alloys undergo morphological and crystallographic changes upon deformation, corresponding to the associated microstructural strain fields. The multiple length and time scales involved therein create immense complexity, especially when microstructural damage mechanisms are also activated. An understanding of the relationship between microstructure and damage initiation can often not be achieved by post-mortem microstructural characterization alone. Here, we present a novel multi-probe analysis approach. It couples various scanning electron microscopy methods to microscopic-digital image correlation (μ-DIC), to overcome various challenges associated with concurrent mapping of the deforming microstructure along with the associated microstrain fields. For this purpose a contrast- and resolution-optimized μ-DIC patterning method and a selective pattern/microstructure imaging strategy were developed. They jointly enable imaging of (i) microstructure-independent pattern maps and (ii) pattern-independent microstructure maps. We apply this approach here to the study of damage nucleation in ferrite/martensite dual-phase (DP) steel. The analyses provide four specific design guidelines for developing damage-resistant DP steels. © 2015 Acta Materialia Inc.
AUTHOR KEYWORDS: Damage; Digital image correlation; Dual-phase; EBSD; In situ
DOCUMENT TYPE: Article
SOURCE: Scopus

Springer, H., Szczepaniak, A., Raabe, D.
On the role of zinc on the formation and growth of intermetallic phases during interdiffusion between steel and aluminium alloys
(2015) Acta Materialia, 96, pp. 203-211. Cited 9 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84935024540&doi=10.1016%2fj.actamat.2015.06.028&partnerID=40&md5=8a6adc591826c7a5867405d0c4e3bcdb

DOI: 10.1016/j.actamat.2015.06.028
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

ABSTRACT: The effect of Zn - both within Al and as a coating on steel - on the intermetallic phase formation and growth was systematically studied in controlled experiments, simulating the interfacial reactions taking place in dissimilar solid/solid and solid/liquid joining procedures. Independent from the reaction temperature, the addition of 1.05 at.% Zn (2.5 wt.%) to Al had no effect on the reaction layers' build-up with the η phase (Al<inf>5</inf>Fe<inf>2</inf>) as the dominant component, but accelerated their parabolic growth up to a factor of 13. While Zn-coatings on steel were found to be beneficial for the regular and even formation of intermetallic reaction zones in solid/liquid joining procedures, their role in solid-state processes was found to be more complex and, if no countermeasures are taken, extremely detrimental to the joint properties. Possible reasons for the Zn-induced growth acceleration are discussed, as well as consequences for possible optimisation steps for reducing harmful effects of Zn in dissimilar joints between Al alloys and steel.
AUTHOR KEYWORDS: Aluminising; Interdiffusion; Interface; Joining; Zinc coatings
DOCUMENT TYPE: Article
SOURCE: Scopus

DOI: 10.1016/j.actamat.2015.05.005
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany;
ThyssenKrupp Steel Europe AG, Duisburg, Germany;
Salzgitter-Mannesmann Forschung, Duisburg, Germany
ABSTRACT: In dual-phase (DP) steels, inherited microstructures and elemental distributions affect the kinetics and morphology of phase transformation phenomena and the mechanical properties of the final material. In order to study the inheritance process, we selected two model materials with the same average DP steel composition but with different initial microstructures, created by coiling at different temperatures after hot rolling. These samples were submitted to a DP-steel heat treatment consisting of a short isothermal annealing in the pure austenite region and a quenching process. The evolution of microstructure, chemical composition and mechanical properties (hardness) during this treatment was investigated. The initial samples had a bainitic-martensitic (B + M) microstructure for the material coiled at lower temperature and a ferritic-pearlitic (P + F) microstructure for that coiled at higher temperature. The P + F microstructure had a much more inhomogeneous distribution of substitutional elements (in particular of Mn) and of carbon. After complete heat treatment, both materials showed a typical DP microstructure (martensite islands embedded in ferrite) but the P + F material showed lower hardness compared to the B + M material. It was found that the inhomogeneous elemental distribution prevailed in the P + F material. The inheritance process was studied by combining measurements of the elemental distribution by Wavelength-Dispersive X-ray spectroscopy (WDX), simulations of the evolution of the elemental composition via the DICTRA (diffusion-controlled reactions) computer programme, dilatometry to observe the kinetics of phase transformation, and observation and quantification of the microstructures by Electron Backscatter Diffraction (EBSD) measurements. For the P + F material it was found that the α-γ transformation during annealing is slowed down in regions of lower Mn content and is therefore not completed. During the subsequent cooling the incompletely autenitized material does not require ferrite nucleation and the γ-α transformation starts at relative high temperatures. For B + M, in contrast, nucleation of ferrite is needed and the transformation starts at lower temperatures. As a

result the B + M material develops a higher martensite content as well as a higher density of geometrically necessary dislocations (GNDs). It is speculated that for the B + M material the γ-α transformation occurs through a bainitic (i.e. partly displacive) process while the transformation at higher temperatures in the P + F material proceeds exclusively in a diffusive way. © 2015 Acta Materialia Inc.
AUTHOR KEYWORDS: DICTRA; DP steel; Gamma-alpha phase transformation; Geometrically necessary dislocations; Mn distribution
DOCUMENT TYPE: Article
SOURCE: Scopus

Morsdorf, L., Tasan, C.C., Ponge, D., Raabe, D.
3D structural and atomic-scale analysis of lath martensite: Effect of the transformation sequence
(2015) Acta Materialia, 95, pp. 366-377. Cited 21 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84935825866&doi=10.1016%2fj.actamat.2015.05.023&partnerID=40&md5=3bbb48e7a9d93fd05de117d4c13c7891

DOI: 10.1016/j.actamat.2015.05.023
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: To improve the fundamental understanding of the multi-scale characteristics of martensitic microstructures and their micro-mechanical properties, a multi-probe methodology is developed and applied to low-carbon lath martensitic model alloys. The approach is based on the joint employment of electron channeling contrast imaging (ECCI), electron backscatter diffraction (EBSD), transmission electron microscopy (TEM), atom probe tomography (APT) and nanoindentation, in conjunction with high precision and large field-of-view 3D serial sectioning. This methodology enabled us to resolve (i) size variations of martensite sub-units, (ii) associated dislocation sub-structures, (iii) chemical heterogeneities, and (iv) the resulting local mechanical properties. The identified interrelated microstructure heterogeneity is discussed and related to the martensitic transformation sequence, which is proposed to intrinsically lead to formation of a nano-composite structure in low-carbon martensitic steels. © 2015 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
AUTHOR KEYWORDS: 3D; Atom probe tomography; EBSD; ECCI; Lath martensite
DOCUMENT TYPE: Article
SOURCE: Scopus

Springer, H., Aparicio Fernandez, R., Duarte, M.J., Kostka, A., Raabe, D.
Microstructure refinement for high modulus in-situ metal matrix composite steels via controlled solidification of the system Fe-TiB<inf>2</inf>
(2015) Acta Materialia, 96, pp. 47-56. Cited 10 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84935830018&doi=10.1016%2fj.actamat.2015.06.017&partnerID=40&md5=707a656e6f8ee03a02f430b5bb1e9365

DOI: 10.1016/j.actamat.2015.06.017
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: Microstructures of Fe-TiB<inf>2</inf> metal-matrix-composites formed in-situ from Fe-Ti-B melts were investigated for hypo- and hyper-eutectic concentrations down to atomic-scale resolution. Special emphasis is laid on the influence of the solidification rate on particle size, morphology and distribution as well as their relation to mechanical properties. Innovative routes for the cost-effective production of stiff and ductile high modulus steels for lightweight structural applications are discussed, focusing on hyper-eutectic compositions due to their high stiffness/density ratio: firstly, very slow cooling allows the primary particles floating to the top of the cast, from which they can either be easily removed for retaining bulk material containing only fine-dispersed

eutectic particles, or be kept and utilised as a wear resistant surface. Secondly, annealing of amorphous matrix material obtained from very fast solidification leads to fine dispersed nano-scaled precipitation of TiB<inf>2</inf> particles. © 2015 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
AUTHOR KEYWORDS: Density; Elastic modulus; Liquid metallurgy; Metal-matrix-composites; Steel
DOCUMENT TYPE: Article
SOURCE: Scopus

Matuszewski, K., Rettig, R., Matysiak, H., Peng, Z., Povstugar, I., Choi, P., Müller, J., Raabe, D., Spiecker, E., Kurzydłowski, K.J., Singer, R.F.
Effect of ruthenium on the precipitation of topologically close packed phases in Ni-based superalloys of 3rd and 4th generation
(2015) Acta Materialia, 95, pp. 274-283. Cited 18 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84931266119&doi=10.1016%2fj.actamat.2015.05.033&partnerID=40&md5=19ef6a8f99a9c58f4d075a3bea3bef94

DOI: 10.1016/j.actamat.2015.05.033
AFFILIATIONS: University of Erlangen-Nuremberg FAU, Department of Materials Science and Engineering, Institute of Science and Technology of Metals WTM, Martensstr. 5, Erlangen, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Department of Microstructure Physics and Alloy Design, Max-Planck-Str. 1, Düsseldorf, Germany;
University of Erlangen-Nuremberg FAU, Department of Materials Science and Engineering, Center for Nanoanalysis and Electron Microscopy, Cauerstr. 6, Erlangen, Germany;
Warsaw University of Technology, Faculty of Materials Science and Engineering, Materials Design Division, Woloska 141, Warsaw, Poland
ABSTRACT: The precipitation of topologically close packed (TCP) phases is detrimental for the high temperature strength of high refractory Ni-based superalloys. The beneficial influence of Ru with respect to this so called instability is nowadays well accepted. In the present paper the precipitation of topologically close packed (TCP) phases is studied quantitatively in two experimental alloys (one Ru-free and one with addition of Ru) to clarify the mechanism of the Ru effect. It is confirmed that the TCP phase precipitates undergo sequential phase transformation with the tetragonal σ-phase precipitating first. Ru retards the phase transformation and leads to decreased equilibrium volume fraction of TCP phases. The results clearly indicate that Ru decreases the driving force for TCP phase precipitation. Investigations of crystallography and chemistry of the TCP/matrix interface point to an additional effect by increase of misfit strain energy. © 2015 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
AUTHOR KEYWORDS: Ni-based superalloys; Precipitation; Ruthenium effect; Thermodynamics; Topologically close packed (TCP) phases
DOCUMENT TYPE: Article
SOURCE: Scopus

Lai, M.J., Tasan, C.C., Zhang, J., Grabowski, B., Huang, L.F., Raabe, D.
Origin of shear induced β to ω transition in Ti-Nb-based alloys
(2015) Acta Materialia, 92, pp. 55-63. Cited 17 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84927666163&doi=10.1016%2fj.actamat.2015.03.040&partnerID=40&md5=b1cc74976a84937d44a57bc677343435

DOI: 10.1016/j.actamat.2015.03.040
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: Ti-Nb-based alloys are essential materials for biomedical implant and aerospace applications. They reveal complex phase transformation

behavior. Here, a {2 1 1}<inf>β</inf> ⟨1 1 1⟩ <inf>β</inf> twinning induced β (body-centered cubic phase) to ω (hexagonal phase) transition in Ti-Nb-based alloys is demonstrated by transmission electron microscopy and analyzed employing ab initio calculations and the linear elastic inclusion theory. Our theoretical results reveal a distinct energy barrier for the β to ω transition, where the contribution from lattice rearrangement, rather than the elastic contribution associated with lattice parameter mismatch, plays the major role. It is shown that this energy barrier can be overcome by {2 1 1}<inf>β</inf> ⟨1 1 1⟩ <inf>β</inf> shear, explaining why {2 1 1}<inf>β</inf> ⟨1 1 1⟩ <inf>β</inf> twinning or, alternatively, the β to α″ (orthorhombic phase) transition promotes local formation of the ω phase.
AUTHOR KEYWORDS: Ab initio; Phase transformation; TEM; Titanium; ω phase
DOCUMENT TYPE: Article
SOURCE: Scopus

Prakash, A., Guénolé, J., Wang, J., Müller, J., Spiecker, E., Mills, M.J., Povstugar, I., Choi, P., Raabe, D., Bitzek, E.
Atom probe informed simulations of dislocation-precipitate interactions reveal the importance of local interface curvature
(2015) Acta Materialia, 92, pp. 33-45. Cited 15 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84927673954&doi=10.1016%2fj.actamat.2015.03.050&partnerID=40&md5=73e104a26bd6f76a25c7685a810457d0

DOI: 10.1016/j.actamat.2015.03.050
AFFILIATIONS: Department of Materials Science and Engineering, Institute i, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany;
Department of Materials Science and Engineering, Institute IX, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany;
Department of Materials Science and Engineering, Ohio State University, Columbus, OH, United States;
Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
ABSTRACT: The interaction of dislocations with precipitates is an essential strengthening mechanism in metals, as exemplified by the superior high-temperature strength of Ni-base superalloys. Here we use atomistic simulation samples generated from atom probe tomography data of a single crystal superalloy to study the interactions of matrix dislocations with a γ′ precipitate in molecular dynamics simulations. It is shown that the precipitate morphology, in particular its local curvature, and the local chemical composition significantly alter both, the misfit dislocation network which forms at the precipitate interface, and the core structure of the misfit dislocations. Simulated tensile tests reveal the atomic scale details of many experimentally observed dislocation-precipitate interaction mechanisms, which cannot be reproduced by idealized simulation setups with planar interfaces. We thus demonstrate the need to include interface curvature in the study of semicoherent precipitates and introduce as an enabling method atom probe tomography-informed atomistic simulations.
AUTHOR KEYWORDS: Atom probe tomography (APT); Atomistic simulation; Misfit dislocation network; Ni-base superalloys; Precipitation hardening
DOCUMENT TYPE: Article
SOURCE: Scopus

Zilnyk, K.D., Oliveira, V.B., Sandim, H.R.Z., Möslang, A., Raabe, D.
Martensitic transformation in Eurofer-97 and ODS-Eurofer steels: A comparative study
(2015) Journal of Nuclear Materials, 462, pp. 360-367. Cited 7 times.

https://www.scopus.com/inward/record.uri?eid=2-s2.0-84930924402&doi=10.1016%2fj.jnucmat.2014.12.112&partnerID=40&md5=46fb6c5508c1401c080ac3f68432ba41

DOI: 10.1016/j.jnucmat.2014.12.112
AFFILIATIONS: Escola de Engenharia de Lorena, University of Sao Paulo, Brazil;
Karlsruher Institut für Technologie, KIT, Germany;
Max-Planck Institut für Eisenforschung, MPIE, Germany
ABSTRACT: (Figure Presented). Reduced-activation ferritic-martensitic Eurofer-97 and ODS-Eurofer steels are potential candidates for structural applications in advanced nuclear reactors. Samples of both steel grades in the as-tempered condition were austenitized in vacuum for 1 h from 900 °C to 1300 °C followed by air cooling to room temperature. The microstructure was characterized by dilatometry, electron backscatter diffraction (EBSD), and X-ray diffraction (XRD). Thermodynamic calculations provided by Thermo-Calc software were used to determine their transformation temperatures. Even having similar chemical composition, important changes were observed after martensitic transformation in these steels. Significant austenitic grain growth was observed in Eurofer-97 steel leading to the development of coarser martensitic packets. Contrastingly, austenitic grain growth was prevented in ODS-Eurofer steel due to fine and stable dispersion of Y-based particles.
DOCUMENT TYPE: Article
SOURCE: Scopus

Zhang, J.-L., Zaefferer, S., Raabe, D.
A study on the geometry of dislocation patterns in the surrounding of nanoindents in a TWIP steel using electron channeling contrast imaging and discrete dislocation dynamics simulations
(2015) Materials Science and Engineering A, 636, pp. 231-242. Cited 11 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84927770039&doi=10.1016%2fj.msea.2015.03.078&partnerID=40&md5=c119130359e6dfa2592e5b77b99f8fb1

DOI: 10.1016/j.msea.2015.03.078
AFFILIATIONS: Max-Planck-lnstitut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: Electron channeling contrast imaging under controlled diffraction conditions (cECCI) enables observation of crystal defects, especially dislocations, stacking faults and nano-twins, close to the surface of bulk samples. In this work cECCI has been employed to observe defects around nanoindents into the surface of {100}-, {110}-, {111}-oriented grains in a Fe-22Mn-0.65C (wt%) TWIP steel sample (fcc crystal structure, stacking fault energy ~20. mJ/m) using a cone-spherical indenter. The dislocation patterns show four- and two-fold symmetries for the {100}- and {110}-orientation, and a three-fold symmetry for the {111}-orientation which is, however, difficult to observe. Discrete dislocation dynamics (DDD) simulations of the indentation were carried out to complement the static experimental investigations. The simulations were carried out with both, cross-slip disabled and enabled conditions, where the former were found to match to the experimental results better, as may be expected for an fcc material with low stacking fault energy. The 3-dimensional geometry of the dislocation patterns of the different indents was analysed and discussed with respect to pattern formation mechanisms. The force-displacement curves obtained during indentation showed a stronger strain hardening for the {111} oriented crystal than that for the other orientations. This is in contrast to the behaviour of, for example, copper and is interpreted to be due to planar slip. Irrespective of orientation and indentation depth the radius of the plastically deformed area was found to be approximately 4 times larger than that of the indenter contact area.

AUTHOR KEYWORDS: Discrete dislocation dynamics (DDD); Dislocation patterning; Dislocations; Electron channeling; Nanoindentation; Plastic zone
DOCUMENT TYPE: Article
SOURCE: Scopus

Ram, F., Zaefferer, S., Jäpel, T., Raabe, D.
Error analysis of the crystal orientations and disorientations obtained by the classical electron backscatter diffraction technique
(2015) Journal of Applied Crystallography, 48, pp. 797-813. Cited 11 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84930624555&doi=10.1107%2fS1600576715005762&partnerID=40&md5=228f49333d6ea9be8182020778f5697d

DOI: 10.1107/S1600576715005762
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, Düsseldorf, Germany;
EO Elektronen-Optik-Service GmbH, Zum Lonnenhohl 46, Dortmund, Germany
ABSTRACT: The fidelity - that is, the error, precision and accuracy - of the crystallographic orientations and disorientations obtained by the classical two-dimensional Hough-transform-based analysis of electron backscatter diffraction patterns (EBSPs) is studied. Using EBSPs simulated based on the dynamical electron diffraction theory, the fidelity analysis that has been previously performed using the patterns simulated based on the theory of kinematic electron diffraction is improved. Using the same patterns, the efficacy of a Fisher-distribution-based analytical accuracy measure for orientation and disorientation is verified.
AUTHOR KEYWORDS: accuracy; crystallographic disorientation; crystallographic orientation; electron backscatter diffraction (EBSD); error analysis; pattern projection center; precision
DOCUMENT TYPE: Article
SOURCE: Scopus

Zambaldi, C., Zehnder, C., Raabe, D.
Orientation dependent deformation by slip and twinning in magnesium during single crystal indentation
(2015) Acta Materialia, 91, pp. 267-288. Cited 22 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84961291551&doi=10.1016%2fj.actamat.2015.01.046&partnerID=40&md5=b5cf8ac23b608a1da67a9cbf946cc80d

DOI: 10.1016/j.actamat.2015.01.046
AFFILIATIONS: MPI für Eisenforschung, Düsseldorf, Germany
ABSTRACT: We present the orientation dependent indentation response of pure magnesium during single grain indentation. A conical indenter and maximum loads between 50 mN and 900 mN were employed. Indent topographies were acquired by confocal microscopy. The indents were also characterized by electron backscatter orientation microscopy for their microstructures. Pronounced activation of specific twinning systems was observed around the impressions. The resulting data were compiled into the inverse pole figure presentation of indent microstructures and topographies after Zambaldi and Raabe, Acta Mater. (2010). Three-dimensional crystal plasticity finite element simulation of the indentation deformation supports the interpretation of the orientation dependent slip and twinning patterns around the indents. The match between the activation of observed and simulated twinning variants is discussed with respect to the conditions for nucleation and growth of extension twins. Furthermore, the compatibility of the twinning strains with the imposed deformation is discussed based on the expanding cavity model of indentation. The orientation dependent response of magnesium during indentation is compared to the literature data for indentation of alpha-titanium and beryllium. Recommendations are given on how to exploit the characteristic nature of the observed indentation patterns to rapidly assess the relative activity of deformation mechanisms

and their critical shear stresses during alloy development. © 2015 Acta Materialia Inc.
AUTHOR KEYWORDS: Anisotropy; EBSD; Indentation; Nucleation; Twinning
DOCUMENT TYPE: Article
SOURCE: Scopus

Shen, Y.F., Qiu, L.N., Sun, X., Zuo, L., Liaw, P.K., Raabe, D.
Effects of retained austenite volume fraction, morphology, and carbon content on strength and ductility of nanostructured TRIP-assisted steels
(2015) Materials Science and Engineering A, 636, pp. 551-564. Cited 25 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84928397672&doi=10.1016%2fj.msea.2015.04.030&partnerID=40&md5=a0e23f803c1dd432d3a22a0fa17f6cfc

DOI: 10.1016/j.msea.2015.04.030
AFFILIATIONS: Key Laboratory for Anisotropy and Texture of Materials (MOE), Northeastern University, 3 Wenhua Road, Shenyang, China;
Pacific Northwest National Laboratory, PO Box 999, Richland, WA, United States;
Department of Materials Science and Engineering, The University of Tennessee, Knoxville, TN, United States;
Max-Planck-Institut fuer Eisenforschung, Max-Planck-Str. 18, Düsseldorf, Germany
ABSTRACT: With a suite of multi-modal and multi-scale characterization techniques, the present study unambiguously proves that a substantially-improved combination of ultrahigh strength and good ductility can be achieved by tailoring the volume fraction, morphology, and carbon content of the retained austenite (RA) in a transformation-induced-plasticity (TRIP) steel with the nominal chemical composition of 0.19C-0.30Si-1.76Mn-1.52Al (weight percent, wt%). After intercritical annealing and bainitic holding, a combination of ultimate tensile strength (UTS) of 1100. MPa and true strain of 50% has been obtained, as a result of the ultrafine RA lamellae, which are alternately arranged in the bainitic ferrite around junction regions of ferrite grains. For reference, specimens with a blocky RA, prepared without the bainitic holding, yield a low ductility (35%) and a low UTS (800. MPa). The volume fraction, morphology, and carbon content of RA have been characterized using various techniques, including the magnetic probing, scanning electron microscopy (SEM), electron-backscatter-diffraction (EBSD), and transmission electron microscopy (TEM). Interrupted tensile tests, mapped using EBSD in conjunction with the kernel average misorientation (KAM) analysis, reveal that the lamellar RA is the governing microstructure component responsible for the higher mechanical stability, compared to the blocky one. By coupling these various techniques, we quantitatively demonstrate that in addition to the RA volume fraction, its morphology and carbon content are equally important in optimizing the strength and ductility of TRIP-assisted steels. © 2015 Elsevier B.V.
AUTHOR KEYWORDS: Ductility; Mechanical stability; Morphology; Retained austenite; Strength
DOCUMENT TYPE: Article
SOURCE: Scopus

Deng, Y., Tasan, C.C., Pradeep, K.G., Springer, H., Kostka, A., Raabe, D.
Design of a twinning-induced plasticity high entropy alloy
(2015) Acta Materialia, 94, pp. 124-133. Cited 68 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84929313620&doi=10.1016%2fj.actamat.2015.04.014&partnerID=40&md5=f85cf9c1b53ee3249b15bf57730299de

DOI: 10.1016/j.actamat.2015.04.014
AFFILIATIONS: Max-Planck-lnstitut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;

Department of Engineering Design and Materials, Norwegian University of Science and Technology, Trondheim, Norway;
Materials Chemistry, RWTH Aachen University, Kopernikusstr.10, Aachen, Germany
ABSTRACT: We introduce a liquid metallurgy synthesized, non-equiatomic Fe<inf>40</inf>Mn<inf>40</inf>Co<inf>10</inf>Cr<inf>10</inf> high entropy alloy that is designed to undergo mechanically-induced twinning upon deformation at room temperature. Microstructure characterization, carried out using SEM, TEM and APT shows a homogeneous fcc structured single phase solid solution in the as-cast, hot-rolled and homogenized states. Investigations of the deformation substructures at specific strain levels with electron channeling contrast imaging (ECCI) combined with EBSD reveal a clear change in the deformation mechanisms of the designed alloy starting from dislocation slip to twinning as a function of strain. Such twinning induced plasticity has only been observed under cryogenic conditions in the equiatomic FeMnNiCoCr high entropy alloy. Thus, despite the decreased contribution of solid solution strengthening, the tensile properties of the introduced lean alloy at room temperature are found to be comparable to that of the well-studied five component FeMnNiCoCr system.
AUTHOR KEYWORDS: EBSD; ECCI; High entropy alloy; Lean; Twinning
DOCUMENT TYPE: Article
SOURCE: Scopus

Isik, M.I., Kostka, A., Yardley, V.A., Pradeep, K.G., Duarte, M.J., Choi, P.P., Raabe, D., Eggeler, G.
The nucleation of Mo-rich Laves phase particles adjacent to M23C6 micrograin boundary carbides in 12% Cr tempered martensite ferritic steels
(2015) Acta Materialia, 90, pp. 94-104. Cited 28 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84924244323&doi=10.1016%2fj.actamat.2015.01.027&partnerID=40&md5=6247e935911e5e2d37a9e9e95bef1eff

DOI: 10.1016/j.actamat.2015.01.027
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Institut für Werkstoffe, Ruhr-Universität Bochum, Bochum, Germany;
Lehrstuhl für Werkstoffchemie, RWTH Aachen University, Aachen, Germany
ABSTRACT: We study the nucleation of Mo-rich Laves phase particles during aging and creep of 12 wt.% Cr tempered martensite ferritic steels (TMFS). Recently, in Isik et al. (2014) we reported that Laves phase particles tend to form at micrograin boundaries of TMFSs after Mo and Si had segregated from the ferritic matrix to these internal interfaces. In the present work, we employ transmission electron microscopy (TEM) and atom probe tomography (APT) to study the formation of Laves phase particles. We investigate the preference of Laves phase particles to nucleate next to M23C6 micrograin boundary carbides. Our results suggest that this joint precipitation effect is due to the combined segregation of Mo and Si from the matrix to the micrograin boundaries and Si and P enrichment around the growing carbides.
AUTHOR KEYWORDS: Atom probe tomography (APT); Laves phase; M23C6 carbides; Tempered martensite ferritic steels; Transmission electron microscopy (TEM)
DOCUMENT TYPE: Article
SOURCE: Scopus

Nellessen, J., Sandlöbes, S., Raabe, D.
Effects of strain amplitude, cycle number and orientation on low cycle fatigue microstructures in austenitic stainless steel studied by electron channelling contrast imaging
(2015) Acta Materialia, 87, pp. 86-99. Cited 6 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84921662117&doi=10.1016%2fj.actamat.2014.12.024&partnerID=40&md5=8fdb85446d0c7f052ec51f26080dca8d

DOI: 10.1016/j.actamat.2014.12.024
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Department for Microstructure Physics and Alloy Design, Düsseldorf, Germany
ABSTRACT: Substructure analysis on cyclically deformed metals is typically performed by time-consuming transmission electron microscopy probing, thus limiting such studies often to a single parameter. Here, we present a novel approach which consists in combining electron backscatter diffraction (EBSD), digital image correlation and electron channelling contrast imaging (ECCI), enabling us to systematically probe a large matrix of different parameters with the aim of correlating and comparing their interdependence. The main focus here is to identify the influence of cycle number, initial grain orientation and local strain amplitude on the evolving dislocation patterns. Therefore, experiments up to 100 cycles were performed on a polycrystalline austenitic stainless steel with local strain amplitudes between 0.35% and 0.95%. EBSD and ECCI maps reveal the individual influence of each parameter while the others remained constant. We find that the dislocation structures strongly depend on grain orientation. Dislocation structures in grains with double-slip (⟨1 1 2⟩ // LD, ⟨1 2 2⟩ // LD and ⟨0 1 2⟩ // LD) and multiple-slip (⟨1 1 1⟩ // LD, M ⟨0 1 1⟩ // LD and ⟨0 0 1⟩ // LD) orientations with respect to the loading direction (LD) are characterized under the variation of strain amplitude and cycle number.
AUTHOR KEYWORDS: Dislocation structures; Electron channelling contrast imaging (ECCI); Low cycle fatigue (LCF); Stainless steel
DOCUMENT TYPE: Article
SOURCE: Scopus

Konijnenberg, P.J., Zaefferer, S., Raabe, D.
Assessment of geometrically necessary dislocation levels derived by 3D EBSD (2015) Acta Materialia, . Article in Press. Cited 10 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84939129904&doi=10.1016%2fj.actamat.2015.06.051&partnerID=40&md5=59e4786bbeea5d1bbadc64838f4d2ed6

DOI: 10.1016/j.actamat.2015.06.051
AFFILIATIONS: Max-Planck-Inst. für Eisenforschung, Max-Planck-Str 1, 40237 Düsseldorf, Germany;
Bruker Nano GmbH, Am Studio 2D, 12489 Berlin, Germany
ABSTRACT: Existing alternatives for the calculation of geometrically necessary dislocation (GND) densities from orientation fields are discussed. Importantly, we highlight the role of reference frames and consider different sources of error. A well-controlled micro cantilever bending experiment on a copper bicrystal has been analyzed by 3-dimensional electron back scatter diffraction (3D EBSD). The GND density is determined experimentally by two different approaches and assessed theoretically, assuming a homogeneous bending of the cantilever. Experiment and theory agree very well. It is further shown that the deformation is accommodated mainly by GNDs, which carry and store lattice rotation, and not (only) by mobile dislocations that leave a crystal portion inspected, without lattice rotations. A detailed GND analysis reveals a local density minimum close to the grain boundary and a distinct difference in edge to screw ratios for both grains.
AUTHOR KEYWORDS: 3D EBSD; Bending test; Dislocation structure; Geometrically necessary dislocations; Microstructure
DOCUMENT TYPE: Article in Press
SOURCE: Scopus

Guo, W., Yao, J., Jägle, E.A., Choi, P.-P., Herbig, M., Schneider, J.M., Raabe, D.
Deformation induced alloying in crystalline - metallic glass nano-composites

(2015) Materials Science and Engineering A, 628, pp. 269-280. Cited 5 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84923039468&doi=10.1016%2fj.msea.2015.01.062&partnerID=40&md5=2bb380e54961d3d3878d97a04af7e560

DOI: 10.1016/j.msea.2015.01.062
AFFILIATIONS: Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China;
Lehrstuhl für Werkstoffchemie, RWTH Aachen University, Aachen, Germany
ABSTRACT: We study the mechanisms of deformation driven chemical mixing in a metallic nanocomposite model system. More specific, we investigate shear banding at the atomic scale in an amorphous CuZr/ crystalline Cu nanolaminate, deformed by microindentation. Three CuZr/Cu multilayer systems (100 nm Cu/100 nm CuZr, 50 nm Cu/100 nm CuZr, and 10 nm Cu/100 nm CuZr) are fabricated to study the effect of layer thickness on shear band formation and deformation induced alloying. The chemical and structural evolution at different strain levels are traced by atom probe tomography and transmission electron microscopy combined with nano-beam diffraction mapping. The initially pure crystalline Cu and amorphous CuZr layers chemically mix by cross-phase shear banding after reaching a critical layer thickness. The Cu inside the shear bands develops a high dislocation density and can locally undergo transition to an amorphous state when sheared and mixed. We conclude that the severe deformation in the shear bands in the amorphous layer squeeze Zr atoms into the Cu dislocation cores in the Cu layers (thickness <5 nm), resulting in local chemical mixing. © 2015 Elsevier B.V.
AUTHOR KEYWORDS: Atom probe tomography; Deformation induced alloying; Metallic glass; Multilayers; Nanocrystalline; Shear band
DOCUMENT TYPE: Article
SOURCE: Scopus

Tytko, D., Choi, P.-P., Raabe, D.
Thermal dissolution mechanisms of AlN/CrN hard coating superlattices studied by atom probe tomography and transmission electron microscopy
(2015) Acta Materialia, 85, pp. 32-41. Cited 9 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84916899400&doi=10.1016%2fj.actamat.2014.11.004&partnerID=40&md5=7cc141e4bfbeba975ec1865c8497bea9

DOI: 10.1016/j.actamat.2014.11.004
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck Str. 1, Düsseldorf, Germany
ABSTRACT: AlN/CrN superlattices with a B1 cubic crystal structure and a bilayer period of 4 nm were deposited by reactive radiofrequency magnetron sputtering. The coatings were investigated with respect to their thermal stability and changes in microstructure and chemical composition at 900 °C. The AlN layers show high chemical stability but undergo dissolution by pinching off at grain boundaries. A transformation from cubic to hexagonal AlN with subsequent coarsening at grain boundary triple junctions is observed. In contrast to AlN, the CrN layers show poor chemical stability and their compositions are shifted towards Cr2N upon annealing in a protective argon atmosphere due to nitrogen loss. However, even after establishing Cr2N stoichiometry the crystal structure of the layers remains cubic. © 2014 Acta Materialia Inc.
AUTHOR KEYWORDS: AlN/CrN; Atom probe tomography; Hard coatings; Layer pinch-off; Thermal stability
DOCUMENT TYPE: Article
SOURCE: Scopus

Wang, M.-M., Tasan, C.C., Ponge, D., Dippel, A.-Ch., Raabe, D.

Nanolaminate transformation-induced plasticity-twinning-induced plasticity steel with dynamic strain partitioning and enhanced damage resistance
(2015) Acta Materialia, 85, pp. 216-228. Cited 35 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84918576104&doi=10.1016%2fj.actamat.2014.11.010&partnerID=40&md5=b01ba24bff f67b4310aa711e3efe9c7b

DOI: 10.1016/j.actamat.2014.11.010
AFFILIATIONS: Max-Planck-lnstitut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany
ABSTRACT: Conventional martensitic steels have limited ductility due to insufficient microstructural strain-hardening and damage resistance mechanisms. It was recently demonstrated that the ductility and toughness of martensitic steels can be improved without sacrificing the strength, via partial reversion of the martensite back to austenite. These improvements were attributed to the presence of the transformation-induced plasticity (TRIP) effect of the austenite phase, and the precipitation hardening (maraging) effect in the martensitic matrix. However, a full micromechanical understanding of this ductilizing effect requires a systematic investigation of the interplay between the two phases, with regards to the underlying deformation and damage micromechanisms. For this purpose, in this work, a Fe-9Mn-3Ni-1.4Al-0.01C (mass%) medium-Mn TRIP maraging steel is produced and heat-treated under different reversion conditions to introduce well-controlled variations in the austenite-martensite nanolaminate microstructure. Uniaxial tension and impact tests are carried out and the microstructure is characterized using scanning and transmission electron microscopy based techniques and post mortem synchrotron X-ray diffraction analysis. The results reveal that (i) the strain partitioning between austenite and martensite is governed by a highly dynamical interplay of dislocation slip, deformation-induced phase transformation (i.e. causing the TRIP effect) and mechanical twinning (i.e. causing the twinning-induced plasticity effect); and (ii) the nanolaminate microstructure morphology leads to enhanced damage resistance. The presence of both effects results in enhanced strain-hardening capacity and damage resistance, and hence the enhanced ductility. © 2014 Acta Materialia Inc.
AUTHOR KEYWORDS: Damage; Reverted austenite; Strain partitioning; TRIP-maraging; TWIP
DOCUMENT TYPE: Article
SOURCE: Scopus

Ma, D., Friák, M., Von Pezold, J., Raabe, D., Neugebauer, J.
Computationally efficient and quantitatively accurate multiscale simulation of solid-solution strengthening by ab initio calculation
(2015) Acta Materialia, 85, pp. 53-66. Cited 12 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84917691048&doi=10.1016%2fj.actamat.2014.10.044&partnerID=40&md5=c7017c3b6c400882646abb7511374969

DOI: 10.1016/j.actamat.2014.10.044
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany;
Institute of Physics of Materials, Academy of Sciences of the Czech Republic, V.v.i, Zi zkova 22, Brno, Czech Republic
ABSTRACT: We propose an approach for the computationally efficient and quantitatively accurate prediction of solid-solution strengthening. It combines the 2-D Peierls-Nabarro model and a recently developed solid-solution strengthening model. Solid-solution strengthening is examined with Al-Mg and Al-Li as representative alloy systems, demonstrating a good agreement between theory and experiments within the temperature range in which the dislocation motion is overdamped. Through a parametric study, two guideline maps of the misfit parameters against (i) the critical resolved shear stress, τ0, at 0 K and (ii) the energy barrier, ΔEb, against

dislocation motion in a solid solution with randomly distributed solute atoms are created. With these two guideline maps, τ0 at finite temperatures is predicted for other Al binary systems, and compared with available experiments, achieving good agreement. © 2014 Acta Materialia Inc.
AUTHOR KEYWORDS: Ab initio; Al alloys; DFT; Peierls-Nabarro model; Solid-solution strengthening
DOCUMENT TYPE: Article
SOURCE: Scopus

Ayodele, S.G., Raabe, D., Varnik, F.
Shear-flow-controlled mode selection in a nonlinear autocatalytic medium (2015) Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, 91 (2), art. no. 022913, . Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84923169418&doi=10.1103%2fPhysRevE.91.022913&partnerID=40&md5=aeace35d0345ad5936fe403ce47bb486

DOI: 10.1103/PhysRevE.91.022913
AFFILIATIONS: Max-Planck-Institut für Dynamik und Selbstorganisation, Am Fassberg 17, Göttingen, Germany;
Max-Planck Institut für Eisenforschung, Max-Planck Straße 1, Düsseldorf, Germany;
Interdisciplinary Center for Advanced Materials Simulation, Ruhr-Universität-Bochum, Universitätsstraße 150, Bochum, Germany
ABSTRACT: The effect of shear flow on mode selection and the length scale of patterns formed in a nonlinear autocatalytic reaction-diffusion model is investigated. We predict analytically the existence of transverse and longitudinal modes. The type of the selected mode strongly depends on the difference in the flow rates of the participating species, quantified by the differential flow parameter. Spatial structures are obtained by varying the length scale of individual modes and superposing them via the differential flow parameter. Our predictions are in line with numerical results obtained from lattice Boltzmann simulations. © 2015 American Physical Society.
DOCUMENT TYPE: Article
SOURCE: Scopus

Li, Y.J., Kostka, A., Choi, P., Goto, S., Ponge, D., Kirchheim, R., Raabe, D.
Mechanisms of subgrain coarsening and its effect on the mechanical properties of carbon-supersaturated nanocrystalline hypereutectoid steel (2015) Acta Materialia, 84, pp. 110-123. Cited 18 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84911916336&doi=10.1016%2fj.actamat.2014.10.027&partnerID=40&md5=445613117649739624af6416f1bef4fe

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AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany;
Department of Materials Science and Engineering, Faculty of Engineering and Resource Science, Akita University, Tegata Gakuencho, Akita, Japan;
Institut für Materialphysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, Göttingen, Germany
ABSTRACT: Carbon-supersaturated nanocrystalline hypereutectoid steels with a tensile strength of 6.35 GPa were produced from severely cold-drawn pearlite. The nanocrystalline material undergoes softening upon annealing at temperatures between 200 and 450°C. The ductility in terms of elongation to failure exhibits a non-monotonic dependence on temperature. Here, the microstructural mechanisms responsible for changes in the mechanical properties were studied using transmission electron microscopy (TEM), TEM-based automated scanning nanobeam diffraction and atom probe tomography (APT). TEM and APT investigations of the nanocrystalline hypereutectoid steel show subgrain coarsening upon annealing, which leads to strength

reduction following a Hall-Petch law. APT analyzes of the Mn distribution near subgrain boundaries and in the cementite give strong evidence of capillary-driven subgrain coarsening occurring through subgrain boundary migration. The pronounced deterioration of ductility after annealing at temperatures above 350°C is attributed to the formation of cementite at subgrain boundaries. The overall segregation of carbon atoms at ferrite subgrain boundaries gives the nanocrystalline material excellent thermal stability upon annealing.
AUTHOR KEYWORDS: Annealing; Cold-drawn pearlitic steel; Nanocrystalline steels; Strength softening; Subgrain coarsening
DOCUMENT TYPE: Article
SOURCE: Scopus

Jägle, E.A., Sheng, Z., Choi, P.-P., Raabe, D.
Maraging steel produced by laser additive manufacturing: The influence of processing conditions on precipitation and austenite reversion behaviour
(2015) PTM 2015 - Proceedings of the International Conference on Solid-Solid Phase Transformations in Inorganic Materials 2015, pp. 1029-1030.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84962635887&partnerID=40&md5=c746f667e61ed3a9156c80145e3addd6

AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, Düsseldorf, Germany
AUTHOR KEYWORDS: Additive manufacturing; Atom probe tomography; Austenite reversion; Laser metal deposition; Maraging steel; Precipitation; Selective laser melting
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Nikolov, S., Fabritius, H., Friák, M., Raabe, D.
Integrated multiscale modeling approach for hierarchical biological nanocomposites applied to lobster cuticle
(2015) Bulgarian Chemical Communications, 47, pp. 424-433. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84976421915&partnerID=40&md5=c066bed686cd2830463449e09d0cb40f

AFFILIATIONS: Institute of Mechanics, Bulgarian Academy of Sciences, Acad. G. Bontchev Str., Sofia, Bulgaria;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: Biological structural materials (e.g., bone, arthropod cuticles, shells) are organic-inorganic nanocomposites with hierarchically organized microstructure. A powerful tool to obtain the structure/property relations in such materials is multiscale modeling encompassing all length scales. Here we present an integral multiscale modeling approach for computing and prediction of the elastic properties of mineralized biomaterials. We combine ab initio calculations using Density Functional Theory (DFT) at the atomistic scale, step-by-step homogenization modeling at the mesoscale, and full-field spectral method based on Fast Fourier Transforms (FFT) for the macroscopic scale. An essential part of the concept is the experimental input to the model concerning the material structure and composition. We apply our multiscale concept to the cuticle of lobster. The cuticle consists of chitin nanofibrils, proteins, and mineral nanoparticles, and contains numerous pore canals across its thickness. The elastic properties at each hierarchical level are estimated and compared to experimental data for dry cuticle. At the mesoscale, the properties of cuticle proteins are identified and the bulk mineralized tissue is investigated. We find that the Young's modulus of the bulk tissue along the chitin fibrils is ~ 60% larger compared the modulus in direction perpendicular to the fibrils. At the macroscale, the highest stress concentrations in the cuticle in uniaxial in-plane loadings appear in planes where: (i) the major axes of

the ellipsoidal pores (as well as the chitin fibrils) are oriented at about ±45° w.r.t. the loading direction, (ii) the separation regions between the pores are thinnest, and (iii) the shear stresses in the separation regions are close to their maximal values. We suggest that these are the necessary conditions for damage initiation in the lobster cuticle. © 2015 Bulgarian Academy of Sciences, Union of Chemists in Bulgaria.
AUTHOR KEYWORDS: Biomaterials; Computational techniques; Mechanical properties of tissues; Organic-inorganic nanostructures; Simulations; Structural modeling
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Herbig, M., Marceau, R.K.W., Morsdorf, L., Raabe, D.
Spinodal decomposition of Fe-Ni-C martensite by room temperature redistribution of carbon investigated by correlative ECCI/TEM/APT
(2015) PTM 2015 - Proceedings of the International Conference on Solid-Solid Phase Transformations in Inorganic Materials 2015, pp. 299-300. Cited 1 time.
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AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany; Institute for Frontier Materials, Deakin University, Geelong, VIC, Australia
AUTHOR KEYWORDS: Atom probe tomography; Correlative microscopy; Electron channeling contrast imaging; Spinodal decomposition; Transmission electron microscopy
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Bleck, W., Raabe, D., Dong, H.
International high manganese steel conference
(2015) Steel Research International, 86 (10), p. 1126.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84942843468&doi=10.1002%2fsrin.201500237&partnerID=40&md5=ca5fd8639346cca7f04bb419f714872b

DOI: 10.1002/srin.201500237
DOCUMENT TYPE: Editorial
SOURCE: Scopus

Aboulfadl, H., Deges, J., Choi, P., Raabe, D.
Dynamic strain aging studied at the atomic scale
(2015) Acta Materialia, 86, pp. 34-42. Cited 28 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84920477150&doi=10.1016%2fj.actamat.2014.12.028&partnerID=40&md5=a425477fdd868d31c0b7d823f3ad8602

DOI: 10.1016/j.actamat.2014.12.028
AFFILIATIONS: Max-Planck Institut für Eisenforschung GmbH, Department for Microstructure Physics and Alloy Design, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: Dynamic strain aging arises from the interaction between solute atoms and matrix dislocations in strained metallic alloy. It initiates jerky dislocation motion and abrupt softening, causing negative strain rate sensitivity. This effect leads to instable flow phenomena at the macroscopic scale, appearing as a serrated stress-strain response and deformation banding. These macroscopic features are referred to as the Portevin-Le Chatelier effect (PLC). Here we study the atomistic origin of dynamic strain aging in an Al-4.8 at.% Mg alloy using atom probe tomography (APT) and transmission electron microscopy (TEM). Samples were prepared from as-cold rolled (90% thickness reduction), stabilized (120 °C, 20 h) and recrystallized sheets (400°C, 10 min), respectively. In the stabilized

state, Mg was found to decorate <1 1 0> aligned dislocations with up to ~12.5 at.%. Tensile tests in combination with thermographic and laser speckle observations were used to map the deformation bands for the site-specific extraction of APT samples from regions inside the PLC bands. We observed an asymmetrical Mg distribution along some of the dislocations, matching model predictions for high dislocation speeds at peak drag stress by Zhang and Curtin. In this case, the Mg distribution is characterized by depletion in the compressive regime above the dislocation slip plane and enrichment in the dilatation region below the slip plane. Mg also depletes in a tail-like form behind fast-moving dislocations, further promoting slip localization.
AUTHOR KEYWORDS: Atom probe tomography; Dynamic strain aging; Portevin-Le Chatelier effect
DOCUMENT TYPE: Article
SOURCE: Scopus

Kim, J.-K., Sandlöbes, S., Raabe, D.
On the room temperature deformation mechanisms of a Mg-Y-Zn alloy with long-period-stacking-ordered structures
(2015) Acta Materialia, 82, pp. 414-423. Cited 26 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84908324001&doi=10.1016%2fj.actamat.2014.09.036&partnerID=40&md5=2c6241ab5666c7a89a1a04488a79c937

DOI: 10.1016/j.actamat.2014.09.036
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: We present a transmission electron microscopy study on the room temperature deformation mechanisms in a Mg97Y2Zn1 (at.%) alloy with long-period-stacking-order (LPSO) phase. The alloy consists of α-Mg matrix with platelet-shaped LPSO precipitates 3-5 nm thick and interdendritic LPSO (18R structures) phase grains. The interdendritic LPSO phase was found to deform either by kink-banding in conjunction with basal <a> slip or by basal <a> slip and the formation of dislocation walls. No orientation dependence of these different deformation modes was observed. The α-Mg matrix deforms by basal <a> slip and pyramidal <c + a> slip. No twinning was observed in the α-Mg matrix during room temperature deformation. The elastic modulus mismatch between α-Mg matrix and LPSO plates is suggested to be the main source for activating non-basal dislocations. The combination of the soft α-Mg matrix strengthened by LPSO precipitates and harder "bulk" interdendritic LPSO grains is suggested to contribute to the well-known good mechanical properties of Mg-LPSO alloys at room temperature.
AUTHOR KEYWORDS: Deformation structures; Dislocations; Long-period-stacking-ordered structure; Magnesium alloy; Transmission electron microscopy
DOCUMENT TYPE: Article
SOURCE: Scopus

Raabe, D., Tasan, C.C., Springer, H., Bausch, M.
From high-entropy alloys to high-entropy steels
(2015) Steel Research International, 86 (10), pp. 1127-1138. Cited 18 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84942986775&doi=10.1002%2fsrin.201500133&partnerID=40&md5=cea0b1d6571167b0bf39e22d62523270

DOI: 10.1002/srin.201500133

AFFILIATIONS: Max-Planck-InstitutfürEisenforschung, Department for Microstructure Physics and Alloy Design, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: Inspired by high-entropy alloys, we study the design of steels that are based on high configurational entropy for stabilizing a single-phase solid solution matrix. The focus is placed on the system Fe-Mn-Al-Si-C but we also present trends in the alloy system Fe-Mn-Al-C. Unlike in conventional high-entropy alloys, where five or more equiatomically proportioned components are used, we exploit the flat configurational entropy plateau in transition metal mixtures, stabilizing solid solutions also for lean, non-equiatomic compositions. This renders the high-entropy alloying concept, where none of the elements prevails, into a class of Fe-based materials which we refer to as high-entropy steels. A point that has received little attention in high-entropy alloys is the use of interstitial elements. Here, we address the role of C in face-centered cubic solid solution phases. High-entropy steels reveal excellent mechanical properties, namely, very high ductility and toughness; excellent high rate and low-temperature ductility; high strength of up to 1 GPa; up to 17% reduced mass density; and very high strain hardening. The microstructure stability can be tuned by adjusting the stacking fault energy. This enables to exploit deformation effects such as the TRIP, TWIP, or precipitation determined mechanisms. We present a class of massive solid solution steels with high configurational entropy. Focus is placed on the system Fe-Mn-Al-Si-C, i.e., considering also C interstitials. By exploiting the flat configurational entropy plateau in metal mixtures, solid solutions of lean, non-equiatomic compositions can be stabilized. This renders the high-entropy alloying concept, where none of the elements prevails, into high-entropy steels.
AUTHOR KEYWORDS: high-entropy alloys; low-density steels; TRIP; strain hardening; TWIP
DOCUMENT TYPE: Article
SOURCE: Scopus

Li, Y.J., Ponge, D., Choi, P., Raabe, D.
Segregation of boron at prior austenite grain boundaries in a quenched martensitic steel studied by atom probe tomography
(2015) Scripta Materialia, 96 (C), pp. 13-16. Cited 14 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84927738717&doi=10.1016%2fj.scriptamat.2014.09.031&partnerID=40&md5=445f8b8c4943c026a0f6a80c98fe2c70

DOI: 10.1016/j.scriptamat.2014.09.031
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: The distribution of B and other alloying elements (C, Cr, Mo) at prior austenite grain boundaries (PAGBs) and in the matrix was quantified by atom probe tomography in a quenched martensitic steel. B and Mo were observed to be segregated only at PAGBs and to be absent at martensite-martensite boundaries. C is segregated both at PAGBs and at martensite-martensite boundaries, whereas Cr is homogeneously distributed in the probed volume. Our results indicate that B undergoes a non-equilibrium segregation.
AUTHOR KEYWORDS: Atom probe tomography; Grain boundary segregation; Martensitic steels; Non-equilibrium segregation; Prior austenite grain boundaries
DOCUMENT TYPE: Article
SOURCE: Scopus

Dmitrieva, O., Raabe, D., Müller, S., Dondl, P.W.
Microstructure in plasticity, a comparison between theory and experiment
(2015) Lecture Notes in Applied and Computational Mechanics, 78, pp. 205-218. Cited 4 times.

https://www.scopus.com/inward/record.uri?eid=2-s2.0-84928671115&doi=10.1007%2f978-3-319-18242-1_8&partnerID=40&md5=b1efdbcaefd61c2ba2085d8cb15af541

DOI: 10.1007/978-3-319-18242-1_8
AFFILIATIONS: Max-Planck-Institut fuer Eisenforschung, Duesseldorf, Germany;
Hausdorff Center for Mathematics and Institute for Applied Mathematics, University Bonn, Bonn, Germany;
Department of Mathematical Sciences, Durham University, Durham, United Kingdom
ABSTRACT: We review aspects of pattern formation in plastically deformed single crystals, in particular as described in the investigation of a copper single crystal shear experiment in [DDMR09]. In this experiment, the specimen showed a band-like microstructure consisting of alternating crystal orientations. Such a formation of microstructure is often linked to a lack of convexity in the free energy describing the system. The specific parameters of the observed bands, namely the relative crystal orientation as well as the normal direction of the band layering, are thus compared to the predictions of the theory of kinematically compatible microstructure oscillating between low-energy states of the non-convex energy. We conclude that this theory is suitable to describe the experimentally observed band-like structure. Furthermore, we link these findings to the models used in studies of relaxation and evolution of microstructure.
DOCUMENT TYPE: Article
SOURCE: Scopus

Belde, M., Springer, H., Inden, G., Raabe, D.
Multiphase microstructures via confined precipitation and dissolution of vessel phases: Example of austenite in martensitic steel
(2015) Acta Materialia, 86, pp. 1-14. Cited 10 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84920454236&doi=10.1016%2fj.actamat.2014.11.025&partnerID=40&md5=38869abfe325286bb72cca1c06176041

DOI: 10.1016/j.actamat.2014.11.025
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: We present a novel method to locally control the constitution, morphology, dispersion and transformation behavior of multiphase materials. The approach is based on the targeted, site-specific formation and confined dissolution of precipitated carbides or intermetallic phases. These dispersoids act as "vessels" or "containers" for specific alloying elements forming controlled chemical gradients within the microstructure upon precipitation and subsequent (partial) dissolution at elevated temperatures. The basic processing sequence consists of three subsequent steps, namely: (i) matrix homogenization (conditioning step); (ii) nucleation and growth of the vessel phases (accumulation step); and (iii) (partial) vessel dissolution (dissolution step). The vessel phase method offers multiple pathways to create dispersed microstructures by the variation of plain thermomechanical parameters such as time, temperature and deformation. This local microstructure design enables us to optimize the mechanical property profiles of advanced structural materials such as high strength steels at comparatively lean alloy compositions. The approach is demonstrated on a 11.6Cr-0.32C (wt.%) steel, where by using M23C6 carbides as a vessel phase, Cr and C can be locally enriched so that the thus-lowered martensite start temperature allows the formation of a significant quantity of retained austenite (up to 14 vol.%) of fine dispersion and controlled morphology. The effects of processing parameters on the obtained microstructures are investigated, with a focus on the dissolution kinetics of the vessel carbides. The approach is referred to as vessel microstructure design.

AUTHOR KEYWORDS: Carbides; High strength steels; Microstructure design; Multiphase materials
DOCUMENT TYPE: Article
SOURCE: Scopus

Springer, H., Tasan, C., Raabe, D.
A novel roll-bonding methodology for the cross-scale analysis of phase properties and interactions in multiphase structural materials
(2015) International Journal of Materials Research, 106 (1), pp. 3-14. Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84928395704&doi=10.3139%2f146.111156&partnerID=40&md5=4d8f1af99d469e96c82874f35f40480f

DOI: 10.3139/146.111156
AFFILIATIONS: Max-Planck-Institut Für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: We introduce a new thermo-mechanical approach for producing layered bulk samples built-up from the constituent phases of structural materials for the analysis of multiphase co-deformation phenomena. Following a thermo-mechani- cally controlled roll-bonding procedure, the intrinsic properties of the microstructural components as well as their mutual mechanical interaction and interfacial phenomena can be systematically investigated in highly controlled model microstructures of reduced complexity. The effectiveness of the approach is demonstrated on two examples where austenite or martensite layers, respectively, are introduced in a bulk ferritic matrix, representing in either case components of high strength steels. Special emphasis is laid on how the plasticity of martensite within ferrite, as a key parameter required for understanding and optimising dual phase steels, can be investigated following the proposed approach.
AUTHOR KEYWORDS: Dual-phase steel; Micro-mechanical testing; Microstructure design; Multiphase materials; Steels
DOCUMENT TYPE: Article
SOURCE: Scopus

Kuzmina, M., Ponge, D., Raabe, D.
Grain boundary segregation engineering and austenite reversion turn embrittlement into toughness: Example of a 9 wt.% medium Mn steel
(2015) Acta Materialia, 86, pp. 182-192. Cited 32 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84920764130&doi=10.1016%2fj.actamat.2014.12.021&partnerID=40&md5=a027ab4f97748ea171579fda0d1214c6

DOI: 10.1016/j.actamat.2014.12.021
AFFILIATIONS: Max-Planck Institut für Eisenforschung GmbH, Max-Planck Strainnodatabetae 1, Düsseldorf, Germany
ABSTRACT: We study grain boundary embrittlement in a quenched and tempered Fe-Mn high-purity model martensite alloy using Charpy impact tests and grain boundary characterization by atom probe tomography. We observe that solute Mn directly embrittles martensite grain boundaries while reversion of martensite to austenite at high-angle grain boundaries cleans the interfaces from solute Mn by partitioning the Mn into the newly formed austenite, hence restoring impact toughness. Microalloying with B improves the impact toughness in the quenched state and delays temper embrittlement at 450 °C. Tempering at 600 °C for 1 min significantly improves the impact toughness and further tempering at lower temperature does not cause the embrittlement to return. At higher temperatures, regular austenite nucleation and growth takes place, whereas at lower temperature, Mn directly promotes its growth.
AUTHOR KEYWORDS: 3-d atom probe tomography; Austenite reversion; Embrittlement; Grain boundary segregation; Medium fe-mn alloy

DOCUMENT TYPE: Article
SOURCE: Scopus

Hamza, M., Hatem, T.M., Raabe, D., El-Awady, J.A.
Hydrogen diffusion and segregation in alpha iron ∑ 3 (111) grain boundaries
(2015) ASME International Mechanical Engineering Congress and Exposition, Proceedings (IMECE), 9-2015, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84981218622&doi=10.1115%2fIMECE2015-53118&partnerID=40&md5=259d48a0c9450fd82ab07e98687e9f9a

DOI: 10.1115/IMECE2015-53118
AFFILIATIONS: Department of Mechanical Engineering, Johns Hopkins University, Baltimore, MD, United States;
Department of Mechanical Engineering, British University in Egypt, Cairo, Egypt;
Microstructure Physics and Alloy Design, Department Max-Planck-Institut fur, Eisenforschung GmbH, Dösseldorf, Germany
ABSTRACT: Polycrystalline material generally exhibits degradation in its mechanical properties and shows more tendency for intergranular fracture due to segregation and diffusion of hydrogen on the grain boundaries (GBs). Understanding the parameters affecting the diffusion and binding of hydrogen within GBs will allow enhancing the mechanical properties of the commercial engineering materials and developing interface dominant materials. In practice during forming processes, the coincidence site lattice (CSL) GBs are experiencing deviations from their ideal configurations. Consequently, this will change the atomic structural integrity by superposition of sub-boundary dislocation networks on the ideal CSL interfaces. For this study, the ideal ∑ 3 111 [11 0] GB structure and its angular deviations in BCC iron within the range of Brandon criterion will be studied comprehensively using molecular statics (MS) simulations. The clean GB energy will be quantified, followed by the GB and free surface segregation energies calculations for hydrogen atoms. Rice-Wang model will be used to assess the embrittlement impact variation over the deviation angles. The results showed that the ideal GB structure is having the greatest resistance to embrittlement prior GB hydrogen saturation, while the 3° deviated GB is showing the highest susceptibility to embrittlement. Upon saturation, the 5° deviated GB appears to have the highest resistance instead due to the lowest stability of hydrogen atoms observed in the free surfaces of its simulation cell. Molecular dynamics (MD) simulations are then applied to calculate hydrogen diffusivity within the ideal and deviated GB structure. It is shown that hydrogen diffusivity decreases significantly in the deviated GB models. In addition, the 5° deviated GB is representing the local minimum for diffusivity results suggesting the existence of the highest atomic disorder and excessive secondary dislocation accommodation within this interface.
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Springer, H., Aparicio-Fernandez, R., Duarte, M.J., Zhang, H., Baron, C., Kostka, A., Raabe, D.
Alloy design and processing routes for novel high modulus steels
(2015) PTM 2015 - Proceedings of the International Conference on Solid-Solid Phase Transformations in Inorganic Materials 2015, p. 981.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84962762490&partnerID=40&md5=6bd00c78d76b1ce4e22ab1706d985463

AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, Germany
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Kim, J.-H., Kim, B.K., Kim, D.-I., Choi, P.-P., Raabe, D., Yi, K.-W.
The role of grain boundaries in the initial oxidation behavior of austenitic stainless steel containing alloyed Cu at 700°C for advanced thermal power plant applications
(2015) Corrosion Science, 96, pp. 52-66. Cited 9 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84929503997&doi=10.1016%2fj.corsci.2015.03.014&partnerID=40&md5=fb8c0ec90545aada4558b1c1ab20f431

DOI: 10.1016/j.corsci.2015.03.014
AFFILIATIONS: High Temperature Energy Materials Research Center, Korea Institute of Science and Technology, Hwarangno 14-gil 5, Seongbuk-gu, Seoul, South Korea;
Department of Materials Science and Engineering, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul, South Korea;
Department of Microstructure Physics and Alloy Design, Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, Düsseldorf, Germany
ABSTRACT: The role of grain boundaries during the early stages of oxidation in austenitic stainless steels containing alloyed Cu was investigated using APT, TEM, EBSD, EPMA, and XRD. The oxidation experiments were performed at 700°C in air with 20% water vapor. Within 4μm from the grain boundaries, the oxide layer exhibits a dual-layer structure consisting of a thin Fe-rich spinel oxide on a protective Cr<inf>2</inf>O<inf>3</inf> oxide. Away from the grain boundaries, non-protective spinel oxide layers are formed as the outer and inner oxide layers. A critical grain size that prevents the formation of fast-growing spinel oxides is discussed. © 2015 Elsevier Ltd.
AUTHOR KEYWORDS: A. stainless steel; B. SEM; B. TEM; C. oxidation
DOCUMENT TYPE: Article
SOURCE: Scopus

Koyama, M., Bashir, A., Rohwerder, M., Merzlikin, S.V., Akiyama, E., Tsuzaki, K., Raabe, D.
Spatially and kinetically resolved mapping of hydrogen in a twinning-induced plasticity steel by use of Scanning Kelvin Probe Force Microscopy
(2015) Journal of the Electrochemical Society, 162 (12), pp. C638-C647. Cited 16 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84942570902&doi=10.1149%2f2.0131512jes&partnerID=40&md5=7c6c359c28ce829f764dfdb7115cb633

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AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Department of Mechanical Engineering, Kyushu University, Nishi-ku, Fukuoka, Japan;
Christian Doppler Laboratory for Diffusion and Segregation Mechanisms, Düsseldorf, Germany;
National Institute for Materials Science, Ibaraki, Japan
ABSTRACT: The hydrogen distribution in a hydrogen-charged Fe-18Mn-1.2C (wt%) twinning-induced plasticity austenitic steel was studied by Scanning Kelvin Probe Force Microscopy (SKPFM). We observed that 1-2 days after the hydrogen-charging, hydrogen showed a higher activity at twin boundaries than inside the matrix. This result indicates that hydrogen at the twin boundaries is diffusible at room temperature, although the twin boundaries act as deeper trap sites compared to typical diffusible hydrogen trap sites such as dislocations. After about 2 weeks the hydrogen activity in the twin boundaries dropped and was indistinguishable from that in the matrix. These SKPFM results were supported by thermal desorption spectrometry and scanning electron microscopic observations of deformation-induced surface cracking parallel to deformation twin boundaries. With this joint approach, two main challenges in the field of hydrogen embrittlement research can be overcome, namely, the detection of hydrogen with high local and chemical sensitivity and the microstructure-dependent and spatially resolved

observation of the kinetics of hydrogen desorption. © 2015 The Electrochemical Society.
DOCUMENT TYPE: Article
SOURCE: Scopus

Zhang, H., Pradeep, K.G., Mandal, S., Ponge, D., Springer, H., Raabe, D.
Dynamic strain-induced transformation: An atomic scale investigation
(2015) Scripta Materialia, 109, art. no. 10722, pp. 23-27. Cited 10 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84940186744&doi=10.1016%2fj.scriptamat.2015.07.010&partnerID=40&md5=5332918f2c176991899e20e25b8f21a8

DOI: 10.1016/j.scriptamat.2015.07.010
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck Str 1, Düsseldorf, Germany;
Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, Aachen, Germany
ABSTRACT: Phase transformations provide the most versatile access to the design of complex nanostructured alloys in terms of grain size, morphology, local chemical constitution etc. Here we study a special case of deformation induced phase transformation. More specifically, we investigate the atomistic mechanisms associated with dynamic strain-induced transformation (DSIT) in a dual-phased multicomponent iron-based alloy at high temperatures. DSIT phenomena and the associated secondary phase nucleation were observed at atomic scale using atom probe tomography. The obtained local chemical composition was used for simulating the nucleation process which revealed that DSIT, occurring during load exertion, proceeds by a diffusion-controlled nucleation process. © 2015 Acta Materialia Inc.
AUTHOR KEYWORDS: Diffusion; Nucleation; Phase transformations; Thermodynamics; Three-dimensional atom probe (3DAP)
DOCUMENT TYPE: Article
SOURCE: Scopus

Cereceda, D., Diehl, M., Roters, F., Shanthraj, P., Raabe, D., Perlado, J.M., Marian, J.
Linking atomistic, kinetic Monte Carlo and crystal plasticity simulations of single-crystal tungsten strength
(2015) GAMM Mitteilungen, 38 (2), pp. 213-227.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84941054217&doi=10.1002%2fgamm.201510012&partnerID=40&md5=107947bb1a47155160faf76b3d930de3

DOI: 10.1002/gamm.201510012
AFFILIATIONS: Materials Science and Engineering Department, University of California, Los Angeles, CA, United States;
Instituto de Fusiõn Nuclear, Universidad Politécnica de Madrid, Madrid, Spain;
Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, Livermore, CA, United States;
Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
Aachen Institute for Advanced Study in Computational Engineering Science, RWTH Aachen University, Schinkelstraße 2, Aachen, Germany
ABSTRACT: Understanding and improving the mechanical properties of tungsten is a critical task for the materials fusion energy program. The plastic behavior in body-centered cubic (bcc) metals like tungsten is governed primarily by screw dislocations on the atomic scale and by ensembles and interactions of dislocations at larger scales. Modeling this behavior requires the application of methods capable of resolving each relevant scale. At the small scale, atomistic methods are used to study single dislocation properties, while at the coarse-scale, continuum models are used to cover the interactions between dislocations. In this work we present a multiscale model that comprises atomistic, kinetic Monte Carlo

(kMC) and continuum-level crystal plasticity (CP) calculations. The function relating dislocation velocity to applied stress and temperature is obtained from the kMC model and it is used as the main source of constitutive information into a dislocation-based CP framework. The complete model is used to perform material point simulations of single-crystal tungsten strength. We explore the entire crystallographic orientation space of the standard triangle. Non-Schmid effects are inlcuded in the model by considering the twinning-antitwinning (T/AT) asymmetry in the kMC calculations. We consider the importance of ?111?{110} and 111 {112} slip systems in the homologous temperature range from 0.08T<inf>m</inf> to 0.33T<inf>m</inf>, where T<inf>m</inf> =3680 K is the melting point in tungsten.
AUTHOR KEYWORDS: bcc; Crystal plasticity; multiscale; non-Schmid; screw dislocation; single crystal; slip; tungsten; uniaxial
DOCUMENT TYPE: Article
SOURCE: Scopus

Cojocaru-Mirédin, O., Fu, Y., Kostka, A., Sáez-Araoz, R., Beyer, A., Knaub, N., Volz, K., Fischer, C.-H., Raabe, D.
Interface engineering and characterization at the atomic-scale of pure and mixed ion layer gas reaction buffer layers in chalcopyrite thin-film solar cells
(2015) Progress in Photovoltaics: Research and Applications, 23 (6), pp. 705-716. Cited 4 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84928634715&doi=10.1002%2fpip.2484&partnerID=40&md5=6f17d86c9130df2924a314115a932b72

DOI: 10.1002/pip.2484
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany;
Helmholtz-Zentrum Berlin für Materialien, Energie Institute of Heterogeneous Materials Systems, Hahn-Meitner-Platz 1, Berlin, Germany;
Philipps-Universität Marburg, Hans-Meerwein-Straße, Marburg, Germany
ABSTRACT: In this work, we investigate the p-n junction region for two different buffer/Cu(In,Ga)(Se,S)<inf>2</inf> (CIGSSe) samples having different conversion efficiencies (the cell with pure In<inf>2</inf>S<inf>3</inf> buffer shows a lower efficiency than the nano-ZnS/In<inf>2</inf>S<inf>3</inf> buffered one). To explain the better efficiency of the sample with nano-ZnS/In<inf>2</inf>S<inf>3</inf> buffer layer, combined transmission electron microscopy, atom probe tomography, and X-ray photoelectron spectroscopy studies were performed. In the pure In<inf>2</inf>S<inf>3</inf> buffered sample, a CuIn<inf>3</inf>Se<inf>5</inf> ordered-defect compound is observed at the CIGSSe surface, whereas in the nano-ZnS/In<inf>2</inf>S<inf>3</inf> buffered sample no such compound is detected. The absence of an ordered-defect compound in the latter sample is explained either by the presence of the ZnS nanodots, which may act as a barrier layer against Cu diffusion in CIGSSe hindering the formation of CuIn<inf>3</inf>Se<inf>5</inf>, or by the presence of Zn at the CIGSSe surface, which may disturb the formation of this ordered-defect compound. In the nano-ZnS/In<inf>2</inf>S<inf>3</inf> sample, Zn was found in the first monolayers of the absorber layer, which may lead to a downward band bending at the surface. This configuration is very stable (Fermi level pinning at the conduction band, as observed for Cd in Cu(In,Ga)Se<inf>2</inf>) and reduces the recombination rate at the interface. This effect may explain why the sample with ZnS nanodots possesses a higher efficiency. This work demonstrates the capability of correlative transmission electron microscopy, atom probe tomography, and X-ray photoelectron spectroscopy studies in investigating buried interfaces. The study provides essential information for understanding and modeling the p-n junction at the nanoscale in CIGSSe solar cells. Copyright © 2014 John Wiley & Sons, Ltd.

AUTHOR KEYWORDS: atom probe tomography; ILGAR; In<inf>2</inf>S<inf>3</inf> alternative buffer layer; ordered-defect compound; transmission electron microscopy; X-ray photoelectron spectroscopy; ZnS nanodots
DOCUMENT TYPE: Article
SOURCE: Scopus

Lübke, A., Enax, J., Loza, K., Prymak, O., Gaengler, P., Fabritius, H.-O., Raabe, D., Epple, M.
Dental lessons from past to present: Ultrastructure and composition of teeth from plesiosaurs, dinosaurs, extinct and recent sharks
(2015) RSC Advances, 5 (76), pp. 61612-61622. Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84937501356&doi=10.1039%2fc5ra11560d&partnerID=40&md5=ea33db2599c2e7c5f81db3e888f8125c

DOI: 10.1039/c5ra11560d
AFFILIATIONS: Institute of Inorganic Chemistry, Center for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, Universitaetsstr. 5-7, Essen, Germany;
ORMED, Institute for Oral Medicine, University of Witten/Herdecke, Alfred-Herrhausen-Straße 45, Witten, Germany;
Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: Teeth represent the hardest tissue in vertebrates and appear very early in their evolution as an ancestral character of the Eugnathostomata (true jawed vertebrates). In recent vertebrates, two strategies to form and mineralize the outermost functional layer have persisted. In cartilaginous fish, the enameloid is of ectomesenchymal origin with fluoroapatite as the mineral phase. All other groups form enamel of ectodermal origin using hydroxyapatite as the mineral phase. The high abundance of teeth in the fossil record is ideal to compare structure and composition of teeth from extinct groups with those of their recent successors to elucidate possible evolutionary changes. Here, we studied the chemical composition and the microstructure of the teeth of six extinct shark species, two species of extinct marine reptiles and two dinosaur species using high-resolution chemical and microscopic methods. Although many of the ultrastructural features of fossilized teeth are similar to recent ones (especially for sharks where the ultrastructure basically did not change over millions of years), we found surprising differences in chemical composition. The tooth mineral of all extinct sharks was fluoroapatite in both dentin and enameloid, in sharp contrast to recent sharks where fluoroapatite is only found in enameloid. Unlike extinct sharks, recent sharks use hydroxyapatite as mineral in dentin. Most notably and hitherto unknown, all dinosaur and extinct marine reptile teeth contained fluoroapatite as mineral in dentin and enamel. Our results indicate a drastic change in the tooth mineralization strategy especially for terrestrial vertebrates that must have set in after the cretaceous period. Possibly, this is related to hitherto unconsidered environmental changes that caused unfavourable conditions for the use of fluoroapatite as tooth mineral.
DOCUMENT TYPE: Article
SOURCE: Scopus

Peng, Z., Povstugar, I., Matuszewski, K., Rettig, R., Singer, R., Kostka, A., Choi, P.-P., Raabe, D.
Effects of Ru on elemental partitioning and precipitation of topologically close-packed phases in Ni-based superalloys
(2015) Scripta Materialia, 101, pp. 44-47. Cited 13 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84924580467&doi=10.1016%2fj.scriptamat.2015.01.014&partnerID=40&md5=1802b786a1872d3ab2997e70db5d6332

DOI: 10.1016/j.scriptamat.2015.01.014
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Department of Microstructure Physics and Alloy Design, Max-Planck-Str. 1, Düsseldorf, Germany;
University of Erlangen-Nuremberg FAU, Department of Materials Science and Engineering, Institute of Science and Technology of Metals WTM, Martensstr. 5, Erlangen, Germany
ABSTRACT: Two Ni-based superalloys (one Ru-free and one containing 1 at.% Ru) were comparatively studied by Atom Probe Tomography and complimentary techniques. Ru addition impedes precipitation of the σ phase at 950 °C. Ru partitions nearly equally to the γ and σ phase. Neither reverse elemental partitioning nor destabilization of the γ' phase is detected when adding Ru. We propose an increase in the γ/σ lattice misfit caused by Ru as a major reason for impeded nucleation of the σ phase. © 2015 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
AUTHOR KEYWORDS: Atom Probe Tomography; Precipitation; Superalloy; Topologically close-packed phases
DOCUMENT TYPE: Article
SOURCE: Scopus

Parsa, A.B., Wollgramm, P., Buck, H., Somsen, C., Kostka, A., Povstugar, I., Choi, P.-P., Raabe, D., Dlouhy, A., Müller, J., Spiecker, E., Demtroder, K., Schreuer, J., Neuking, K., Eggeler, G.
Advanced scale bridging microstructure analysis of single crystal Ni-base superalloys
(2015) Advanced Engineering Materials, 17 (2), pp. 216-230. Cited 22 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84920892735&doi=10.1002%2fadem.201400136&partnerID=40&md5=6b099dbd8b86630411c84436fbc4ad94

DOI: 10.1002/adem.201400136
AFFILIATIONS: Institut für Werkstoffe, Ruhr-Universität Bochum, Universitätstr. 150, Bochum, Germany;
Max-Planck-Institut für Eisenforschung, Max Planck Str. 1, Dusseldorf, Germany;
Institute of Physics of Materials, Zizkova 22, Brno, Czech Republic;
Center for Nanoanalysis and Electron Microscopy, Friedrich-Alexander Universität Erlangen-Nürnberg, Cauerstr. 6, Erlangen, Germany;
Institut für Geowissenschaften, Ruhr-Universität Bochum, Universitätstr. 150, Bochum, Germany
ABSTRACT: In the present work, we show how conventional and advanced mechanical, chemical, and microstructural methods can be used to characterize cast single crystal Ni-base superalloy (SX) plates across multiple length scales. Two types of microstructural heterogeneities are important, associated with the castmicrostructure (dendrites (D) and interdendritic (ID) regions - large scale heterogeneity) and with the well-known γ/γ′ microstructure (small scale heterogeneity). Using electron probe microanalysis (EPMA), we can showthat elements such as Re, Co, andCr partition to the dendrites while ID regions contain more Al, Ta, and Ti. Analytical transmission electron microscopy and atom probe tomography (APT) show that Al, Ta, and Ti partition to the γ′ cubes while g channels show higher concentrations of Co, Cr, Re, andW.We can combine large scale (EPMA) and small-scale analytical methods (APT) to obtain reasonable estimates for γ′ volume fractions in the dendrites and in the ID regions. The chemical and mechanical properties of the SX plates studied in the present work are homogeneous, when they are determined from volumes with dimensions, which are significantly larger than the dendrite spacing. For the SX plates (140mm x 100mm x 20mm) studied in the present work this holds for the average chemical composition as well as for elastic behavior and local creep properties. We highlight the potential of HRTEM and APT to contribute to a better understanding of the role of dislocations during coarsening of the γ′ phase and the effect of cooling rates after high temperature exposure on the microstructure. © 2014 Wiley-VCH Verlag GmbH & Co. KGaA.

DOCUMENT TYPE: Article
SOURCE: Scopus

Raabe, D.
Recovery and Recrystallization: Phenomena, Physics, Models, Simulation
(2014) Physical Metallurgy: Fifth Edition, 1, pp. 2291-2397. Cited 11 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84942645800&doi=10.1016%2fB978-0-444-53770-6.00023-X&partnerID=40&md5=a089cb772c4f02d9c65498c72a75f024

DOI: 10.1016/B978-0-444-53770-6.00023-X
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
ABSTRACT: Recovery, recrystallization and grain growth are among the most important metallurgical heat treatment processes to soften cold worked metals and design desired microstructures and textures. Specifically the reduction in grain size can be efficiently achieved by recrystallization. While plastic cold working increases the stored energy of metals, mainly through dislocation accumulation, recovery and specifically recrystallization lead to it reduction. While recovery describes the gradual re-ordering and annihilation of the stored dislocations, primary recrystallization proceeds discontinuously by the formation and motion of high angle grain boundaries which discontinuously sweep the deformation substructure. Grain growth describes the process of competitive capillary driven coarsening of the average grain size. This chapter reviews the main mechanisms, lattice defects, and driving forces associated with recovery, recrystallization and grain growth and provides an introduction to the simulation of these phenomena.
AUTHOR KEYWORDS: Cellular automata; Grain boundary; Grain growth; Nucleation; Potts model; Recovery; Recrystallization; Simulation; Subgrain coarsening
DOCUMENT TYPE: Book Chapter
SOURCE: Scopus

Povstugar, I., Choi, P.-P., Neumeier, S., Bauer, A., Zenk, C.H., Göken, M., Raabe, D.
Elemental partitioning and mechanical properties of Ti- and Ta-containing Co-Al-W-base superalloys studied by atom probe tomography and nanoindentation
(2014) Acta Materialia, 78, pp. 78-85. Cited 46 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84904225970&doi=10.1016%2fj.actamat.2014.06.020&partnerID=40&md5=360f09b3818aba9ed060a29a5388dc0a

DOI: 10.1016/j.actamat.2014.06.020
AFFILIATIONS: Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Materials Science and Engineering, Institute i, Martensstr. 5, 91058 Erlangen, Germany
ABSTRACT: Elemental partitioning and hardness in Ti- and Ta-containing Co-base superalloys, strengthened by γ′-Co3(Al, W) precipitates, have been studied by local measurements. Using atom probe tomography, we detect strong partitioning of W (partitioning coefficients from 2.4 to 3.4) and only slight partitioning of Al (partitioning coefficients ≤1.1) to the γ′-Co3(Al, W) phase. Al segregates to the γ/γ′ phase boundaries, whereas W is depleted at the γ side of the boundaries after aging at 900 °C and slow air cooling. This kind of Al segregation and W depletion is much less pronounced when water quenching is applied. As a result, these effects are considered to be absent at high temperatures and therefore should not influence the creep properties. Ti and Ta additions are found to strongly partition to the γ′ phase and greatly increase the γ′ volume fraction. Our results indicate that the alloying elements Al, W, Ti and Ta all occupy the

B sublattice of the A 3B structure (L12 type) and affect the partitioning behavior of each other. Nanoindentation measurements show that Ta also increases the hardness of the γ′ phase, while the hardness of the γ channels remains nearly constant in all alloys. The change in hardness of the γ′ phase can be ascribed to the substitution of Al and W atoms by Ti and/or Ta.
AUTHOR KEYWORDS: Atom probe tomography (APT); Cobalt-base superalloys; Nanoindentation
DOCUMENT TYPE: Article
SOURCE: Scopus

Mattern, N., Han, J.H., Pradeep, K.G., Kim, K.C., Park, E.M., Kim, D.H., Yokoyama, Y., Raabe, D., Eckert, J.
Structure of rapidly quenched (Cu0.5Zr0.5) 100-xAgx alloys (x = 0-40 at.%)
(2014) Journal of Alloys and Compounds, 607, pp. 285-290. Cited 8 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84900411894&doi=10.1016%2fj.jallcom.2014.04.047&partnerID=40&md5=d4ba6440989ea3c789923cb5b38d8014

DOI: 10.1016/j.jallcom.2014.04.047
AFFILIATIONS: IFW Dresden, Institute for Complex Materials, Helmholtzstr. 20, 01069 Dresden, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany;
Center for Non-crystalline Materials, Yonsei University, 134 Shinchon-dong, Seodaemun-ku, Seoul 120-749, South Korea;
Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan;
TU Dresden, Institute of Materials Science, Helmholtzstr. 7, 01069 Dresden, Germany
ABSTRACT: The influence of Ag addition on the microstructure of rapidly quenched (Cu0.5Zr0.5)100-xAg x melts was investigated (x = 0-40 at.%). Fully glassy alloys were obtained for 0 ≤ x ≤ 20 at.% Ag, which are characterized by a homogeneous microstructure without any indication of phase separation. For 30 ≤ x ≤ 40 at.% Ag a composite structure is formed consisting of fcc-Ag nano-crystallites 5 nm in size and an amorphous matrix phase Cu40Zr40Ag 20. With higher Ag-content the volume fraction of the fcc-Ag phase becomes increased mainly due to crytal growth during quenching. The primary formation of fcc-Ag for 30 ≤ x ≤ 40 at.% Ag is confirmed by the analysis of the microstructure of mold cast bulk samples which were fully crystalline. From the experimental results we conclude that the miscibility gap of the liquid phase of the ternary Ag-Cu-Zr system may occur only for x > 40 at.% Ag. For the bulk glass forming quaternary Cu40Zr40Al 10Ag10 alloy a homogeneous element distribution is observed in accordance with the microstructure of ternary (Cu 0.5Zr0.5)100-xAg x glasses (x = 10, 20 at.%).

AUTHOR KEYWORDS: Ag-Cu-Zr; Atom Probe Tomography; Metallic glass; Phase separation
DOCUMENT TYPE: Article
SOURCE: Scopus

Li, Y., Raabe, D., Herbig, M., Choi, P.-P., Goto, S., Kostka, A., Yarita, H., Borchers, C., Kirchheim, R.
Segregation stabilizes nanocrystalline bulk steel with near theoretical strength
(2014) Physical Review Letters, 113 (10), art. no. 106104, . Cited 63 times.
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DOI: 10.1103/PhysRevLett.113.106104

AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck-Strasse 1, Düsseldorf, Germany;
Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, Göttingen, Germany;
Akita University, Tegata Gakuencho, Akita, Japan;
Suzuki Metal Industry Co. LTD., Narashino, Chiba, Japan
ABSTRACT: Grain refinement through severe plastic deformation enables synthesis of ultrahigh-strength nanostructured materials. Two challenges exist in that context: First, deformation-driven grain refinement is limited by dynamic dislocation recovery and crystal coarsening due to capillary driving forces; second, grain boundary sliding and hence softening occur when the grain size approaches several nanometers. Here, both challenges have been overcome by severe drawing of a pearlitic steel wire (pearlite: lamellar structure of alternating iron and iron carbide layers). First, at large strains the carbide phase dissolves via mechanical alloying, rendering the initially two-phase pearlite structure into a carbon-supersaturated iron phase. This carbon-rich iron phase evolves into a columnar nanoscaled subgrain structure which topologically prevents grain boundary sliding. Second, Gibbs segregation of the supersaturated carbon to the iron subgrain boundaries reduces their interface energy, hence reducing the driving force for dynamic recovery and crystal coarsening. Thus, a stable cross-sectional subgrain size <10nm is achieved. These two effects lead to a stable columnar nanosized grain structure that impedes dislocation motion and enables an extreme tensile strength of 7 GPa, making this alloy the strongest ductile bulk material known.
DOCUMENT TYPE: Article
SOURCE: Scopus

Jia, N., Raabe, D., Zhao, X.
Texture and microstructure evolution during non-crystallographic shear banding in a plane strain compressed Cu-Ag metal matrix composite
(2014) Acta Materialia, 76, pp. 238-251. Cited 11 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84902028820&doi=10.1016%2fj.actamat.2014.05.036&partnerID=40&md5=a00d58707e3f75ee1e655da5b031d2ce

DOI: 10.1016/j.actamat.2014.05.036
AFFILIATIONS: Key Laboratory for Anisotropy and Texture of Materials (MOE), Northeastern University, Shenyang 110819, China;
Max-Planck-Institut für Eisenforschung, D-40237 Düsseldorf, Germany
ABSTRACT: We studied the texture and microstructure evolution in a plane strain compressed Cu-Ag metal matrix composite (MMC) with a heterophase microstructure using crystal plasticity finite element simulations. Lattice reorientations induced by both crystallographic (dislocation slip and twinning) and non-crystallographic (shear banding) mechanisms are addressed. First, simulations on a polycrystalline composite are made. Quite similar texture trends are observed for the composites and for the individual single-phase materials, namely, copper-type texture components in the Cu phase and brass-type texture components in the Ag phase. This result differs from experimental data that show less copper-type and more brass-type textures in both phases for the composite materials. To explore co-deformation mechanisms that lead to the specific crystallographic textures in the MMC, bicrystal simulations for the composite with specific initial orientation combinations are performed. The bicrystal simulations reproduce the experimentally observed trends of texture evolution in the respective phases of the composite, indicating that the localized stress and strain fields as well as the co-deformation mechanisms within the actual heterophase microstructure are well captured. The modeling shows that to accommodate plastic deformation between adjacent phases in the bicrystals, pronounced shear bands are triggered by stress concentration at the hetero-interfaces. With further deformation the bands penetrate through the phase boundaries and lead to larger lattice rotations. The simulations

confirm that the shear banding behavior in heterophase composites is different from that in single-phase metals and the texture evolution in composite materials is strongly influenced by the starting texture, the local constraints exerted from the phase boundaries and the constitutive properties of the abutting phases.
AUTHOR KEYWORDS: Crystal plasticity finite element analysis; Metal matrix composites; Shear band; Texture
DOCUMENT TYPE: Article
SOURCE: Scopus

Millán, J., Sandlöbes, S., Al-Zubi, A., Hickel, T., Choi, P., Neugebauer, J., Ponge, D., Raabe, D.
Designing Heusler nanoprecipitates by elastic misfit stabilization in Fe-Mn maraging steels
(2014) Acta Materialia, 76, pp. 94-105. Cited 25 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84901905564&doi=10.1016%2fj.actamat.2014.05.016&partnerID=40&md5=de97b1c08a4eefd90f24527d57627041

DOI: 10.1016/j.actamat.2014.05.016
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Department for Microstructure Physics and Alloy Design, Max-Planck-Str. 1, 40477 Düsseldorf, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Department for Computational Materials Design, Max-Planck-Str. 1, 40477 Düsseldorf, Germany;
Universidad Simón Bolívar, Departamento de Ciencia de Los Materiales, Valle de Sartenejas, Baruta 1086, Estado-Miranda, Caracas, Venezuela;
Peter Grünberg Institut, Institute of Advanced Simulation, JARA, D-52425 Jülich, Germany
ABSTRACT: B2 NiMn and Ni2MnAl Heusler nanoprecipitates are designed via elastic misfit stabilization in Fe-Mn maraging steels by combining transmission electron microscopy (TEM) correlated atom probe tomography (APT) with ab initio simulations. Guided by these predictions, the Al content of the alloys is systematically varied, and the influence of the Al concentration on structure stability, size and distribution of precipitates formed during ageing at 450 °C is studied using scanning electron microscopy-electron backscatter diffraction, TEM and APT. Specifically, the Ni2MnAl Heusler nanoprecipitates exhibit the finest sizes and highest dispersion and hence lead to significant strengthening. The formation of the different types of precipitates and their structure, size, dispersion and effect on the mechanical properties of the alloys are discussed.
AUTHOR KEYWORDS: Ab initio predictions; Atom probe tomography; Heusler nanoprecipitates; Maraging TRIP steels; Transmission electron microscopy
DOCUMENT TYPE: Article
SOURCE: Scopus

Zhang, H., Ponge, D., Raabe, D.
Designing quadplex (four-phase) microstructures in an ultrahigh carbon steel
(2014) Materials Science and Engineering A, 612, pp. 46-53. Cited 5 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84903529741&doi=10.1016%2fj.msea.2014.06.023&partnerID=40&md5=bbea4770238561dc2b2ffcaa473223dc

DOI: 10.1016/j.msea.2014.06.023
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck Str 1, 40237 Düsseldorf, Germany
ABSTRACT: Here we present an approach to design a ferrite-based quadplex microstructure (ferrite/martensite/carbide/austenite) using a lean alloyed Mn-Si-Cr-Al ultrahigh carbon steel. The material has 1500MPa tensile strength and 11% elongation. The thermomechanical processing includes two

main steps, namely, first, the formation of a ferrite plus carbide duplex microstructure by warm rolling below Ae1; and second, annealing just above Ae1 for a short time (~20min). The quadplex microstructure consists of 57vol% ultrafine ferrite (mean grain size ~1.5μm), 29vol% martensite, 12vol% spherical carbide and 2vol% austenite. Fracture analysis after tensile deformation reveals a mixed ductile and brittle failure mode without necking. Scanning electron microscopy (SEM), electron backscatter diffraction (EBSD) and dilatometry tests were conducted to map the microstructure characteristics and the contribution of each phase to the overall deformation. © 2014 Elsevier B.V.
AUTHOR KEYWORDS: Electron backscatter diffraction (EBSD); Quadplex microstructure; Steel; Strain; Thermomechanical processing
DOCUMENT TYPE: Article
SOURCE: Scopus

Liu, B., Raabe, D., Roters, F., Arsenlis, A.
Interfacial dislocation motion and interactions in single-crystal superalloys
(2014) Acta Materialia, 79, pp. 216-233. Cited 17 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84905602653&doi=10.1016%2fj.actamat.2014.06.048&partnerID=40&md5=58b4c5caa3a24c2b8adec827c4656be4

DOI: 10.1016/j.actamat.2014.06.048
AFFILIATIONS: Lawrence Livermore National Laboratory, Livermore, CA 94550, United States;
Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany
ABSTRACT: The early stage of high-temperature low-stress creep in single-crystal superalloys is characterized by the rapid development of interfacial dislocation networks. Although interfacial motion and dynamic recovery of these dislocation networks have long been expected to control the subsequent creep behavior, direct observation and hence in-depth understanding of such processes has not been achieved. Incorporating recent developments of discrete dislocation dynamics models, we simulate interfacial dislocation motion in the channel structures of single-crystal superalloys, and investigate how interfacial dislocation motion and dynamic recovery are affected by interfacial dislocation interactions and lattice misfit. Different types of dislocation interactions are considered: self, collinear, coplanar, Lomer junction, glissile junction, and Hirth junction. The simulation results show that strong dynamic recovery occurs due to the short-range reactions of collinear annihilation and Lomer junction formation. The misfit stress is found to induce and accelerate dynamic recovery of interfacial dislocation networks involving self-interaction and Hirth junction formation, but slow down the steady interfacial motion of coplanar and glissile junction forming dislocation networks. The insights gained from these simulations on high-temperature low-stress creep of single-crystal superalloys are also discussed. © 2014 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
AUTHOR KEYWORDS: Dislocation dynamics; Dislocation interactions; High-temperature low-stress creep; Interfacial dislocation motion; Superalloys
DOCUMENT TYPE: Article
SOURCE: Scopus

Wang, M.-M., Tasan, C.C., Ponge, D., Kostka, A., Raabe, D.
Smaller is less stable: Size effects on twinning vs. transformation of reverted austenite in TRIP-maraging steels
(2014) Acta Materialia, 79, pp. 268-281. Cited 45 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84905776834&doi=10.1016%2fj.actamat.2014.07.020&partnerID=40&md5=8f0a531f74df7c832066432e984198c1

DOI: 10.1016/j.actamat.2014.07.020

AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany
ABSTRACT: Steels containing reverted nanoscale austenite (γRN) islands or films dispersed in a martensitic matrix show excellent strength, ductility and toughness. The underlying microstructural mechanisms responsible for these improvements are not yet understood, but are observed to be strongly connected to the γRN island or film size. Two main micromechanical effects are conceivable in this context, namely: (i) interaction of γRN with microcracks from the matrix (crack blunting or arresting); and (ii) deformation-induced phase transformation of γRN to martensite (TRIP effect). The focus here is on the latter phenomenon. To investigate size effects on γRN transformation independent of other factors that can influence austenite stability (composition, crystallographic orientation, defect density, surrounding phase, etc.), a model (TRIP-maraging steel) microstructure is designed with support from diffusion simulations (using DICTRA software) to have the same, homogeneous chemical composition in all γRN grains. Characterization is conducted by in-situ tension and bending experiments in conjunction with high-resolution electron backscatter diffraction mapping and scanning electron microscopy imaging, as well as post-mortem transmission electron microscopy and synchrotron X-ray diffraction analysis. Results reveal an unexpected "smaller is less stable" effect due to the size-dependent competition between mechanical twinning and deformation-induced phase transformation.
AUTHOR KEYWORDS: In-situ EBSD; Reverted austenite; Size effect; TRIP-maraging steel; Twinning
DOCUMENT TYPE: Article
SOURCE: Scopus

Hickel, T., Sandlöbes, S., Marceau, R.K.W., Dick, A., Bleskov, I., Neugebauer, J., Raabe, D.
Impact of nanodiffusion on the stacking fault energy in high-strength steels
(2014) Acta Materialia, 75, pp. 147-155. Cited 21 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84901384777&doi=10.1016%2fj.actamat.2014.04.062&partnerID=40&md5=3dcadcc407e7b19b4103bcf6fcd13b2b

DOI: 10.1016/j.actamat.2014.04.062
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany
ABSTRACT: A key requirement of modern steels - the combination of high strength and high deformability - can best be achieved by enabling a local adaptation of the microstructure during deformation. A local hardening is most efficiently obtained by a modification of the stacking sequence of atomic layers, resulting in the formation of twins or martensite. Combining ab initio calculations with in situ transmission electron microscopy, we show that the ability of a material to incorporate such stacking faults depends on its overall chemical composition and, importantly, the local composition near the defect, which is controlled by nanodiffusion. Specifically, the role of carbon for the stacking fault energy in high-Mn steels is investigated. Consequences for the long-term mechanical properties and the characterisation of these materials are discussed.
AUTHOR KEYWORDS: Carbon; DFT; In situ TEM; Iron; Stacking fault energy
DOCUMENT TYPE: Article
SOURCE: Scopus

Guo, W., Jägle, E.A., Choi, P.-P., Yao, J., Kostka, A., Schneider, J.M., Raabe, D.
Erratum: Shear-induced mixing governs codeformation of crystalline-amorphous nanolaminates (Physical Review Letters (2014) 113 (035501))
(2014) Physical Review Letters, 113 (6), art. no. 069903, . Cited 8 times.

https://www.scopus.com/inward/record.uri?eid=2-s2.0-84906070935&doi=10.1103%2fPhysRevLett.113.069903&partnerID=40&md5=7cafbdedb1c7242f8952f02ef09eeeae

DOI: 10.1103/PhysRevLett.113.069903
DOCUMENT TYPE: Erratum
SOURCE: Scopus

Haley, D., Merzlikin, S.V., Choi, P., Raabe, D.
Atom probe tomography observation of hydrogen in high-Mn steel and silver charged via an electrolytic route
(2014) International Journal of Hydrogen Energy, 39 (23), pp. 12221-12229. Cited 16 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84904719528&doi=10.1016%2fj.ijhydene.2014.05.169&partnerID=40&md5=8a7c91f0aa45e3feacfb263f2d27daef

DOI: 10.1016/j.ijhydene.2014.05.169
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, D-40237 Düsseldorf, Germany
ABSTRACT: We investigate an electrolytic route for hydrogen charging of metals and its detection in Atom Probe Tomography (APT) experiments. We charge an austenitic Fe-30Mn-8Al-1.2C (wt.%) weight reduced high-Mn steel and subsequently demonstrate the detectability of deuterium in an APT experiment. The experiment is repeated with a deposited Ag film upon an APT tip of a high-Mn steel. It is shown that a detectable deuterium signal can be seen in the high-Mn steel, and a D:H ratio of 0.84 can be reached in Ag films. Additionally, it was found that the predicted time constraint on detectability of D in APT was found to be lower than predicted by bulk diffusion for the high-Mn steel.
AUTHOR KEYWORDS: Atom probe; Electrolytic charging; High-Mn steel
DOCUMENT TYPE: Article
SOURCE: Scopus

Zhang, H., Ponge, D., Raabe, D.
Superplastic Mn-Si-Cr-C duplex and triplex steels: Interaction of microstructure and void formation
(2014) Materials Science and Engineering A, 610, pp. 355-369. Cited 3 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84902210040&doi=10.1016%2fj.msea.2014.05.061&partnerID=40&md5=9245500e31b7fa7dcfe0b23922bc237f

DOI: 10.1016/j.msea.2014.05.061
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: Duplex and triplex microstructures consisting initially of ferrite plus carbide or of martensite, ferrite plus carbide, respectively, can undergo strain induced austenite formation during superplastic deformation at 30K below Ae1 (Ae1: equilibrium pearlite-austenite transformation temperature) and low strain rate (e.g. 2×10-3s-1). The effect leads to excellent superplasticity of the materials (elongation ~500%, flow stress <50MPa) through fine austenite grains (~10μm). Using a deformation temperature just below Ae1 leads to a weak driving force for both, carbide dissolution and austenite formation. Thereby a sufficient volume fraction of carbides (1-2μm, 15vol%) is located at austenite grain boundaries suppressing austenite grain growth during superplastic deformation. Also, void nucleation and growth in the superplastic regime are slowed down within the newly transformed austenite plus carbide microstructure. In contrast, austenite grains and voids grow fast at a high deformation temperature (120K above Ae1). At a low deformation temperature (130K below Ae1), strain induced austenite formation does not occur and the

nucleation of multiple voids at the ferrite-carbide interfaces becomes relevant. The fast growth of grains and voids as well as the formation of multiple voids can trigger premature failure during tensile testing in the superplastic regime. EBSD is used to analyze the microstructure evolution and void formation during superplastic deformation, revealing optimum microstructural and forming conditions for superplasticity of Mn-Si-Cr-C steels. The study reveals that excellent superplasticity can be maintained even at 120K above Ae1 by designing an appropriate initial duplex ferrite plus carbide microstructure. © 2014 Elsevier B.V.
AUTHOR KEYWORDS: Electron backscatter diffraction (EBSD); Microstructure design; Steel; Superplasticity; Void
DOCUMENT TYPE: Article
SOURCE: Scopus

Mandal, S., Lang, S., Gross, M., Oettel, M., Raabe, D., Franosch, T., Varnik, F.
Multiple reentrant glass transitions in confined hard-sphere glasses
(2014) Nature Communications, 5, art. no. 4435, . Cited 18 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84904620849&doi=10.1038%2fncomms5435&partnerID=40&md5=9dc128200bf15b6da5b49e1f0c0f7a94

DOI: 10.1038/ncomms5435
AFFILIATIONS: Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Universitätsstrae 150, D-44780 Bochum, Germany;
Max-Planck-Institut für Eisenforschung, Max-Planck-Strae 1, D-40237, Düsseldorf, Germany;
Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Technikerstrae 25/2, A-6020 Innsbruck, Austria;
Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstrae 7, D-91058 Erlangen, Germany;
Institut für Angewandte Physik, Eberhard Karls-Universität Tübingen, Auf der Morgenstelle 10, D-72076 Tübingen, Germany
ABSTRACT: Glass-forming liquids exhibit a rich phenomenology upon confinement. This is often related to the effects arising from wall-fluid interactions. Here we focus on the interesting limit where the separation of the confining walls becomes of the order of a few particle diameters. For a moderately polydisperse, densely packed hard-sphere fluid confined between two smooth hard walls, we show via event-driven molecular dynamics simulations the emergence of a multiple reentrant glass transition scenario upon a variation of the wall separation. Using thermodynamic relations, this reentrant phenomenon is shown to persist also under constant chemical potential. This allows straightforward experimental investigation and opens the way to a variety of applications in micro-and nanotechnology, where channel dimensions are comparable to the size of the contained particles. The results are in line with theoretical predictions obtained by a combination of density functional theory and the mode-coupling theory of the glass transition. © 2014 Macmillan Publishers Limited.
DOCUMENT TYPE: Article
SOURCE: Scopus

Guo, W., Jägle, E.A., Choi, P.-P., Yao, J., Kostka, A., Schneider, J.M., Raabe, D.
Shear-induced mixing governs codeformation of crystalline-amorphous nanolaminates
(2014) Physical Review Letters, 113 (3), art. no. 035501, . Cited 28 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84904554001&doi=10.1103%2fPhysRevLett.113.035501&partnerID=40&md5=f156731e58febd5fbc6590e424eb5c22

DOI: 10.1103/PhysRevLett.113.035501

AFFILIATIONS: Max Planck Institut für Eisenforschung, Düsseldorf 40237, Germany;
Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China;
Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, D-52074 Aachen, Germany
ABSTRACT: Deformation of ductile crystalline-amorphous nanolaminates is not well understood due to the complex interplay of interface mechanics, shear banding, and deformation-driven chemical mixing. Here we present indentation experiments on 10 nm nanocrystalline Cu-100 nm amorphous CuZr model multilayers to study these mechanisms down to the atomic scale. By using correlative atom probe tomography and transmission electron microscopy we find that crystallographic slip bands in the Cu layers coincide with noncrystallographic shear bands in the amorphous CuZr layers. Dislocations from the crystalline layers drag Cu atoms across the interface into the CuZr layers. Also, crystalline Cu blocks are sheared into the CuZr layers. In these sheared and thus Cu enriched zones the initially amorphous CuZr layer is rendered into an amorphous plus crystalline nanocomposite.
DOCUMENT TYPE: Article
SOURCE: Scopus

Mandal, S., Pradeep, K.G., Zaefferer, S., Raabe, D.
A novel approach to measure grain boundary segregation in bulk polycrystalline materials in dependence of the boundaries' five rotational degrees of freedom
(2014) Scripta Materialia, 81, pp. 16-19. Cited 28 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84898776381&doi=10.1016%2fj.scriptamat.2014.02.016&partnerID=40&md5=3e75414cad39dc7508465f01b3fd5782

DOI: 10.1016/j.scriptamat.2014.02.016
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: We demonstrate a simplified nondestructive 3-D electron backscatter diffraction (EBSD) methodology that enables the measurement of all five degrees of freedom of grain boundaries (GBs) combined with segregation analysis using atom probe tomography (APT). The approach is based on two 2-D EBSD measurements on orthogonal surfaces at a sharp edge of the specimen followed by site-specific GB composition analysis using APT. An example of an asymmetric Σ9 boundary exhibiting GB segregation emphasizes the need for complete GB characterization in this context.
AUTHOR KEYWORDS: Atom probe tomography; Electron backscatter diffraction; Grain boundary crystallography; Segregation
DOCUMENT TYPE: Article
SOURCE: Scopus

Koyama, M., Tasan, C.C., Akiyama, E., Tsuzaki, K., Raabe, D.
Hydrogen-assisted decohesion and localized plasticity in dual-phase steel
(2014) Acta Materialia, 70, pp. 174-187. Cited 67 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84896415682&doi=10.1016%2fj.actamat.2014.01.048&partnerID=40&md5=7611db3abf76139c232303165ff2958c

DOI: 10.1016/j.actamat.2014.01.048
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany;
National Institute for Materials Science, 1-2-1, Sengen, Tsukuba, Ibaraki 305-0047, Japan;
Department of Mechanical Engineering, Kyushu University, 744 Motooka, Nishi-ku, Fukuoka 819-0395, Japan

ABSTRACT: Hydrogen embrittlement affects high-strength ferrite/martensite dual-phase (DP) steels. The associated micromechanisms which lead to failure have not been fully clarified yet. Here we present a quantitative micromechanical analysis of the microstructural damage phenomena in a model DP steel in the presence of hydrogen. A high-resolution scanning electron microscopy-based damage quantification technique has been employed to identify strain regimes where damage nucleation and damage growth take place, both with and without hydrogen precharging. The mechanisms corresponding to these regimes have been investigated by employing post-mortem electron channeling contrast imaging and electron backscatter diffraction analyses, as well as additional in situ deformation experiments. The results reveal that damage nucleation mechanism (i.e. martensite decohesion) and the damage growth mechanisms (e.g. interface decohesion) are both promoted by hydrogen, while the crack-arresting capability of the ferrite is significantly reduced. The observations are discussed on the basis of the hydrogen-enhanced decohesion and hydrogen-enhanced localized plasticity mechanisms. We discuss corresponding microstructure design strategies for better hydrogen-related damage tolerance of DP steels.
AUTHOR KEYWORDS: Damage; Dual-phase steel; Ferrite; Hydrogen embrittlement; Martensite
DOCUMENT TYPE: Article
SOURCE: Scopus

Sandlöbes, S., Pei, Z., Friák, M., Zhu, L.-F., Wang, F., Zaefferer, S., Raabe, D., Neugebauer, J.
Ductility improvement of Mg alloys by solid solution: Ab initio modeling, synthesis and mechanical properties
(2014) Acta Materialia, 70, pp. 92-104. Cited 58 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84896356920&doi=10.1016%2fj.actamat.2014.02.011&partnerID=40&md5=782d7621b0102ca23cbb6ea81419a066

DOI: 10.1016/j.actamat.2014.02.011
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, D-40237 Düsseldorf, Germany;
Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Schinkelstraße 2, D-52062 Aachen, Germany;
Institute of Physics of Materials, Academy of Sciences of the Czech Republic, V.v.i., Žižkova 22, 6161 62 Brno, Czech Republic
ABSTRACT: The I1 intrinsic stacking fault energy (I1 SFE) serves as an alloy design parameter for ductilizing Mg alloys. In view of this effect we have conducted quantum-mechanical calculations for Mg15X solid-solution crystals (X = Dy, Er, Gd, Ho, Lu, Sc, Tb, Tm, Nd, Pr, Be, Ti, Zr, Zn, Tc, Re, Co, Ru, Os, Tl). We find that Y, Sc and all studied lanthanides reduce the I1 SFE and render hexagonal closed-packed (hcp) and double hcp phases thermodynamically, structurally and elastically similar. Synthesis, experimental testing and characterization of some of the predicted key alloys (Mg-3Ho, Mg-3Er, Mg-3Tb, Mg-3Dy) indeed confirm reduced I1 SFEs and significantly improved room-temperature ductility by up to 4-5 times relative to pure Mg, a finding that is attributed to the higher activity of non-basal dislocation slip.
AUTHOR KEYWORDS: Ab initio; Ductility; Magnesium; Modeling; Rare-earth elements
DOCUMENT TYPE: Article
SOURCE: Scopus

Zilnyk, K.D., Sandim, H.R.Z., Bolmaro, R.E., Lindau, R., Möslang, A., Kostka, A., Raabe, D.
Long-term microstructural stability of oxide-dispersion strengthened Eurofer steel annealed at 800 °c

(2014) Journal of Nuclear Materials, 448 (1-3), pp. 33-42. Cited 8 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84894061626&doi=10.1016%2fj.jnucmat.2014.01.032&partnerID=40&md5=dfb699f5e1dd3e74d1d464784ddc58dc

DOI: 10.1016/j.jnucmat.2014.01.032
AFFILIATIONS: Escola de Engenharia de Lorena, USP, 12600-970 Lorena, SP, Brazil;
Instituto de Física Rosario, CONICET-UNR, 2000 Rosario, Argentina;
Karlsruher Institut für Technologie, KIT, IAM-AWP, D-72061 Karlsruhe, Germany;
Max-Planck Institut für Eisenforschung, MPI-E, D-40237 Düsseldorf, Germany
ABSTRACT: Oxide-dispersion strengthened ferritic martensitic steels such as ODS-Eurofer grade are good candidates for structural applications in future fusion power reactors. Long-term annealing treatments in vacuum were carried out in cold-rolled samples (80% reduction in thickness) from 1 h up to 4320 h (6 months) at 800 °C, i.e. the maximum temperature in the ferritic phase field, to follow its softening behavior. The microstructural stability of this steel was mapped using several characterization techniques including scanning electron microscopy, transmission electron microscopy, electron backscatter diffraction, Vickers microhardness testing, X-ray diffraction texture measurements, low-temperature electrical resistivity, and magnetic coercive field measurements. ODS-Eurofer steel displays good microstructural stability. Discontinuous recrystallization occurs at the early stages of annealing resulting in a low volume fraction of recrystallized grains. Extended recovery is the predominant softening mechanism at this temperature for longer times.
DOCUMENT TYPE: Article
SOURCE: Scopus

Pradeep, K.G., Herzer, G., Choi, P., Raabe, D.
Atom probe tomography study of ultrahigh nanocrystallization rates in FeSiNbBCu soft magnetic amorphous alloys on rapid annealing
(2014) Acta Materialia, 68, pp. 295-309. Cited 26 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84896698861&doi=10.1016%2fj.actamat.2014.01.031&partnerID=40&md5=3fdab50a1168c2dbe9a277f0da7007c0

DOI: 10.1016/j.actamat.2014.01.031
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Vacuumschmelze GmbH and Co. KG, Grüner Weg 37, 63450 Hanau, Germany
ABSTRACT: Rapid annealing (4-10 s) induced primary crystallization of soft magnetic Fe-Si nanocrystals in a Fe73.5Si15.5Cu1Nb 3B7 amorphous alloy has been systematically studied by atom probe tomography in comparison with conventional annealing (30-60 min). It was found that the nanostructure obtained after rapid annealing is basically the same, irrespective of the different time scales of annealing. This underlines the crucial role of Cu during structure formation. Accordingly, the clustering of Cu atoms starts at least 50 C below the onset temperature of primary crystallization. As a consequence, coarsening of Cu atomic clusters also starts prior to crystallization, resulting in a reduction of available nucleation sites during Fe-Si nanocrystallization. Furthermore, the experimental results explicitly show that these Cu clusters initially induce a local enrichment of Fe and Si in the amorphous matrix. These local chemical heterogeneities are proposed to be the actual nuclei for subsequent nanocrystallization. Nevertheless, rapid annealing in comparison with conventional annealing results in the formation of ~30% smaller Fe-Si nanocrystals, but of identical structure, volume fraction and chemical composition, indicating the limited influence of thermal treatment on nanocrystallization, owing to

the effect of Cu.
AUTHOR KEYWORDS: Atom probe tomography; Coarsening; Crystallization; Nanocrystalline microstructure; Soft magnets
DOCUMENT TYPE: Article
SOURCE: Scopus

Pierce, D.T., Jiménez, J.A., Bentley, J., Raabe, D., Oskay, C., Wittig, J.E.
The influence of manganese content on the stacking fault and austenite/ε-martensite interfacial energies in Fe-Mn-(Al-Si) steels investigated by experiment and theory
(2014) Acta Materialia, 68, pp. 238-253. Cited 57 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84894327757&doi=10.1016%2fj.actamat.2014.01.001&partnerID=40&md5=bf4c3fae4af86e69e1026f4af8d2a51f

DOI: 10.1016/j.actamat.2014.01.001
AFFILIATIONS: Vanderbilt University, PMB 351683, 2301 Vanderbilt Place, Nashville, TN 37232, United States;
Advanced Steel Processing and Products Research Center, Colorado School of Mines, Golden, CO 80401, United States;
Centro Nacional de Investigaciones Metalurgicas (CSIC), Avda. Gregorio del Amo, 8, 28040 Madrid, Spain;
Microscopy and Microanalytical Sciences, P.O. Box 7103, Oak Ridge, TN 37831-7103, United States;
Max-Planck-Institut für Eisenforschung, Max-Planck Str. 1, D-40237 Düsseldorf, Germany
ABSTRACT: The stacking fault and interfacial energies of three transformation- and twinning-induced plasticity steels (TRIP/TWIP) (Fe-22/25/28Mn-3Al-3Si wt.%) were determined by experimental and theoretical methods. Analysis of Shockley partial dislocation configurations in the three alloys using weak-beam dark-field transmission electron microscopy yielded stacking fault energy (SFE) values of 15 ± 3, 21 ± 3 and 39 ± 5 mJ m-2 for alloys with 22, 25 and 28 wt.% Mn, respectively. The experimental SFE includes a coherency strain energy of ~1-4 mJ m-2, determined by X-ray diffraction, which arises from the contraction in volume of the stacking fault upon the face-centered cubic (fcc) to hexagonal close-packed (hcp) phase transformation. The ideal SFE, computed as the difference between the experimental SFE and the coherency strain energy, is equal to14 ± 3, 19 ± 3 and 35 ± 5 mJ m-2, respectively. These SFE values were used in conjunction with a thermodynamic model developed in the present work to calculate the free energy difference of the fcc and hcp phases and to determine a probable range for the fcc/hcp interfacial energy in the three Fe-Mn-(Al-Si) steels investigated. In addition, the interfacial energies of three Fe-18Mn-0.6C-0/1.5(Al/Si) TWIP and five Fe-16/18/20/22/25Mn binary alloys were also determined from experimental data in the literature. The interfacial energy ranged from 8 to 12 mJ m-2 in the TRIP/TWIP steels and from 15 to 33 mJ m-2 in the binary Fe-Mn alloys. The interfacial energy exhibits a strong dependence on the difference in Gibbs energy of the individual fcc and hcp phases. Accordingly, an empirical description of this parameter is proposed to improve the accuracy of thermodynamic SFE calculations.
AUTHOR KEYWORDS: Interface energy; Partial dislocation; Phase stability; Stacking fault energy; TWIP steel
DOCUMENT TYPE: Article
SOURCE: Scopus

Varnik, F., Mandal, S., Chikkadi, V., Denisov, D., Olsson, P., Vågberg, D., Raabe, D., Schall, P.
Correlations of plasticity in sheared glasses

(2014) Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, 89 (4), art. no. 040301, . Cited 11 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84899740629&doi=10.1103%2fPhysRevE.89.040301&partnerID=40&md5=c3ac9a320fb364fca4eb5ed389aa880e

DOI: 10.1103/PhysRevE.89.040301
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck Straße 1, 40237 Düsseldorf, Germany;
Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Universitätsstraße 150, 44780 Bochum, Germany;
Institute of Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, Netherlands;
Department of Theoretical Physics, Umeå University, 901 87 Umeå, Sweden
ABSTRACT: In a recent paper [Mandal, Phys. Rev. E 88, 022129 (2013)PLEEE81539-375510. 1103/PhysRevE.88.022129], the nature of spatial correlations of plasticity in hard-sphere glasses was addressed both via computer simulations and in experiments. It was found that the experimentally obtained correlations obey a power law, whereas the correlations from simulations are better fitted by an exponential decay. We here provide direct evidence - via simulations of a hard-sphere glass in two dimensions (2D) - that this discrepancy is a consequence of the finite system size in the 3D simulations. By extending the study to a 2D soft disk model at zero temperature [Durian, Phys. Rev. Lett. 75, 4780 (1995)PRLTAO0031-900710.1103/PhysRevLett.75.4780], the robustness of the power-law decay in sheared amorphous solids is underlined. Deviations from a power law occur when either reducing the packing fraction towards the supercooled regime in the case of hard spheres or changing the dissipation mechanism from contact dissipation to a mean-field-type drag in the case of soft disks. © 2014 American Physical Society.
DOCUMENT TYPE: Article
SOURCE: Scopus

Koyama, M., Springer, H., Merzlikin, S.V., Tsuzaki, K., Akiyama, E., Raabe, D.
Hydrogen embrittlement associated with strain localization in a precipitation-hardened Fe-Mn-Al-C light weight austenitic steel
(2014) International Journal of Hydrogen Energy, 39 (9), pp. 4634-4646. Cited 51 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84895455730&doi=10.1016%2fj.ijhydene.2013.12.171&partnerID=40&md5=ded55304e8037dfa879640cb93fe5e42

DOI: 10.1016/j.ijhydene.2013.12.171
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany;
National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan;
Department of Mechanical Engineering, Kyushu University, 744 Motooka, Nishi-ku, Fukuoka 819-0395, Japan
ABSTRACT: Hydrogen embrittlement of a precipitation-hardened Fe-26Mn-11Al-1.2C (wt.%) austenitic steel was examined by tensile testing under hydrogen charging and thermal desorption analysis. While the high strength of the alloy (>1 GPa) was not affected, hydrogen charging reduced the engineering tensile elongation from 44 to only 5%. Hydrogen-assisted cracking mechanisms were studied via the joint use of electron backscatter diffraction analysis and orientation-optimized electron channeling contrast imaging. The observed embrittlement was mainly due to two mechanisms, namely, grain boundary triple junction cracking and slip-localization-induced intergranular cracking along micro-voids formed on grain boundaries. Grain boundary triple junction cracking occurs preferentially, while the microscopically ductile slip-localization-induced intergranular cracking assists crack growth during plastic deformation resulting in

macroscopic brittle fracture appearance.
AUTHOR KEYWORDS: Austenitic steel; Electron channeling contrast imaging; Hydrogen embrittlement; Precipitation hardening; Tension test
DOCUMENT TYPE: Article
SOURCE: Scopus

Kapoor, R., Sarkar, A., Singh, J., Samajdar, I., Raabe, D.
Effect of strain rate on twinning in a Zr alloy
(2014) Scripta Materialia, 74, pp. 72-75. Cited 10 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84891011357&doi=10.1016%2fj.scriptamat.2013.10.025&partnerID=40&md5=10d379c8bb0b5851b640c6c141439907

DOI: 10.1016/j.scriptamat.2013.10.025
AFFILIATIONS: Mechanical Metallurgy Division, Bhabha Atomic Research Centre, Mumbai 400085, India;
Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai 400076, India;
Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany
ABSTRACT: Zr-1Nb alloy uniaxially compressed at room temperature at 10-2 and 103 s-1 exhibited twinning and a three-stage strain-hardening behavior. At 103 s-1 the twin fraction initially increased to 0.3, decreasing to 0.02 at higher strains. Despite the difference in texture at intermediate strains, the final texture was similar at both strain rates. The increasing strain-hardening rate in the second stage was attributed to strengthening from grain boundaries and dislocations, and softening from reorientation due to twinning. © 2013 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
AUTHOR KEYWORDS: High strain rate; Strain hardening; Tensile twin; Zr alloy
DOCUMENT TYPE: Article
SOURCE: Scopus

Toji, Y., Matsuda, H., Herbig, M., Choi, P.-P., Raabe, D.
Atomic-scale analysis of carbon partitioning between martensite and austenite by atom probe tomography and correlative transmission electron microscopy
(2014) Acta Materialia, 65, pp. 215-228. Cited 58 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84905215255&doi=10.1016%2fj.actamat.2013.10.064&partnerID=40&md5=af511a0f52111d0ce2201f557c7069bc

DOI: 10.1016/j.actamat.2013.10.064
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Steel Research Laboratory, JFE Steel Corporation, 1 Kawasaki-cho, Chuo-ku, Chiba 260-0835, Japan
ABSTRACT: Carbon partitioning between ferritic and austenitic phases is essential for austenite stabilization in the most advanced steels such as those produced by the quenching and partitioning (Q&P) process. The atomistic analysis of the carbon partitioning in Q&P alloys is, however, difficult owing to the simultaneous occurrence of bainite transformation, which can also contribute to carbon enrichment into remaining austenite and hence overlap with the carbon partitioning from martensite into austenite. Therefore, we provide here a direct atomic-scale evidence of carbon partitioning from martensite into austenite without the presence of bainite transformation. Carbon partitioning is investigated by means of atom probe tomography and correlative transmission electron microscopy. A model steel (Fe-0.59 wt.% C (2.7 at.% C)-2.0 wt.% Si-2.9 wt.% Mn) with martensite finish temperature below room temperature was designed and used in order to clearly separate the carbon partitioning between martensite and austenite from the bainite transformation. The steel was austenitized at 900°C, then

water-quenched and tempered at 400°C. Approximately 8 vol.% retained austenite existed in the asquenched state. We confirmed by X-ray diffraction and dilatometry that austenite decomposition via bainite transformation did not occur during tempering. No carbon enrichment in austenite was observed in the as-quenched specimen. On the other hand, clear carbon enrichment in austenite was observed in the 400°C tempered specimens with a carbon concentration inside the austenite of 5-8 at.%. The results hence quantitatively revealed carbon partitioning from martensite to austenite, excluding bainite transformation during the Q&P heat treatment.
AUTHOR KEYWORDS: Atom probe tomography; Austenite; Bainite; Martensite; Quenching and partitioning
DOCUMENT TYPE: Article
SOURCE: Scopus

Ram, F., Zaefferer, S., Raabe, D.
Kikuchi bandlet method for the accurate deconvolution and localization of Kikuchi bands in Kikuchi diffraction patterns
(2014) Journal of Applied Crystallography, 47 (1), pp. 264-275. Cited 9 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84893340414&doi=10.1107%2fS1600576713030446&partnerID=40&md5=2f3a2162915db505f320209997e87ff9

DOI: 10.1107/S1600576713030446
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany
ABSTRACT: In order to retrieve crystallographic information from an electron backscatter Kikuchi diffraction pattern, its Kikuchi bands have to be localized. One of the main reasons for the limited precision of the present Kikuchi band localization methods is that the diffuse edges of a Kikuchi band are convoluted by many other Kikuchi bands that intersect them. To improve the localization accuracy, Kikuchi bands have to be deconvoluted. In this article, a new method for the deconvolution and localization of Kikuchi bands is presented. The deconvolution is based on the fact that, in a Kikuchi pattern, there are a number of Kikuchi bands that are not parallel to the bands that intersect them. It is performed in Fourier space. After deconvolution, localization is carried out by a quantitative shape analysis of the intensity profiles of the deconvoluted Kikuchi bands. Using the introduced method, for a real electron backscatter Kikuchi diffraction pattern with 45° half capture angle and 0.12°per pixel maximum scale factor, the characteristic hyperbolic features of the Kikuchi bands can be localized with a precision of better than 0.1°in reflection angle.
AUTHOR KEYWORDS: deconvolution; electron backscatter diffraction; Fourier transforms; frequency space; intensity profile shape analysis; Kikuchi bands; Kikuchi patterns
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Yao, M.J., Pradeep, K.G., Tasan, C.C., Raabe, D.
A novel, single phase, non-equiatomic FeMnNiCoCr high-entropy alloy with exceptional phase stability and tensile ductility
(2014) Scripta Materialia, 72-73, pp. 5-8. Cited 104 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84889091858&doi=10.1016%2fj.scriptamat.2013.09.030&partnerID=40&md5=11a8bfe461b9c13f10cf697a66ac9231

DOI: 10.1016/j.scriptamat.2013.09.030
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany

ABSTRACT: A non-equiatomic FeMnNiCoCr alloy is introduced and characterized at multiple scales employing various characterization techniques (e.g. atom probe tomography, electron channeling contrast imaging, electron backscatter diffraction, etc.) to elucidate (i) the role of configurational entropy and (ii) the intrinsic tensile ductility of high-entropy alloys. Results reveal that the new material is a true high-entropy alloy with a stable random solid solution despite its comparably low configurational entropy, and that it has excellent tensile ductility irrespective of the substantial lattice distortion.
AUTHOR KEYWORDS: Atom probe tomography; Ductility; ECCI; High-entropy alloy; Non-equiatomic
DOCUMENT TYPE: Article
SOURCE: Scopus

Hafez Haghighat, S.M., Schäublin, R., Raabe, D.
Atomistic simulation of the a0 ⟨1 0 0⟩ binary junction formation and its unzipping in body-centered cubic iron
(2014) Acta Materialia, 64, pp. 24-32. Cited 9 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84890282705&doi=10.1016%2fj.actamat.2013.11.037&partnerID=40&md5=35e868a6069b0c3dca8bbaf4aba6748c

DOI: 10.1016/j.actamat.2013.11.037
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Ecole Polytechnique Fédérale de Lausanne (EPFL), Centre de Recherches en Physique des Plasmas, Association Euratom-Confédération Suisse, CH 5232 Villigen PSI, Switzerland
ABSTRACT: Molecular dynamics simulation is used to study the formation of the a 0 ⟨1 0 0⟩ binary dislocation junction in body-centered cubic Fe. Results show that under an applied strain two intersecting 1/2 a 0 ⟨1 1 1⟩ dislocations, one mobile edge and one immobile screw, form an a0 ⟨1 0 0⟩ binary junction of mixed character in the glide plane of the mobile edge dislocation. It appears, however, that the binary junction does not necessarily lay in one of the three possible {1 1 0} glide planes of the screw dislocation. The binary junction starts to unzip as the impinging edge dislocation bows around and moves away, which results in the formation of a screw dipole along its Burgers vector. The dipole eventually annihilates, completing the unzipping process of the junction, which liberates the edge dislocation. The effects of temperature and strain rate on the unzipping of the junction are quantified by the critical release stress needed to detach the edge dislocation from the screw one. The critical stress decreases when the temperature increases from 10 to 300 K, whereas it increases with increasing applied strain rate, or dislocation speed. The interaction mechanism and strength of the a0 ⟨1 0 0⟩ binary junction as an obstacle to the edge dislocation are compared to that of other types of defect, namely nanosized voids, Cu and Cr precipitates, and dislocation loops in Fe. It appears that the binary junction strength is in the lowest range, comparable to that of a coherent Cr precipitate.
AUTHOR KEYWORDS: Binary junction; Dislocations interaction; Iron; Molecular dynamics (MD); Strength
DOCUMENT TYPE: Article
SOURCE: Scopus

Zhang, H., Pradeep, K.G., Mandal, S., Ponge, D., Choi, P., Tasan, C.C., Raabe, D.
Enhanced superplasticity in an Al-alloyed multicomponent Mn-Si-Cr-C steel
(2014) Acta Materialia, 63, pp. 232-244. Cited 15 times.

https://www.scopus.com/inward/record.uri?eid=2-s2.0-84888294180&doi=10.1016%2fj.actamat.2013.10.034&partnerID=40&md5=d9a2a3340b5a91a348e172ae582cb691

DOI: 10.1016/j.actamat.2013.10.034
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: Excellent superplasticity (elongation ~720%) is observed in a novel multi-component (Mn-S-Cr-Al alloyed) ultrahigh carbon steel during tensile testing at a strain rate of 2 × 10-3 s-1 and a temperature of 1053 K (just above the equilibrium austenite-pearlite transformation temperature). In order to understand superplasticity in this material and its strong Al dependence, the deformation-induced microstructure evolution is characterized at various length scales down to atomic resolution, using X-ray diffraction, scanning electron microscopy, electron backscatter diffraction, energy-dispersive X-ray spectroscopy and atom probe tomography. The results reveal that 1 wt.% Al addition influences various microprocesses during deformation, e.g. it impedes Ostwald ripening of carbides, carbide dissolution, austenite nucleation and growth and void growth. As a result, the size of the austenite grains and voids remains relatively fine (<10 μm) during superplastic deformation, and fine-grained superplasticity is enabled without premature failure.
AUTHOR KEYWORDS: Aluminum; Grain growth; Steel; Superplasticity; Void
DOCUMENT TYPE: Article
SOURCE: Scopus

Friák, M., Zhu, L.-F., Lymperakis, L., Titrian, H., Aydin, U., Janus, A.M., Fabritius, H.-O., Ziegler, A., Nikolov, S., Hemzalová, P., Raabe, D., Neugebauer, J.
Quantum-mechanical study of single-crystalline and polycrystalline elastic properties of Mg-substituted calcite crystals
(2014) Key Engineering Materials, 592-593, pp. 335-341. Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84891859913&doi=10.4028%2fwww.scientific.net%2fKEM.592-593.335&partnerID=40&md5=db57f22ea1af6993827cdbdc99e5c606

DOI: 10.4028/www.scientific.net/KEM.592-593.335
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, Düsseldorf 40237, Germany;
University Duisburg-Essen, Germany;
Central Facility for Electron Microscopy, University of Ulm, Albert-Einstein-Allee 11, Ulm 89069, Germany;
Bulgarian Academy of Sciences, Institute of Mechanics, Acad. G. Bonchev Str. Bl. 4, 1113 Sofia, Bulgaria;
Masaryk University, Kotlářská 2, Brno 61137, Czech Republic
ABSTRACT: We use quantum-mechanical calculations to study single-crystalline elastic properties of (Ca,Mg)CO3 crystals with concentrations ranging from calcite CaCO3 to magnesite MgCO3. By analyzing results for a dense set of distributions of Ca and Mg atoms within 30-atom supercells, our theoretical study shows that those atomic configurations, that minimize the total energy for a given concentration, are characterized by elastic constants that either increase with the Mg content or remain nearly constants. Employing these ab initio calculated single-crystalline elastic parameters, the polycrystalline elastic properties of (Ca,Mg)CO3 aggregates are determined using a mean-field self-consistent homogenization method. The computed integral elastic moduli (bulk and shear) show a significant stiffening impact of Mg atoms on calcite crystals. Our analysis also demonstrates that it is not advantageous to use a granular two-phase composite of stoichiometric calcite and magnesite instead of substituting individual Ca and Mg atoms. Such two-phase aggregates are not significantly

thermodynamically favorable and do not offer any strong additional stiffening effect. © (2014) Trans Tech Publications.
AUTHOR KEYWORDS: Ab initio; Bio-materials; Calcite; Elasticity; Homogenization; Multi-phase
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Gutierrez-Urrutia, I., Raabe, D.
Study of dislocation substructures in high-Mn steels by electron channeling contrast imaging
(2014) Materials Science Forum, 783-786, pp. 750-754.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84904544244&partnerID=40&md5=a4f9a76580d90b5d1b1651e5abee153e

AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany
ABSTRACT: We have investigated the formation of dislocation substructures in high-Mn steels by electron channeling contrast imaging in the SEM. The coupling of electron channeling contrast imaging (ECCI) with electron backscatter diffraction (EBSD) provides an efficient and fast approach to characterize dislocation substructures under controlled diffraction conditions with enhanced contrast. The dislocation substructure of high-Mn steels at intermediate strain levels is characterized by cells and cell blocks with strong crystallographic orientation dependence. We observe a significant effect of strain path on dislocation patterning. Microband formation is enabled under shearing conditions. We explain this effect on terms of Schmid's law. © (2014) Trans Tech Publications, Switzerland.
AUTHOR KEYWORDS: Dislocation substructure; EBSD; Electron channeling contrast imaging; High-Mn TWIP steels
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Gutierrez-Urrutia, I., Raabe, D.
High strength and ductile low density austenitic FeMnAlC steels: Simplex and alloys strengthened by nanoscale ordered carbides
(2014) Materials Science and Technology (United Kingdom), 30 (9), pp. 1099-1104. Cited 28 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84901785876&doi=10.1179%2f1743284714Y.0000000515&partnerID=40&md5=d55f5eed7dccfaf636d61143551af4f3

DOI: 10.1179/1743284714Y.0000000515
AFFILIATIONS: Max-Planck-Institut füR Eisenforschung, Max-Planck Str. 1, D-40237 Düsseldorf, Germany
ABSTRACT: We introduce the alloy design concepts of high performance austenitic FeMnAlC steels, namely, Simplex and alloys strengthened by nanoscale ordered k-carbides. Simplex steels are characterised by an outstanding strain hardening capacity at room temperature. This is attributed to the multiple stage strain hardening behaviour associated to dislocation substructure refinement and subsequent activation of deformation twinning, which leads to a steadily increase of the strain hardening. Al additions higher that 5 wt-% promote the precipitation of nanoscale L912 ordered precipitates (so called k-carbides) resulting in high strength (yield stress ~ 1.0 GPa) and ductile (elongation to fracture 7sim; 30%) steels. Novel insights into dislocation-particle interactions in a Fe- 30.5Mn-8.0Al-1.2C (wt-%) steel strengthened by nanoscale k-carbides are discussed. © 2014 Institute of Materials, Minerals and Mining.
AUTHOR KEYWORDS: Deformation mechanisms; High Mn steels; K-carbides; Low density steels; Microstructure control; Strain hardening
DOCUMENT TYPE: Article
SOURCE: Scopus

Gutierrez-Urrutia, I., Raabe, D.
Study of dislocation substructures in high-Mn steels by electron channeling contrast imaging
(2014) Advanced Materials Research, 783-786, pp. 750-754. Cited 3 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84902260755&doi=10.4028%2fwww.scientific.net%2fMSF.783-786.750&partnerID=40&md5=21b5d0af2139156791730b3ba6bef832

DOI: 10.4028/www.scientific.net/MSF.783-786.750
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany
ABSTRACT: We have investigated the formation of dislocation substructures in high-Mn steels by electron channeling contrast imaging in the SEM. The coupling of electron channeling contrast imaging (ECCI) with electron backscatter diffraction (EBSD) provides an efficient and fast approach to characterize dislocation substructures under controlled diffraction conditions with enhanced contrast. The dislocation substructure of high-Mn steels at intermediate strain levels is characterized by cells and cell blocks with strong crystallographic orientation dependence. We observe a significant effect of strain path on dislocation patterning. Microband formation is enabled under shearing conditions. We explain this effect on terms of Schmid's law. © (2014) Trans Tech Publications, Switzerland.
AUTHOR KEYWORDS: Dislocation substructure; EBSD; Electron channeling contrast imaging; High-Mn TWIP steels
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Jägle, E.A., Choi, P.-P., Raabe, D.
The maximum separation cluster analysis algorithm for atom-probe tomography: Parameter determination and accuracy
(2014) Microscopy and Microanalysis, 20 (6), pp. 1662-1671. Cited 9 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84919465754&doi=10.1017%2fS1431927614013294&partnerID=40&md5=c6076bca8241cbd066eeb47a9d8e258d

DOI: 10.1017/S1431927614013294
AFFILIATIONS: Metal Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, Düsseldorf, Germany
ABSTRACT: Atom-probe tomography is a materials characterization method ideally suited for the investigation of clustering and precipitation phenomena. To distinguish the clusters from the surrounding matrix, the maximum separation algorithm is widely employed. However, the results of the cluster analysis strongly depend on the parameters used in the algorithm and hence, a wrong choice of parameters leads to erroneous results, e.g., for the cluster number density, concentration, and size. Here, a new method to determine the optimum value of the parameter d max is proposed, which relies only on information contained in the measured atom-probe data set. Atom-probe simulations are employed to verify the method and to determine the sensitivity of the maximum separation algorithm to other input parameters. In addition, simulations are used to assess the accuracy of cluster analysis in the presence of trajectory aberrations caused by the local magnification effect. In the case of Cu-rich precipitates (Cu concentration 40-60 at% and radius 0.25-1.0 nm) in a bcc Fe-Si-Cu matrix, it is shown that the error in concentration is below 10 at% and the error in radius is <0.15 nm for all simulated conditions, provided that the correct value for d max, as determined with the newly proposed method, is employed. © Microscopy Society of America 2014.
AUTHOR KEYWORDS: atom-probe tomography; cluster analysis; clustering; electrical steel; field evaporation simulation
DOCUMENT TYPE: Article
SOURCE: Scopus

Jägle, E.A., Choi, P.-P., Van Humbeeck, J., Raabe, D.

Precipitation and austenite reversion behavior of a maraging steel produced by selective laser melting
(2014) Journal of Materials Research, 29 (17), pp. 2072-2079. Cited 22 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84911962015&doi=10.1557%2fjmr.2014.204&partnerID=40&md5=104fc475efc0b127a3037d1aa69394d3

DOI: 10.1557/jmr.2014.204
AFFILIATIONS: Department Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany; Department of Metallurgy and Materials Engineering, KU Leuven, Leuven, Belgium
ABSTRACT: Materials produced by selective laser melting (SLM) experience a thermal history that is markedly different from that encountered by conventionally produced materials. In particular, a very high cooling rate from the melt is combined with cyclical reheating upon deposition of subsequent layers. Using atom-probe tomography (APT), we investigated how this nonconventional thermal history influences the phase-transformation behavior of maraging steels (Fe-18Ni-9Co-3.4Mo-1.2Ti) produced by SLM. We found that despite the "intrinsic heat treatment" and the known propensity of maraging steels for rapid clustering and precipitation, the material does not show any sign of phase transformation in the as-produced state. Upon aging, three different types of precipitates, namely (Fe,Ni,Co)3(Ti,Mo), (Fe,Ni,Co)3(Mo,Ti), and (Fe,Ni,Co)7Mo6 (μ phase), were observed as well as martensite-to-austenite reversion around regions of the retained austenite. The concentration of the newly formed phases as quantified by APT closely matches thermodynamic equilibrium calculations.

DOCUMENT TYPE: Article
SOURCE: Scopus

Gutierrez-Urrutia, I., Marceau, R., Herbig, M., Raabe, D.
Revealing the strain-hardening mechanisms of advanced high-Mn steels by multi-scale microstructure characterization
(2014) Advanced Materials Research, 783-786, pp. 755-760. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84902287317&doi=10.4028%2fwww.scientific.net%2fMSF.783-786.755&partnerID=40&md5=cdd6f690efe0989d3ee79b4e0f0942ca

DOI: 10.4028/www.scientific.net/MSF.783-786.755
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany
ABSTRACT: We have investigated the strain-hardening mechanisms across the relevant scales in a Fe-22Mn-0.6C (wt.%) twinning induced plasticity steel by multi-scale microstructure characterization. The approach makes use of electron microscopy techniques such as electron channeling contrast imaging (ECCI) to characterize microstructure features at the micro/nano scale, and atomic-scale investigations of partitioning behavior across interfaces and solid solution/clustering effects by atom probe tomography (APT). The contribution of most relevant microstructure features to strain hardening is analyzed.
AUTHOR KEYWORDS: Atom probe tomography; Electron channeling contrast imaging; High-Mn TWIP steels; Strain-hardening
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Gutierrez-Urrutia, I., Marceau, R., Herbig, M., Raabe, D.
Revealing the strain-hardening mechanisms of advanced high-Mn steels by multi-scale microstructure characterization
(2014) Materials Science Forum, 783-786, pp. 755-760.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84904538799&partnerID=40&md5=067c19a7244360a09cf10b648c4a98c3

AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany
ABSTRACT: We have investigated the strain-hardening mechanisms across the relevant scales in a Fe-22Mn-0.6C (wt.%) twinning induced plasticity steel by multi-scale microstructure characterization. The approach makes use of electron microscopy techniques such as electron channeling contrast imaging (ECCI) to characterize microstructure features at the micro/nano scale, and atomic-scale investigations of partitioning behavior across interfaces and solid solution/clustering effects by atom probe tomography (APT). The contribution of most relevant microstructure features to strain hardening is analyzed. © (2014) Trans Tech Publications, Switzerland.
AUTHOR KEYWORDS: Atom probe tomography; Electron channeling contrast imaging; High-Mn TWIP steels; Strain-hardening
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Alankar, A., Field, D.P., Raabe, D.
Plastic anisotropy of electro-deposited pure α-iron with sharp crystallographic <1 1 1>// texture in normal direction: Analysis by an explicitly dislocation-based crystal plasticity model
(2014) International Journal of Plasticity, 52, pp. 18-32. Cited 17 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84888197399&doi=10.1016%2fj.ijplas.2013.03.006&partnerID=40&md5=cd4ab307e4694bc2d9914f06bc6d6899

DOI: 10.1016/j.ijplas.2013.03.006
AFFILIATIONS: MST-8, Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87545, United States;
School of Mechanical and Materials Engineering, Washington State University, Box 642920, Pullman, WA 99164, United States;
Microstructure Physics and Alloy Design, Max-Planck Institut für Eisenforschung GmbH, 40235 Düsseldorf, Germany
ABSTRACT: We present a single crystal plasticity model based on edge and screw dislocation densities for body centered cubic (bcc) crystals. In a bcc crystal screw dislocations experience high lattice friction due to their non-planar core. Hence, they have much slower velocity compared to edge dislocations. This phenomenon is modeled by accounting for the motion of screw dislocations via nucleation and expansion of kink-pairs. The model, embedded as a constitutive law into a crystal plasticity framework, is able to predict the crystallographic texture of a bcc polycrystal subjected to 70%, 80% and 90% thickness reduction. We perform a parametric study based on the velocities of edge and screw dislocations to analyze the effect on plastic anisotropy of electro-deposited pure iron with long needle-shaped grains having sharp crystallographic <1 1 1>//ND texture (ND: normal direction). The model shows a large change in the r-value (Lankford value, planar anisotropy ratio) for pure iron when the texture changes from random to <1 1 1>//ND. For different simulated cases where the crystallites have an orientation deviation of 1, 3 and 5, respectively, from the ideal <1 1 1>//ND axis, the simulations predict r-values between 4.0 and 7.0 which is in excellent agreement with data observed in experiments by Yoshinaga et al. (ISIJ Intern.; 48 (2008) 667-670). For these specific orientations of grains, we also model the effect of long needle shaped grains via a procedure that excludes dislocation annihilation. © 2013 Elsevier Ltd. All rights reserved.
AUTHOR KEYWORDS: α-Iron; Crystallographic texture; Dislocations; Kink-pairs; Metal sheet forming
DOCUMENT TYPE: Article
SOURCE: Scopus

He, D., Zhu, J., Zaefferer, S., Raabe, D.
Effect of retained beta layer on slip transmission in Ti-6Al-2Zr-1Mo-1V near alpha titanium alloy during tensile deformation at room temperature

(2014) Materials and Design, 56, pp. 937-942. Cited 15 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84891103993&doi=10.1016%2fj.matdes.2013.12.018&partnerID=40&md5=148dbb0bb838d7289bb67e0824da2ed0

DOI: 10.1016/j.matdes.2013.12.018
AFFILIATIONS: State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China;
National Key Laboratory for Precision Hot Processing of Metals, Harbin Institute of Technology, Harbin 150001, China;
Max-Planck-Institut für Eisenforschung, Abteilung Mikrostrukturphysik und Umformtechnik, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany
ABSTRACT: Slip is the main plastic deformation mechanism in titanium alloys at room temperature. This is especially so for near alpha titanium alloy like Ti-6Al-2Zr-1Mo-1V, which contains low beta stabilizing and high aluminum (alpha stabilizing) element additions. The effects of retained beta layers on slip transmission across α/β interfaces in Ti-6Al-2Zr-1Mo-1V during tensile deformation have been studied in the current work. High resolution scanning electron microscopy (HR-SEM) and electron backscatter diffraction (EBSD) techniques were used to study the deformation microstructure. The results indicate that the full Burgers crystal orientation relationship (OR) between the α and the thin retained β phase layers facilitates slip transition but is not the necessary requirement/restriction. Some novel slip trace morphologies that are characterized by deflection and bifurcation (fork-like morphology) are revealed in the retained β layers between two abutting α grains. The possible reasons for these different slip transmission patterns are analyzed by EBSD results and a schematic model is proposed. © 2013 Elsevier Ltd.
AUTHOR KEYWORDS: Burgers orientation relationship; Retained beta; Slip transmission; Tensile deformation; Titanium alloys
DOCUMENT TYPE: Article
SOURCE: Scopus

Reuber, C., Eisenlohr, P., Roters, F., Raabe, D.
Dislocation density distribution around an indent in single-crystalline nickel: Comparing nonlocal crystal plasticity finite-element predictions with experiments
(2014) Acta Materialia, 71, pp. 333-348. Cited 27 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84897364469&doi=10.1016%2fj.actamat.2014.03.012&partnerID=40&md5=1b961bc58cadb64acdcfd9606013768b

DOI: 10.1016/j.actamat.2014.03.012
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Microstructure Physics and Alloy Design, Max-Planck-Straße 1, 40237 Düsseldorf, Germany;
Michigan State University, Chemical Engineering and Materials Science, East Lansing, MI 48824, United States
ABSTRACT: We present a physics-based constitutive model of dislocation glide in metals that explicitly accounts for the redistribution of dislocations due to their motion. The model parameterizes the complex microstructure by dislocation densities of edge and screw character, which either occur with monopolar properties, i.e. a single dislocation with positive or negative line sense, or with dipolar properties, i.e. two dislocations of opposite line sense combined. The advantage of the model lies in the description of the dislocation density evolution, which comprises the usual rate equations for dislocation multiplication and annihilation, and formation and dissociation of dislocation dipoles. Additionally, the spatial redistribution of dislocations by slip is explicitly accounted for. This is achieved by introducing an advection term for the dislocation density that turns the evolution equations for the dislocation density from ordinary into partial differential equations. The associated spatial gradients of the dislocation slip render the model

nonlocal. The model is applied to wedge indentation in single-crystalline nickel. The simulation results are compared to published experiments (Kysar et al., 2010) in terms of the spatial distribution of lattice rotations and geometrically necessary dislocations. In agreement with experiment, the predicted dislocation fluxes lead to accumulation of geometrically necessary dislocations around a vertical geometrical border with a high orientation gradient below the indenter that is decisive for the overall plastic response. A local model variant without dislocation transport is not able to predict the influence of this geometrical transition zone correctly and is shown to behave markedly softer.
AUTHOR KEYWORDS: Crystal plasticity; Dislocations; Geometrically necessary dislocations; Indentation; Microstructure
DOCUMENT TYPE: Article
SOURCE: Scopus

Gutierrez-Urrutia, I., Böttcher, A., Lahn, L., Raabe, D.
Microstructure-magnetic property relations in grain-oriented electrical steels: Quantitative analysis of the sharpness of the Goss orientation
(2014) Journal of Materials Science, 49 (1), pp. 269-276. Cited 7 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84891345069&doi=10.1007%2fs10853-013-7701-2&partnerID=40&md5=222cd97100ce6a9fb3d1e66d84593e62

DOI: 10.1007/s10853-013-7701-2
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck Str. 1, 40237 Düsseldorf, Germany;
ThyssenKrupp Electrical Steel, Kurt-Schumacher-St. 95, 45881 Gelsenkirchen, Germany
ABSTRACT: We have investigated microstructure-magnetic property relations in several high-permeability grain-oriented steels by large-area electron backscatter diffraction (EBSD) mapping. The evaluation of the Goss sharpness determined from orientation distribution functions provides a more quantitative and detailed texture analysis than conventional pole figure estimates. Accordingly, it results in a more quantitative treatment of texture-magnetic property relations. The analysis of crystal-orientation distribution by a statistical binning method provides further insights into the occurrence of secondary texture components. Specifically, we have found the formation of two weak secondary components rotated about 4°-6° and 8°-10° from the texture center, respectively. These texture components have a strong influence on the magnetic polarization but a small influence on the core loss. We explain this effect in terms of the magneto-crystalline anisotropy energy of a cubic crystal and magnetic domain-microstructure feature interactions.
DOCUMENT TYPE: Article
SOURCE: Scopus

Zhang, H., Pradeep, K.G., Mandal, S., Ponge, D., Raabe, D.
New insights into the austenitization process of low-alloyed hypereutectoid steels: Nucleation analysis of strain-induced austenite formation
(2014) Acta Materialia, 80, pp. 296-308. Cited 5 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84906527591&doi=10.1016%2fj.actamat.2014.07.073&partnerID=40&md5=782850073f8c9e6461f93fa72cec6d19

DOI: 10.1016/j.actamat.2014.07.073
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck Str 1, 40237 Düsseldorf, Germany;
Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, D-52074 Aachen, Germany
ABSTRACT: Austenite formation, which originated from a fined-grained ferrite plus carbide microstructure, was observed during tensile testing at 973 K (60 K below Ae1, the equilibrium austenite-pearlite transformation

temperature). Scanning electron microscopy, electron backscatter diffraction and atom probe tomography results reveal the mechanism of austenitic transformation below Ae1. The initial fine-grained microstructure, in combination with the warm deformation process, determines the occurrence of strain-induced austenite formation below Ae1. The initial fine-grained microstructure essentially contains a higher dislocation density to facilitate the formation of Cottrell atmospheres and a larger area fraction of ferrite/carbide interfaces which serve as austenite nucleation sites. The warm deformation promotes the Ostwald ripening process and the increase in dislocation density, and hence promotes the accumulation of local high carbon concentrations in the form of Cottrell atmospheres to reach a sufficiently high thermodynamic driving force for austenite nucleation. The critical carbon concentration required for the nucleation of austenite was calculated using classical nucleation theory, which correlated well with the experimental observations.
AUTHOR KEYWORDS: Atom probe tomography (APT); Austenite; Carbon; Nucleation; Steel
DOCUMENT TYPE: Article
SOURCE: Scopus

Zhu, M., Sun, D., Pan, S., Zhang, Q., Raabe, D.
Modelling of dendritic growth during alloy solidification under natural convection
(2014) Modelling and Simulation in Materials Science and Engineering, 22 (3), art. no. 034006, . Cited 8 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84898684038&doi=10.1088%2f0965-0393%2f22%2f3%2f034006&partnerID=40&md5=486b85b1fe4c0a5997349a386573f6e9

DOI: 10.1088/0965-0393/22/3/034006
AFFILIATIONS: Jiangsu Key Laboratory for Advanced Metallic Materials, Southeast University, Nanjing, 211189, China;
School of Mechanical Engineering, Southeast University, Nanjing 211189, China;
Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany
ABSTRACT: A two-dimensional (2D) lattice Boltzmann method (LBM)-cellular automaton model is presented to investigate the dendritic growth of binary alloys in the presence of natural convection. The kinetic-based LBM is adopted to calculate the transport phenomena by the evolution of distribution functions of moving pseudo-particles. To numerically solve natural convection thermal and solute transport simultaneously, three sets of distribution functions are employed in conjunction with the lattice Bhatnagar-Gross-Krook scheme. Based on the LBM calculated local temperature and concentration at the solid/liquid interface, the kinetics of dendritic growth is determined according to a local solute equilibrium approach. Thus, the physics of a complete time-dependent interaction of natural convection, thermal and solutal transport, and dendritic growth during alloy solidification is embedded in the model. Model validation is performed by comparing the simulated results with literature data and analytical predictions. The model is applied to simulate dendritic growth in binary alloys under the influence of natural convection. The effects of Rayleigh numbers and initial undercooling on dendrite growth are investigated. The results show that natural buoyancy flow, induced by thermal and solutal gradients under gravity, transports the heat and solute from the lower region to the upper region. The dendritic growth is thus accelerated in the downward direction, whereas it is inhibited in the upward direction, yielding asymmetrical dendrite patterns. Increasing the Rayleigh number and undercooling will enhance and reduce, respectively, the influence of natural flow on the dendritic growth.
AUTHOR KEYWORDS: cellular automaton; dendritic growth; lattice Boltzmann method; natural convection; solidification

DOCUMENT TYPE: Article
SOURCE: Scopus

Enax, J., Janus, A.M., Raabe, D., Epple, M., Fabritius, H.-O.
Ultrastructural organization and micromechanical properties of shark tooth enameloid
(2014) Acta Biomaterialia, 10 (9), pp. 3959-3968. Cited 16 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84905562273&doi=10.1016%2fj.actbio.2014.04.028&partnerID=40&md5=6edb4938be59c7c8d24b3d97e6487339

DOI: 10.1016/j.actbio.2014.04.028
AFFILIATIONS: Institute of Inorganic Chemistry, Center for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, Universitaetsstr. 5-7, 45117 Essen, Germany;
Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: The outer part of shark teeth is formed by the hard and mineral-rich enameloid that has excellent mechanical properties, which makes it a very interesting model system for the development of new bio-inspired dental materials. We characterized the microstructure, chemical composition and resulting local mechanical properties of the enameloid from teeth of Isurus oxyrinchus (shortfin mako shark) by performing an in-depth analysis using various high-resolution analytical techniques, including scanning electron microscopy, qualitative energy-dispersive X-ray spectroscopy and nanoindentation. Shark tooth enameloid reveals an intricate hierarchical arrangement of thin (50-80 nm) and long (>1 μm) crystallites of fluoroapatite with a high degree of structural anisotropy, which leads to exceptional mechanical properties. Both stiffness and hardness are surprisingly homogeneous in the shiny layer as well as in the enameloid: although both tooth phases differ in structure and composition, they show almost no orientation dependence with respect to the loading direction of the enameloid crystallites. The results were used to determine the structural hierarchy of shark teeth, which can be used as a base for establishing design criteria for synthetic bio-inspired and biomimetic dental composites.
AUTHOR KEYWORDS: Biomineralization; Calcium phosphate; Nanoindentation; Shark tooth enameloid; Structural hierarchy
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Wen, Y.H., Peng, H.B., Si, H.T., Xiong, R.L., Raabe, D.
A novel high manganese austenitic steel with higher work hardening capacity and much lower impact deformation than Hadfield manganese steel
(2014) Materials and Design, 55, pp. 798-804. Cited 18 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84887517933&doi=10.1016%2fj.matdes.2013.09.057&partnerID=40&md5=23e6f5df64287d823195cfd36670be53

DOI: 10.1016/j.matdes.2013.09.057
AFFILIATIONS: College of Manufacturing Science and Engineering, Sichuan University, 610065 Chengdu, China;
Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: To tackle the problem of poor work hardening capacity and high initial deformation under low load in Hadfield manganese steel, the deformation behavior and microstructures under tensile and impact were investigated in a new high manganese austenitic steel Fe18Mn5Si0.35C (wt.%). The results show that this new steel has higher work hardening capacity at low and high strains than Hadfield manganese steel. Its impact deformation is much lower than that of Hadfield manganese steel. The easy occurrence and rapid increase of the amount of stress-induced ε martensitic

transformation account for this unique properties in Fe18Mn5Si0.35C steel. The results indirectly confirm that the formation of distorted deformation twin leads to the anomalous work hardening in Hadfield manganese steel. © 2013 Elsevier Ltd.
AUTHOR KEYWORDS: Hadfield manganese steel; Interstitials; Martensitic phase transformation; Twinning; Work hardening
DOCUMENT TYPE: Article
SOURCE: Scopus

Wen, Y.H., Peng, H.B., Raabe, D., Gutierrez-Urrutia, I., Chen, J., Du, Y.Y.
Large recovery strain in Fe-Mn-Si-based shape memory steels obtained by engineering annealing twin boundaries
(2014) Nature Communications, 5, art. no. 5964, . Cited 8 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84923282742&doi=10.1038%2fncomms5964&partnerID=40&md5=8b25313bd8798ae97a19f9847f9a2643

DOI: 10.1038/ncomms5964
AFFILIATIONS: College of Manufacturing Science and Engineering, Sichuan University, Chengdu, China;
Max-Planck Institut für Eisenforschung, Max-Planck Strasse 1, Düsseldorf, Germany;
Research Center for Strategic Materials, National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba-city, Ibaraki, Japan
ABSTRACT: Shape memory alloys are a unique class of materials that can recover their original shape upon heating after a large deformation. Ti-Ni alloys with a large recovery strain are expensive, while low-cost conventional processed Fe-Mn-Si-based steels suffer from a low recovery strain (<3%). Here we show that the low recovery strain results from interactions between stress-induced martensite and a high density of annealing twin boundaries. Reducing the density of twin boundaries is thus a critical factor for obtaining a large recovery strain in these steels. By significantly suppressing the formation of twin boundaries, we attain a tensile recovery strain of 7.6% in an annealed cast polycrystalline Fe-20.2Mn-5.6Si-8.9Cr-5.0Ni steel (weight%). Further attractiveness of this material lies in its low-cost alloying components and simple synthesis-processing cycle consisting only of casting plus annealing. This enables these steels to be used at a large scale as structural materials with advanced functional properties
DOCUMENT TYPE: Article
SOURCE: Scopus

Demura, M., Raabe, D., Roters, F., Eisenlohr, P., Xu, Y., Hirano, T., Kishida, K.
Slip system analysis in the cold rolling of a Ni3Al single crystal
(2014) Materials Science Forum, 783-786, pp. 1111-1116.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84904543366&partnerID=40&md5=518393546d612b593aa948b1de291f45

AFFILIATIONS: National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237 Düsseldorf, Germany;
Kyoto University, akyo-ku, Kyoto, 606-8501, Japan
ABSTRACT: The activated slip systems were analyzed in the cold rolling of a Ni3Al single crystal with an initial orientation of ~[-112](512), which showed an irregular rolling deformation, i.e. widening, bending, and shear deformation. A phenomenological crystal plasticity model was applied using a spectral method. The boundary condition was optimized to reproduce the actual rolling deformation, as follows. That is, the orthogonal components of the deformation gradient were given from the measured widening and reduction, and the shear components were iteratively optimized as to that

the final orientation was as close to the experimental one as possible. The calculated result showed that three slip systems, a3, b1, and d1 in the Bishop-Hill notation, were mainly activated in the irregular rolling deformation, which result was consistent to the previous observation of the slip traces [Kishida et al., Philos. Mag. 83 (2003) 3029]. The three activated systems were identical to those activated in the plane-strain condition. However, the quantitative comparison revealed that the activity of b1 was significantly reduced in the irregular rolling deformation, while the activity of d1 was enhanced instead. The less activity of b1 and the enhancement of d1 can be understood assuming a strong interaction between a3 and b1. The reaction of this pair has been reported to form the superlattice intrinsic stacking fault (SISF) in Ni3Al [Chiba and Hanada, Philos. Mag. A. 69 (1994) 751]. It is likely that the formation of the SISF, which are considered immobile in Ni3Al, restrained the activation of b1, leading to the irregular rolling deformation.
AUTHOR KEYWORDS: Crystal plasticity; Intermetallic; Lattice rotation; Slip-slip interaction; Spectral method
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Hafez Haghighat, S.M., Von Pezold, J., Race, C.P., Körmann, F., Friák, M., Neugebauer, J., Raabe, D.
Influence of the dislocation core on the glide of the ⟨1 1 ⟩ {1 1 0} edge dislocation in bcc-iron: An embedded atom method study
(2014) Computational Materials Science, 87, pp. 274-282. Cited 4 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84896346177&doi=10.1016%2fj.commatsci.2014.02.031&partnerID=40&md5=95b328bbe8838cad207055f2467f174c

DOI: 10.1016/j.commatsci.2014.02.031
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Institute of Physics of Materials, Academy of Sciences of the Czech Republic, V.v.i., Žižkova 22, 616 62 Brno, Czech Republic
ABSTRACT: Four commonly used embedded atom method potentials for bcc-Fe by Ackland et al. (1997), Mendelev et al. (2003), Chiesa et al. (2009) and Malerba et al. (2010) are critically evaluated with respect to their description of the edge dislocation core structure and its dynamic behavior. Our results allow us to quantify the transferability of the various empirical potentials in the study of the ⟨1 1 ⟩ {1 1 0} edge dislocation core structure and kinetics. Specifically, we show that the equilibrium dislocation core structure is a direct consequence of the shape of the extended gamma surface. We further find that there is a strong correlation between the structure of the edge dislocation core and its glide stress. An in depth analysis of the dislocation migration results reveals that the dominant migration mechanism is via progressing straight line segments of the dislocation. This is further confirmed by the excellent qualitative agreement of nudged elastic band calculations of the Peierls barrier with the dynamically determined critical shear stresses.
AUTHOR KEYWORDS: Core structure; Dislocation glide; Edge dislocation; Iron; Molecular dynamics
DOCUMENT TYPE: Article
SOURCE: Scopus

Stoffers, A., Cojocaru-Miredin, O., Breitenstein, O., Seifert, W., Zaefferer, S., Raabe, D.
Grain boundary characterization in multicrystalline silicon using joint EBSD, EBIC, and atom probe tomography
(2014) 2014 IEEE 40th Photovoltaic Specialist Conference, PVSC 2014, art. no. 6925089, pp. 42-46. Cited 2 times.

https://www.scopus.com/inward/record.uri?eid=2-s2.0-84912072478&doi=10.1109%2fPVSC.2014.6925089&partnerID=40&md5=db6f4db229789ec52c951ca6bfcc6cb6

DOI: 10.1109/PVSC.2014.6925089
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
Brandenburgische Technische Universitat, Platz der Deutschen Einheit 1, Cottbus, Germany;
Brandenburgische Technische Universität, Platz der Deutschen Einheit 1, Cottbus, Germany;
IHP, Im Technologiepark 25, Frankfurt (Oder), Germany
ABSTRACT: The efficiency of multicrystalline silicon solar cells suffers from the presence of extended defects like dislocations and grain boundaries. In fact, the defects themselves do not implicitly have to be harmful, but their interaction with impurities makes them detrimental for the cell efficiencies. © 2014 IEEE.
AUTHOR KEYWORDS: atom probe tomography; grain boundaries; impurities; multicrystalline silicon solar cells; recombination activity
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Song, W., Choi, P.-P., Inden, G., Prahl, U., Raabe, D., Bleck, W.
On the spheroidized carbide dissolution and elemental partitioning in high carbon bearing steel 100Cr6
(2014) Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 45 (2), pp. 595-606. Cited 20 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84895922401&doi=10.1007%2fs11661-013-2048-5&partnerID=40&md5=cf1dcf46747972870251b4df5992ed75

DOI: 10.1007/s11661-013-2048-5
AFFILIATIONS: Department of Ferrous Metallurgy, RWTH Aachen University, Aachen, Germany;
AtomProbe Tomography Research GroupLeader, United States;
Max-Planck-Institut für Eisenforschung GmbH, Dusseldorf, Germany
ABSTRACT: We report on the characterization of high carbon bearing steel 100Cr6 using electron microscopy and atom probe tomography in combination with multi-component diffusion simulations. Scanning electron micrographs show that around 14 vol pct spheroidized carbides are formed during soft annealing and only 3 vol pct remain after dissolution into the austenitic matrix through austenitization at 1123 K (850 °C) for 300 seconds. The spheroidized particles are identified as (Fe, Cr)3C by transmission electron microscopy. Atom probe analysis reveals the redistribution and partitioning of the elements involved, i.e., C, Si, Mn, Cr, Fe, in both, the spheroidized carbides and the bainitic matrix in the sample isothermally heat-treated at 773 K (500 °C) after austenitization. Homogeneous distribution of C and a Cr gradient were detected within the spheroidized carbides. Due to its limited diffusivity in (Fe, Cr) 3C, Cr exhibits a maximum concentration at the surface of spheroidized carbides (16 at. pct) and decreases gradually from the surface towards the core down to about 2 at. pct. The atom probe results also indicate that the partially dissolved spheroidized carbides during austenitization may serve as nucleation sites for intermediate temperature cementite within bainite, which results in a relatively softer surface and harder core in spheroidized particles. This microstructure may contribute to the good wear resistance and fatigue properties of the steel. Good agreement between DICTRA simulations and experimental composition profiles is obtained by an increase of mobility of the substitutional elements in cementite by a factor of five, compared to the mobility in the database MOBFE2. © The Minerals, Metals & Materials Society and ASM International 2013.
DOCUMENT TYPE: Article
SOURCE: Scopus

Demura, M., Raabe, D., Roters, F., Eisenlohr, P., Xu, Y., Hirano, T., Kishida, K.
Slip system analysis in the cold rolling of a Ni3Al single crystal
(2014) Advanced Materials Research, 783-786, pp. 1111-1116.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84902280666&doi=10.4028%2fwww.scientific.net%2fMSF.783-786.1111&partnerID=40&md5=8fc14dd2c04c379697964e69ab5bf1ea

DOI: 10.4028/www.scientific.net/MSF.783-786.1111
AFFILIATIONS: National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, D-40237 Düsseldorf, Germany;
Kyoto University, akyo-ku, Kyoto, 606-8501, Japan
ABSTRACT: The activated slip systems were analyzed in the cold rolling of a Ni3Al single crystal with an initial orientation of ~[-112](512), which showed an irregular rolling deformation, i.e. widening, bending, and shear deformation. A phenomenological crystal plasticity model was applied using a spectral method. The boundary condition was optimized to reproduce the actual rolling deformation, as follows. That is, the orthogonal components of the deformation gradient were given from the measured widening and reduction, and the shear components were iteratively optimized as to that the final orientation was as close to the experimental one as possible. The calculated result showed that three slip systems, a3, b1, and d1 in the Bishop-Hill notation, were mainly activated in the irregular rolling deformation, which result was consistent to the previous observation of the slip traces [Kishida et al., Philos. Mag. 83 (2003) 3029]. The three activated systems were identical to those activated in the plane-strain condition. However, the quantitative comparison revealed that the activity of b1 was significantly reduced in the irregular rolling deformation, while the activity of d1 was enhanced instead. The less activity of b1 and the enhancement of d1 can be understood assuming a strong interaction between a3 and b1. The reaction of this pair has been reported to form the superlattice intrinsic stacking fault (SISF) in Ni3Al [Chiba and Hanada, Philos. Mag. A. 69 (1994) 751]. It is likely that the formation of the SISF, which are considered immobile in Ni3Al, restrained the activation of b1, leading to the irregular rolling deformation.
AUTHOR KEYWORDS: Crystal plasticity; Intermetallic; Lattice rotation; Slip-slip interaction; Spectral method
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Wang, F., Sandlöbes, S., Diehl, M., Sharma, L., Roters, F., Raabe, D.
In situ observation of collective grain-scale mechanics in Mg and Mg-rare earth alloys
(2014) Acta Materialia, 80, pp. 77-93. Cited 16 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84906709190&doi=10.1016%2fj.actamat.2014.07.048&partnerID=40&md5=10ddcc9e8e31087cedc1c9496a55ca88

DOI: 10.1016/j.actamat.2014.07.048
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Department for Microstructure Physics and Alloy Design, Max-Planck-Str. 1, Düsseldorf, Germany;
University of Virginia, Materials Science and Engineering, Charlottesville, VA, United States
ABSTRACT: The microstructure evolution of pure Mg and two Mg-rare-earth alloys (Mg-3 wt.% Dy and Mg-3 wt.% Er) was studied during in situ compression tests by electron backscatter diffraction and electron channelling contrast imaging. Strain localization and the formation of an early stage shear band ("pre-shear band") were observed in pure Mg during

compressive deformation below 5% engineering strain. In the experiments percolative grain clusters with prevalent basal slip as a precursor for shear band formation was observed. This collective grain-cluster shear behaviour was analysed in more detail using crystal plasticity simulations, revealing a percolation of intense basal slip activity across grain boundaries as the mechanism for shear band initiation. Plane trace analysis, Schmid factor calculation and deformation transfer analysis at the grain boundaries were performed for the activated twins. It appears that many activated tension twins exhibit pronounced non-Schmid behaviour. Twinning appears to be a process of accommodating local strain rather than a response to macroscopic strain.
AUTHOR KEYWORDS: Crystal plasticity modelling; Deformation twinning; Electron channelling contrast imaging; Magnesium; Shear banding
DOCUMENT TYPE: Article
SOURCE: Scopus

Yan, F.K., Tao, N.R., Archie, F., Gutierrez-Urrutia, I., Raabe, D., Lu, K.
Deformation mechanisms in an austenitic single-phase duplex microstructured steel with nanotwinned grains
(2014) Acta Materialia, 81, pp. 487-500. Cited 25 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84908210904&doi=10.1016%2fj.actamat.2014.08.054&partnerID=40&md5=dd980b22380da6f1fcdf21ca1bb53157

DOI: 10.1016/j.actamat.2014.08.054
AFFILIATIONS: Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China;
Max-Planck-Institut fur Eisenforschung, Max-Planck Str. 1, Dusseldorf, Germany;
Herbert Gleiter Institute of Nanoscience, Nanjing University of Science and Technology, Nanjing, China
ABSTRACT: A novel type of duplex microstructure is generated in a single-phase austenitic steel (AISI 316L; X2CrNiMo19-12), consisting of plastically compliant recrystallized austenitic grains as the matrix containing coarse non-recrystallized grains with a nanotwinned austenitic (nt-γ) structure as strengthening inclusions. This novel type of single-phase yet duplex microstructured steel exhibits an excellent combination of strength and ductility. We study the plastic co-deformation mechanisms between the nanotwinned and the recrystallized grains under tension using electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM). At tensile strains below 5%, the nt-γ grains nearly deform homogeneously in conjunction with the surrounding statically recrystallized (SRX) grains without generating notable strain localization near their interfaces. The anisotropic plastic deformation of the nt-γ grains with predominant shear parallel to the twin boundaries results in a higher dislocation density in the neighboring SRX grains. As the strain exceeds 12%, localized deformation occurs within the nt-γ grains in the form of shear banding. A strain gradient is developed in the surrounding SRX grains as a function of distance from the nt-γ/SRX interface. Deformation twinning is observed in the SRX grains near the nt-γ grains, while away from nt-γ grains dislocation slip dominates the deformation. The strengthening effect of the strong and ductile nt-γ grains may offer a novel approach to strengthen austenitic steels and related alloys by generating a nanotwinned/recrystallized duplex microstructure.
AUTHOR KEYWORDS: Austenitic steels; Nano-twinned structures; Plastic deformation mechanism; TEM and EBSD characterization
DOCUMENT TYPE: Article
SOURCE: Scopus

Tasan, C.C., Hoefnagels, J.P.M., Diehl, M., Yan, D., Roters, F., Raabe, D.

Strain localization and damage in dual phase steels investigated by coupled in-situ deformation experiments and crystal plasticity simulations
(2014) International Journal of Plasticity, 63, pp. 198-210. Cited 88 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84922689409&doi=10.1016%2fj.ijplas.2014.06.004&partnerID=40&md5=2b12a6cf1ec50327d1b7490aa496dfc0

DOI: 10.1016/j.ijplas.2014.06.004
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, Düsseldorf, Germany;
Eindhoven University of Technology, Dep. of Mech. Eng., P.O. Box 513, Eindhoven, Netherlands
ABSTRACT: Ferritic-martensitic dual phase (DP) steels deform spatially in a highly heterogeneous manner, i.e. with strong strain and stress partitioning at the micro-scale. Such heterogeneity in local strain evolution leads in turn to a spatially heterogeneous damage distribution, and thus, plays an important role in the process of damage inheritance and fracture. To understand and improve DP steels, it is important to identify connections between the observed strain and damage heterogeneity and the underlying microstructural parameters, e.g. ferrite grain size, martensite distribution, martensite fraction, etc. In this work we pursue this aim by conducting in-situ deformation experiments on two different DP steel grades, employing two different microscopic-digital image correlation (μDIC) techniques to achieve microstructural strain maps of representative statistics and high-resolution. The resulting local strain maps are analyzed in connection to the observed damage incidents (identified by image post-processing) and to local stress maps (obtained from crystal plasticity (CP) simulations of the same microstructural area). The results reveal that plasticity is typically initiated within "hot zones" with larger ferritic grains and lower local martensite fraction. With increasing global deformation, damage incidents are most often observed in the boundary of such highly plastified zones. High-resolution μDIC and the corresponding CP simulations reveal the importance of martensite dispersion: zones with bulky martensite are more susceptible to macroscopic localization before the full strain hardening capacity of the material is consumed. Overall, the presented joint analysis establishes an integrated computational materials engineering (ICME) approach for designing advanced DP steels.
AUTHOR KEYWORDS: A. Microcracking; A. Voids and inclusions; B. Crystal plasticity; C. Electron microscopy; Digital image correlation
DOCUMENT TYPE: Article
SOURCE: Scopus

Tasan, C.C., Diehl, M., Yan, D., Zambaldi, C., Shanthraj, P., Roters, F., Raabe, D.
Integrated experimental-simulation analysis of stress and strain partitioning in multiphase alloys
(2014) Acta Materialia, 81, pp. 386-400. Cited 74 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84908214186&doi=10.1016%2fj.actamat.2014.07.071&partnerID=40&md5=a67c902b9379d476120f357b96b629fa

DOI: 10.1016/j.actamat.2014.07.071
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany
ABSTRACT: The mechanical response of multiphase alloys is governed by the microscopic strain and stress partitioning behavior among microstructural constituents. However, due to limitations in the characterization of the partitioning that takes place at the submicron scale, microstructure optimization of such alloys is typically based on evaluating the averaged response, referring to, for example, macroscopic stress-strain curves. Here, a novel experimental-numerical methodology is introduced to

strengthen the integrated understanding of the microstructure and mechanical properties of these alloys, enabling joint analyses of deformation-induced evolution of the microstructure, and the strain and stress distribution therein, down to submicron resolution. From the experiments, deformation-induced evolution of (i) the microstructure, and (ii) the local strain distribution are concurrently captured, employing in situ secondary electron imaging and electron backscatter diffraction (EBSD) (for the former), and microscopic-digital image correlation (for the latter). From the simulations, local strain as well as stress distributions are revealed, through 2-D full-field crystal plasticity (CP) simulations conducted with an advanced spectral solver suitable for heterogeneous materials. The simulated model is designed directly from the initial EBSD measurements, and the phase properties are obtained by additional inverse CP simulations of nanoindentation experiments carried out on the original microstructure. The experiments and simulations demonstrate good correlation in the proof-of-principle study conducted here on a martensite-ferrite dual-phase steel, and deviations are discussed in terms of limitations of the techniques involved. Overall, the presented integrated computational materials engineering approach provides a vast amount of well-correlated structural and mechanical data that enhance our understanding as well as the design capabilities of multiphase alloys.
AUTHOR KEYWORDS: Crystal plasticity; Digital image correlation; Dual-phase steel; In situ testing; Spectral method
DOCUMENT TYPE: Article
SOURCE: Scopus

Guo, W., Jägle, E., Yao, J., Maier, V., Korte-Kerzel, S., Schneider, J.M., Raabe, D.
Intrinsic and extrinsic size effects in the deformation of amorphous CuZr/nanocrystalline Cu nanolaminates
(2014) Acta Materialia, 80, pp. 94-106. Cited 38 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84906656042&doi=10.1016%2fj.actamat.2014.07.027&partnerID=40&md5=5e089bf89d02f1d9b23ba115c84fd961

DOI: 10.1016/j.actamat.2014.07.027
AFFILIATIONS: Department of Microstructure Physics and Alloy Design, Max-Planck Institut für Eisenforschung, Düsseldorf 40237, Germany;
Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China;
Lehrstuhl für Allgemeine Werkstoffeigenschaften, FAU Erlangen-Nürnberg, Erlangen 91058, Germany;
Institut für Metallkunde und Metallphysik, RWTH Aachen University, Aachen 52074, Germany;
Lehrstuhl für Werkstoffchemie, RWTH Aachen University, Aachen 52074, Germany
ABSTRACT: Introducing a soft crystalline phase into an amorphous alloy can promote the compound's ductility. Here we synthesized multilayered nanolaminates consisting of alternating amorphous Cu54Zr46 and nanocrystalline Cu layers. The Cu layer thickness was systematically varied in different samples. Mechanical loading was imposed by nanoindentation and micropillar compression. Increasing the Cu layer thickness from 10 to 100 nm led to a transition from sharp, cross-phase shear banding to gradual bending and co-deformation of the two layer types (amorphous/nanocrystalline). Specimens with a sequence of 100 nm amorphous Cu54Zr46 and 50 nm Cu layers show a compressive flow stress of 2.57 ± 0.21 GPa, matching the strength of pure CuZr metallic glass, hence exceeding the linear rule of mixtures. In pillar compression, 40% strain without fracture was achieved by the suppression of percolative shear band propagation. The results show that inserting a ductile nanocrystalline phase into a metallic glass prevents catastrophic shear banding. The mechanical response of such

nanolaminates can be tuned by adjusting the layer thickness.
AUTHOR KEYWORDS: Metallic glass; Nanolaminates; Nanotwins; Shear band
DOCUMENT TYPE: Article
SOURCE: Scopus

Tasan, C.C., Deng, Y., Pradeep, K.G., Yao, M.J., Springer, H., Raabe, D.
Composition Dependence of Phase Stability, Deformation Mechanisms, and Mechanical Properties of the CoCrFeMnNi High-Entropy Alloy System
(2014) JOM, 66 (10), pp. 1993-2001. Cited 47 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84910156576&doi=10.1007%2fs11837-014-1133-6&partnerID=40&md5=c11a465bd4c2f93570cf617165253ae9

DOI: 10.1007/s11837-014-1133-6
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Düsseldorf, Germany; Materials Chemistry, RWTH Aachen University, Aachen, Germany
ABSTRACT: The proposal of configurational entropy maximization to produce massive solid-solution (SS)-strengthened, single-phase high-entropy alloy (HEA) systems has gained much scientific interest. Although most of this interest focuses on the basic role of configurational entropy in SS formability, setting future research directions also requires the overall property benefits of massive SS strengthening to be carefully investigated. To this end, taking the most promising CoCrFeMnNi HEA system as the starting point, we investigate SS formability, deformation mechanisms, and the achievable mechanical property ranges of different compositions and microstructural states. A comparative assessment of the results with respect to room temperature behavior of binary Fe-Mn alloys reveals only limited benefits of massive SS formation. Nevertheless, the results also clarify that the compositional requirements in this alloy system to stabilize the face-centered cubic (fcc) SS are sufficiently relaxed to allow considering nonequiatomic compositions and exploring improved strength–ductility combinations at reduced alloying costs. © 2014, The Minerals, Metals & Materials Society.
DOCUMENT TYPE: Article
SOURCE: Scopus

Sandim, H.R.Z., Bolmaro, R.E., Renzetti, R.A., Sandim, M.J.R., Hartwig, K.T., Vogel, S.C., Raabe, D.
Texture evolution as determined by in situ neutron diffraction during annealing of iron deformed by equal channel angular pressing
(2014) Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 45 (10), pp. 4235-4246. Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84928822996&doi=10.1007%2fs11661-014-2401-3&partnerID=40&md5=5e135ce7c113afdd23dbe7373a3b0ee5

DOI: 10.1007/s11661-014-2401-3
AFFILIATIONS: Escola de Engenharia de Lorena, Universidade de São Paulo, Lorena 12600-970, Brazil;
Instituto de Física Rosario, CONICET - UNR, Rosario 2000, Argentina;
Universidade Federal de Itajubá, Itajubá, Brazil;
Department of Mechanical Engineering, Texas AandM University, College Station, TX 77843-3123, United States;
Los Alamos Neutron Science Center, LANSCE-LANL, Los Alamos, NM 87545, United States;
Max-Planck-Institut für Eisenforschung, Düsseldorf 40237, Germany
ABSTRACT: In situ neutron diffraction experiments were performed to follow the annealing behavior of iron deformed by equal-channel angular pressing at room temperature using route B <inf>c</inf> to a total von Mises strain of ε <inf>vM</inf> = 9.2. The temperature was varied from room temperature to 1223 K (950 °C), while neutron diffraction data for quantitative texture analysis were collected at a given temperature when holding for 5 minutes.

Pole figures and orientation distribution function maps from neutron diffraction and electron backscatter diffraction measurements were used to follow the changes in crystallographic texture and grain size during annealing. In situ neutron diffraction experiments allowed understanding and identifying texture-related changes that occur during recrystallization, grain growth, and phase transformation in iron.
DOCUMENT TYPE: Article
SOURCE: Scopus

Raabe, D., Springer, H., Gutierrez-Urrutia, I., Roters, F., Bausch, M., Seol, J.-B., Koyama, M., Choi, P.-P., Tsuzaki, K.
Alloy Design, Combinatorial Synthesis, and Microstructure–Property Relations for Low-Density Fe-Mn-Al-C Austenitic Steels
(2014) JOM, 66 (9), pp. 1845-1856. Cited 45 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84920252209&doi=10.1007%2fs11837-014-1032-x&partnerID=40&md5=960e44a516521d3293f239900b7478e3

DOI: 10.1007/s11837-014-1032-x
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany; Department of Mechanical Engineering, Kyushu University, 744 Motooka, Nishi-ku, Fukuoka, Fukuoka, Japan
ABSTRACT: We present recent developments in the field of austenitic steels with up to 18% reduced mass density. The alloys are based on the Fe-Mn-Al-C system. Here, two steel types are addressed. The first one is a class of low-density twinning-induced plasticity or single phase austenitic TWIP (SIMPLEX) steels with 25–30 wt.% Mn and <4–5 wt.% Al or even <8 wt.% Al when naturally aged. The second one is a class of κ-carbide strengthened austenitic steels with even higher Al content. Here, κ-carbides form either at 500–600°C or even during quenching for >10 wt.% Al. Three topics are addressed in more detail, namely, the combinatorial bulk high-throughput design of a wide range of corresponding alloy variants, the development of microstructure–property relations for such steels, and their susceptibility to hydrogen embrittlement. © 2014, The Minerals, Metals & Materials Society.
DOCUMENT TYPE: Article
SOURCE: Scopus

Schwarz, T., Cojocaru-Mirédin, O., Choi, P.-P., Lämmle, A., Würz, R., Mousel, M., Redinger, A., Siebentritt, S., Botti, S., Raabe, D.
Nano-scale characterization of thin-film solar cells
(2014) Microscopy and Microanalysis, 20 (3), pp. 394-395.
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DOI: 10.1017/S1431927614003699
AFFILIATIONS: Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden Württemberg, Stuttgart, Germany;
Laboratory for Photovoltaics, University of Luxembourg, Belvaux, Luxembourg;
LPMCN, CRNS, Université Lyon 1, Villerbanne, France;
Laboratoire des Solides Irradiés and ETSF, École Polytechnique, CNRS, Polaiseau, France
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Duarte, M.J., Kostka, A., Jimenez, J.A., Choi, P., Klemm, J., Crespo, D., Raabe, D., Renner, F.U.

Crystallization, phase evolution and corrosion of Fe-based metallic glasses: An atomic-scale structural and chemical characterization study
(2014) Acta Materialia, 71, pp. 20-30. Cited 14 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84896690263&doi=10.1016%2fj.actamat.2014.02.027&partnerID=40&md5=b9f66cd2fa03f9f34a6b7a38bd8cefe3

DOI: 10.1016/j.actamat.2014.02.027
AFFILIATIONS: Department of Interface Chemistry and Surface Engineering, Max-Planck Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany;
Department of Microstructure Physics and Alloy Design, Max-Planck Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany;
CENIM-CSIC, Avda. Gregorio del Amo 8, 28040 Madrid, Spain;
Departament de Fisica Aplicada, Universitat Politècnica de Catalunya, 08860 Castelldefels, Spain;
Instituut voor Materiaalonderzoek, Universiteit Hasselt, 3590 Diepenbeek, Belgium
ABSTRACT: Understanding phase changes, including their formation and evolution, is critical for the performance of functional as well as structural materials. We analyze in detail microstructural and chemical transformations of the amorphous steel Fe50Cr15Mo14C15B6 during isothermal treatments at temperatures ranging from 550 to 800 °C. By combining high-resolution transmission electron microscopy and Rietveld analyses of X-ray diffraction patterns together with the local chemical data obtained by atom probe tomography, this research provides relevant information at the atomic scale about the mechanisms of crystallization and the subsequent phases evolution. During the initial stages of crystallization a stable (Fe,Cr)23(C,B)6 precipitates as well as two metastable intermediates of M3(C,B) and the intermetallic χ-phase. When full crystallization is reached, only a percolated nano-scale Cr-rich (Fe,Cr)23(C,B)6 and Mo-rich η-Fe3Mo3C structure is detected, with no evidence to suggest that other phases appear at any subsequent time. Finally, the corrosion behavior of the developed phases is discussed from considerations of the obtained atomic information.

AUTHOR KEYWORDS: Atom probe tomography; Crystallization; Metallic glasses; Phase evolution; Transmission electron microscopy
DOCUMENT TYPE: Article
SOURCE: Scopus

Raabe, D., Herbig, M., Sandlöbes, S., Li, Y., Tytko, D., Kuzmina, M., Ponge, D., Choi, P.-P.
Grain boundary segregation engineering in metallic alloys: A pathway to the design of interfaces
(2014) Current Opinion in Solid State and Materials Science, 18 (4), pp. 253-261. Cited 67 times.
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DOI: 10.1016/j.cossms.2014.06.002
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Department for Microstructure Physics and Alloy Design, Max-Planck-Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: Grain boundaries influence mechanical, functional, and kinetic properties of metallic alloys. They can be manipulated via solute decoration enabling changes in energy, mobility, structure, and cohesion or even promoting local phase transformation. In the approach which we refer here to as 'segregation engineering' solute decoration is not regarded as an undesired phenomenon but is instead utilized to manipulate specific grain boundary structures, compositions and properties that enable useful material behavior. The underlying thermodynamics follow the adsorption isotherm. Hence, matrix-solute combinations suited for designing interfaces in metallic alloys can be identified by considering four main aspects,

namely, the segregation coefficient of the decorating element; its effects on interface cohesion, energy, structure and mobility; its diffusion coefficient; and the free energies of competing bulk phases, precipitate phases or complexions. From a practical perspective, segregation engineering in alloys can be usually realized by a modest diffusion heat treatment, hence, making it available in large scale manufacturing.
AUTHOR KEYWORDS: Atom probe tomography; Grain boundary; Phase transformation; Segregation
DOCUMENT TYPE: Article
SOURCE: Scopus

Mehrtens, T., Schowalter, M., Tytko, D., Choi, P., Raabe, D., Hoffmann, L., Jönen, H., Rossow, U., Hangleiter, A., Rosenauer, A.
Measuring composition in InGaN from HAADF-STEM images and studying the temperature dependence of Z-contrast
(2013) Journal of Physics: Conference Series, 471 (1), art. no. 012009, .
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DOI: 10.1088/1742-6596/471/1/012009
AFFILIATIONS: Institute of Solid State Physics, University of Bremen, 28359 Bremen, Germany;
Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany;
Institute of Applied Physics, TU Braunschweig, 38106 Braunschweig, Germany
ABSTRACT: In this contribution, the indium concentration profile of an In xGa1-xN/GaN five-fold multi quantum well structure is measured from high-angle annular dark field scanning transmission electron microscopy (HAADF-STEM) images. The results are compared with an atom probe tomography study. Indium concentrations in the range of 26 at.% to 33 at.% are measured in the centre of the quantum wells. An additional indium layer of 14 at.% has been found on top of the quantum wells. In the second part, the temperature dependence of measured intensities in GaN is investigated. Here, multislice calculations in the frozen lattice approximation are carried out in dependence of specimen thickness and compared to experimental data. An increase of intensity with specimen temperature is found.
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Scheunemann, L., Balzani, D., Brands, D., Schröder, J., Raabe, D.
Statistically similar RVE construction based on 3D dual-phase steel microstructures
(2013) Research and Applications in Structural Engineering, Mechanics and Computation - Proceedings of the 5th International Conference on Structural Engineering, Mechanics and Computation, SEMC 2013, pp. 411-416. Cited 3 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84889065995&partnerID=40&md5=6c01c2888e84d167fa0d265bc00c34ee

AFFILIATIONS: Faculty of Engineering, Institute of Mechanics, University Duisburg-Essen, Essen, Germany;
Department of Microstructure Physics and Alloy Design, Max-Planck-Institut Für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: This contribution presents a method to construct three-dimensional Statistically Similar RVEs (SSRVEs) for the simulation of the mechanical response of dual-phase steel (DP steel). DP steels have enhanced material properties such as high ductility and high strength compared to conventional steels. Since these properties originate in the microstructure of the material, it should be incorporated in the numerical calculations in order to account for these microstructural effects. This can be accomplished by using the FE2 - method, however for an efficient computation SSRVEs with a reduced complexity compared to the real

microstructure have to be defined. These SSRVEs still represent the mechanical response of the material accurately. The method for the construction of SSRVEs is based on a least-square functional considering suitable statistical measures describing the inclusion morphology of the real microstructure. In numerical examples, the mechanical response of the SSRVE is compared to the response of the real microstructure. © 2013 Taylor & Francis Group, London, UK.
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Nakada, N., Tsuchiyama, T., Takaki, S., Ponge, D., Raabe, D.
Transition from diffusive to displacive austenite reversion in low-alloy steel
(2013) ISIJ International, 53 (12), pp. 2275-2277. Cited 14 times.
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DOI: 10.2355/isijinternational.53.2275
AFFILIATIONS: Department of Materials Science and Engineering, Graduate School of Engineering, Kyushu University, 744 Moto-oka, Nishiku, Fukuoka, 819-0395, Japan;
International Institute for Carbon Neutral Energy Research (WPI-I2CNER), Kyushu University, 744 Moto-oka, Nishi-ku, Fukuoka, 819-0395, Japan;
Max-Planck-Institute für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, 40237, Germany
ABSTRACT: For understanding the transition from diffusive to displacive austenite reversion mechanism in steel, the effect of heating rate on austenite reversion behavior was investigated in 0.15%C- 5%Mn steel. Austenite reversion temperature first increased gradually with the heating rate owing to the superheating effect and then remained at a constant temperature above a critical heating rate. In response, the austenite formed by rapid heating exhibited a coarse prior austenite grain structure, indicating the occurrence of displacive reversion even in low-alloy steel. © 2013 ISIJ.
AUTHOR KEYWORDS: Displacive reversion; Heating rate; Low-alloy steel; Transition of reversion mechanism
DOCUMENT TYPE: Article
SOURCE: Scopus

Povstugar, I., Choi, P.-P., Tytko, D., Ahn, J.-P., Raabe, D.
Interface-directed spinodal decomposition in TiAlN/CrN multilayer hard coatings studied by atom probe tomography
(2013) Acta Materialia, 61 (20), pp. 7534-7542. Cited 19 times.
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DOI: 10.1016/j.actamat.2013.08.028
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Department of Microstructure Physics and Alloy Design, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Korea Institute of Science and Technology, Advanced Analysis Center, P.O. Box 131, Cheongryang, 130-650 Seoul, South Korea
ABSTRACT: Microstructural and compositional changes in TiAlN/CrN multilayered films occurring at temperatures up to 1000 C were studied at different length scales by a combination of atom probe tomography, transmission electron microscopy and X-ray diffraction. We observe the onset of decomposition of the multilayer structure at 700 C via the mechanism of interface-directed spinodal decomposition of TiAlN layers, where Al atoms preferentially move toward the nearest interface and segregate there. The interface-directed mechanism later transforms into isotropic spinodal decomposition and is accompanied by intense

interdiffusion between the constituting layers. Distinct compositional gradients across columnar grain boundaries (extending perpendicular to the multilayers) are detected at this stage of decomposition. Drastic differences in decomposition behavior across the film depth were observed at elevated temperatures (800-1000 C): the layered structure completely dissolves in the near-surface part but persists in the regions distant from the surface. The influence of residual stresses caused by the sputter deposition process on the thermally induced evolution of the multilayer thin films is discussed.
AUTHOR KEYWORDS: Atom probe tomography (APT); Multilayer thin films; Nitrides; Residual stresses; Spinodal decomposition
DOCUMENT TYPE: Article
SOURCE: Scopus

Cojocaru-Mirédin, O., Schwarz, T., Choi, P.P., Herbig, M., Wuerz, R., Raabe, D.
Atom probe tomography studies on the Cu(In,ga)Se2 grain boundaries.
(2013) Journal of visualized experiments : JoVE, (74), . Cited 8 times.
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AFFILIATIONS: Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH.
ABSTRACT: Compared with the existent techniques, atom probe tomography is a unique technique able to chemically characterize the internal interfaces at the nanoscale and in three dimensions. Indeed, APT possesses high sensitivity (in the order of ppm) and high spatial resolution (sub nm). Considerable efforts were done here to prepare an APT tip which contains the desired grain boundary with a known structure. Indeed, site-specific sample preparation using combined focused-ion-beam, electron backscatter diffraction, and transmission electron microscopy is presented in this work. This method allows selected grain boundaries with a known structure and location in Cu(In,Ga)Se2 thin-films to be studied by atom probe tomography. Finally, we discuss the advantages and drawbacks of using the atom probe tomography technique to study the grain boundaries in Cu(In,Ga)Se2 thin-film solar cells.
DOCUMENT TYPE: Article
SOURCE: Scopus

Song, W., Von Appen, J., Choi, P., Dronskowski, R., Raabe, D., Bleck, W.
Atomic-scale investigation of ε and θ precipitates in bainite in 100Cr6 bearing steel by atom probe tomography and ab initio calculations
(2013) Acta Materialia, 61 (20), pp. 7582-7590. Cited 19 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84886289410&doi=10.1016%2fj.actamat.2013.08.051&partnerID=40&md5=3276aa7033acb278bd79bf8e5df020a8

DOI: 10.1016/j.actamat.2013.08.051
AFFILIATIONS: Department of Ferrous Metallurgy, RWTH Aachen University, Aachen, Germany;
Institute of Inorganic Chemistry, RWTH Aachen University, Aachen, Germany;
Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
ABSTRACT: Carbide precipitation during upper and lower bainite formation in high-carbon bearing steel 100Cr6 is characterized using transmission electron microscopy and atom probe tomography. The results reveal that both ε and θ carbides precipitate in lower bainite isothermally held at 260 C and only θ precipitates form in upper bainite isothermally held at 500 C. ε and θ precipitate under paraequilibrium condition at 260 C in lower bainite and θ precipitates under negligible partitioning local equilibrium condition in upper bainite at 500 C. In order to theoretically study ε and θ precipitation and the ε → θ transition in bainite, thermodynamic

calculations have been carried out using ab initio techniques. We find that ε and θ carbides in ferrite have almost identical thermodynamic stability, and hence have similar formation probability. In austenite, however, cementite formation is clearly preferred: it is favored by 5 kJ mol-1 at room temperature and still by 4 kJ mol-1 at 500 C. Hence, the thermodynamic predictions agree well with the atom probe tomography results.
AUTHOR KEYWORDS: ε carbide; Ab initio; Atom probe tomography; Cementite
DOCUMENT TYPE: Article
SOURCE: Scopus

Marceau, R.K.W., Gutierrez-Urrutia, I., Herbig, M., Moore, K.L., Lozano-Perez, S., Raabe, D.
Multi-scale correlative microscopy investigation of both structure and chemistry of deformation twin bundles in Fe-Mn-C steel
(2013) Microscopy and Microanalysis, 19 (6), pp. 1581-1585. Cited 5 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84887904550&doi=10.1017%2fS1431927613013494&partnerID=40&md5=21c9e727aa1e2f99add3bcfd3f129eff

DOI: 10.1017/S1431927613013494
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Strae 1, 40237 Düsseldorf, Germany;
Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom
ABSTRACT: A multi-scale investigation of twin bundles in Fe-22Mn-0.6C (wt%) twinning-induced plasticity steel after tensile deformation has been carried out by truly correlative means; using electron channelling contrast imaging combined with electron backscatter diffraction, high-resolution secondary ion mass spectrometry, scanning transmission electron microscopy, and atom probe tomography on the exact same region of interest in the sample. It was revealed that there was no significant segregation of Mn or C to the twin boundary interfaces. Copyright © 2013 Microscopy Society of America.
AUTHOR KEYWORDS: atom probe tomography; austenitic steels; correlative microscopy; electron channelling contrast imaging; high-resolution secondary ion mass spectrometry; scanning transmission electron microscopy; twinning
DOCUMENT TYPE: Article
SOURCE: Scopus

Herbig, M., Raabe, D., Li, Y.J., Choi, P., Zaefferer, S., Goto, S.
Atomic-scale quantification of grain boundary segregation in nanocrystalline material
(2013) Physical Review Letters, 112 (12), art. no. 126103, . Cited 86 times.
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DOI: 10.1103/PhysRevLett.112.126103
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany;
Department of Materials Science and Engineering, Faculty of Engineering and Resource Science, Akita University, Tegata Gakuencho, Akita 010-8502, Japan
ABSTRACT: Grain boundary segregation leads to nanoscale chemical variations that can alter a material's performance by orders of magnitude (e.g., embrittlement). To understand this phenomenon, a large number of grain boundaries must be characterized in terms of both their five crystallographic interface parameters and their atomic-scale chemical composition. We demonstrate how this can be achieved using an approach that combines the accuracy of structural characterization in transmission electron microscopy with the 3D chemical sensitivity of atom probe

tomography. We find a linear trend between carbon segregation and the misorientation angle ω for low-angle grain boundaries in ferrite, which indicates that ω is the most influential crystallographic parameter in this regime. However, there are significant deviations from this linear trend indicating an additional strong influence of other crystallographic parameters (grain boundary plane, rotation axis). For high-angle grain boundaries, no general trend between carbon excess and ω is observed; i.e., the grain boundary plane and rotation axis have an even higher influence on the segregation behavior in this regime. Slight deviations from special grain boundary configurations are shown to lead to unexpectedly high levels of segregation. © 2014 American Physical Society.
DOCUMENT TYPE: Article
SOURCE: Scopus

Hemzalová, P., Friák, M., Šob, M., Ma, D., Udyansky, A., Raabe, D., Neugebauer, J.
Ab initio study of thermodynamic, electronic, magnetic, structural, and elastic properties of Ni4N allotropes
(2013) Physical Review B - Condensed Matter and Materials Physics, 88 (17), art. no. 174103, . Cited 3 times.
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DOI: 10.1103/PhysRevB.88.174103
AFFILIATIONS: Department of Chemistry, Faculty of Science, Masaryk University, Kotlářská 2, CZ-611 37 Brno, Czech Republic;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, D-40237 Düsseldorf, Germany;
Central European Institute of Technology, CEITEC MU, Masaryk University, Kamenice 5, CZ-625 00 Brno, Czech Republic;
Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Žižkova 22, CZ-616 62 Brno, Czech Republic
ABSTRACT: We have employed parameter-free density functional theory calculations to study the thermodynamic stability and structural parameters as well as elastic and electronic properties of Ni4N in eight selected crystallographic phases. In agreement with the experimental findings, the cubic structure with Pearson symbol cP5, space group $Pm\bar{3}m$ (221) is found to be the most stable and it is also the only thermodynamically stable structure at T=0 K with respect to decomposition to the elemental Ni crystal and N2 gas phase. We determine structural parameters, bulk moduli, and their pressure derivatives for all eight allotropes. The thermodynamic stability and bulk modulus is shown to be anticorrelated. Comparing ferromagnetic and nonmagnetic states, we find common features between the magnetism of elemental Ni and studied ferromagnetic Ni4N structures. For the ground-state Ni4N structure and other two Ni4N cubic allotropes, we predict a complete set of single-crystalline elastic constants (in the equilibrium and under hydrostatic pressure), the Young and area moduli, as well as homogenized polycrystalline elastic moduli obtained by different homogenization methods. We demonstrate that the elastic anisotropy of the ground-state Ni4N is qualitatively opposite to that in the elemental Ni, i.e., these materials have hard and soft crystallographic directions interchanged. Moreover, one of the studied metastable cubic phases is found auxetic, i.e., exhibiting negative Poisson ratio. © 2013 American Physical Society.
DOCUMENT TYPE: Article
SOURCE: Scopus

Enax, J., Fabritius, H.-O., Rack, A., Prymak, O., Raabe, D., Epple, M.
Characterization of crocodile teeth: Correlation of composition, microstructure, and hardness
(2013) Journal of Structural Biology, 184 (2), pp. 155-163. Cited 14 times.

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DOI: 10.1016/j.jsb.2013.09.018
AFFILIATIONS: Institute of Inorganic Chemistry and Center for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, Universitaetsstr. 5-7, 45117 Essen, Germany;
Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
European Synchrotron Radiation Facility (ESRF), 6 Rue Jules Horowitz, 38000 Grenoble Cedex, France
ABSTRACT: Structure and composition of teeth of the saltwater crocodile Crocodylus porosus were characterized by several high-resolution analytical techniques. X-ray diffraction in combination with elemental analysis and infrared spectroscopy showed that the mineral phase of the teeth is a carbonated calcium-deficient nanocrystalline hydroxyapatite in all three tooth-constituting tissues: Dentin, enamel, and cementum. The fluoride content in the three tissues is very low (<0.1. wt.%) and comparable to that in human teeth. The mineral content of dentin, enamel, and cementum as determined by thermogravimetry is 71.3, 80.5, and 66.8. wt.%, respectively. Synchrotron X-ray microtomography showed the internal structure and allowed to visualize the degree of mineralization in dentin, enamel, and cementum. Virtual sections through the tooth and scanning electron micrographs showed that the enamel layer is comparably thin (100-200 μm). The crystallites in the enamel are oriented perpendicularly to the tooth surface. At the dentin-enamel-junction, the packing density of crystallites decreases, and the crystallites do not display an ordered structure as in the enamel. The microhardness was 0.60 ± 0.05. GPa for dentin, 3.15 ± 0.15. GPa for enamel, 0.26 ± 0.08. GPa for cementum close to the crown, and 0.31 ± 0.04. GPa for cementum close to the root margin. This can be explained with the different degree of mineralization of the different tissue types and is comparable with human teeth. © 2013 Elsevier Inc.
AUTHOR KEYWORDS: Biomineralization; Calcium phosphate; Crocodiles; Mechanical properties; Synchrotron X-ray microtomography; Teeth
DOCUMENT TYPE: Article
SOURCE: Scopus

Krüger, T., Gross, M., Raabe, D., Varnik, F.
Crossover from tumbling to tank-treading-like motion in dense simulated suspensions of red blood cells
(2013) Soft Matter, 9 (37), pp. 9008-9015. Cited 26 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84883425641&doi=10.1039%2fc3sm51645h&partnerID=40&md5=f2338d2c1c576e7a14f24ceb6a66b25d

DOI: 10.1039/c3sm51645h
AFFILIATIONS: Centre for Computational Science, University College London, 20 Gordon Street, London WC1H 0AJ, United Kingdom;
Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Universitätsstrasse 150, 44780 Bochum, Germany;
Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: Via computer simulations, we provide evidence that the shear rate induced red blood cell tumbling-to-tank-treading transition also occurs at quite high volume fractions, where collective effects are important. The transition takes place as the ratio of effective suspension stress to the characteristic cell membrane stress exceeds a certain value and does not explicitly depend on volume fraction or cell deformability. This value coincides with that for a transition from an orientationally less ordered to a highly ordered phase. The average cell deformation does not show any signature of transition, but rather follows a simple scaling law independent of volume fraction. © 2013 The Royal Society of Chemistry.

DOCUMENT TYPE: Article
SOURCE: Scopus

Springer, H., Belde, M., Raabe, D.
Bulk combinatorial design of ductile martensitic stainless steels through confined martensite-to-austenite reversion
(2013) Materials Science and Engineering A, 582, pp. 235-244. Cited 17 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84881243377&doi=10.1016%2fj.msea.2013.06.036&partnerID=40&md5=571879a430c8427cd51cb5703c7b103d

DOI: 10.1016/j.msea.2013.06.036
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany
ABSTRACT: The effect of local martensite-to-austenite reversion on microstructure and mechanical properties was studied with the aim of designing ductile martensitic steels. Following a combinatorial screening with tensile and hardness testing on a matrix of six alloys (0-5. wt% Mn, 0-2. wt% Si, constant 13.5. wt% Cr and 0.45. wt% C) and seven martensite tempering conditions (300-500. °C, 0-30. min), investigations were focussed on martensite-to-austenite reversion during tempering as function of chemical composition and its correlation with the mechanical properties. While Mn additions promoted austenite formation (up to 35. vol%) leading to a martensitic-austenitic TRIP steel with optimum mechanical properties (1.5. GPa ultimate tensile strength and 18% elongation), Si led to brittle behaviour despite even larger austenite contents. Combined additions of Mn and Si broadened the temperature range of austenite reversion, but also significantly lowered hardness and yield strength at limited ductility. These drastically diverging mechanical properties of the probed steels are discussed in light of microstructure morphology, dispersion and transformation kinetics of the austenite, as a result of the composition effects on austenite retention and reversion. © 2013 Elsevier B.V.
AUTHOR KEYWORDS: Combinatorial alloy design; Mechanical properties; Microstructure; Steels; Transformation induced plasticity
DOCUMENT TYPE: Article
SOURCE: Scopus

Nakada, N., Fukagawa, R., Tsuchiyama, T., Takaki, S., Ponge, D., Raabe, D.
Inheritance of dislocations and crystallographic texture during martensitic reversion into austenite
(2013) ISIJ International, 53 (7), pp. 1286-1288. Cited 12 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84883223081&doi=10.2355%2fisijinternational.53.1286&partnerID=40&md5=7e93052ed83ed0e43b3e522a5860f400

DOI: 10.2355/isijinternational.53.1286
AFFILIATIONS: Department of Materials Science and Engineering, Graduate School of Engineering, Kyushu University, 744 Moto-oka, Nishi-ku, Fukuoka, 819-0395, Japan;
International Institute for Carbon Neutral Energy Research (WPI-I2CNER), Kyushu University, 744 Moto-oka, Nishi-ku, Fukuoka, 819-0395, Japan;
Kyushu University, 744 Moto-oka, Nishi-ku, Fukuoka, 819-0395, Japan;
Max-Planck-Institute Für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: A novel type of heat treatment to control austenite stability by precipitation and dissolution of carbide was applied to a 18%Ni-0.6%C steel. The new method enables to study the inherent characteristics of austenite formed by martensitic reversion. The material selected for this study is a hypereutectoid steel with a large carbon solubility gap depending on the austenitizing temperature. The precipitated carbide immediately dissolves into the austenite matrix again after martensitic reversion in order to restore the Ms and Mf temperatures to their initial

values. The crystallographic orientation of each phase was mapped by means of the electron back scattering diffraction (EBSD) method using a field emission scanning electron microscope. A full fcc-bcc-fcc reversible martensitic transformations cycle was observed. As a result of the specific heat treatment, the austenite that was formed by martensitic reversion remains stable at ambient temperature.
AUTHOR KEYWORDS: Austenite; Ccrystallographic memory effect; Martensitic reversion; Reversible martensitic transformations
DOCUMENT TYPE: Article
SOURCE: Scopus

Gutierrez-Urrutia, I., Zaefferer, S., Raabe, D.
Coupling of electron channeling with EBSD: Toward the quantitative characterization of deformation structures in the sem
(2013) JOM, 65 (9), pp. 1229-1236. Cited 38 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84883222249&doi=10.1007%2fs11837-013-0678-0&partnerID=40&md5=4318c99c95f2d47933442a827f77c7a8

DOI: 10.1007/s11837-013-0678-0
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, 40237 Dusseldorf, Germany
ABSTRACT: The coupling of electron channeling contrast imaging (ECCI) with electron backscatter diffraction (EBSD) provides an efficient and fast approach to perform ECCI of crystal defects, such as dislocations, cells, and stacking faults, under controlled diffraction conditions with enhanced contrast. From a technical point of view, the ECCI technique complements two of the main electron microscopy techniques, namely, EBSD and conventional diffraction-based transmission electron microscopy. In this review, we provide several application examples of the EBSD-based ECCI approach on microstructure characterization, namely, characterization of single dislocations, measurement of dislocation densities, and characterization of dislocation substructures in deformed bulk materials. We make use of a two-beam Bloch wave approach to interpret the channeling contrast associated with crystal defects. The approach captures the main features observed in the experimental contrast associated with stacking faults and dislocations. © 2013 TMS.
DOCUMENT TYPE: Article
SOURCE: Scopus

Marceau, R.K.W., Choi, P., Raabe, D.
Understanding the detection of carbon in austenitic high-Mn steel using atom probe tomography
(2013) Ultramicroscopy, 132, pp. 239-247. Cited 20 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84883786984&doi=10.1016%2fj.ultramic.2013.01.010&partnerID=40&md5=c69b555967a1e96d3f48a16e89eb77a5

DOI: 10.1016/j.ultramic.2013.01.010
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany
ABSTRACT: A high-Mn TWIP steel having composition Fe-22Mn-0.6C (wt%) is considered in this study, where the need for accurate and quantitative analysis of clustering and short-range ordering by atom probe analysis requires a better understanding of the detection of carbon in this system. Experimental measurements reveal that a high percentage of carbon atoms are detected as molecular ion species and on multiple hit events, which is discussed with respect to issues such as optimal experimental parameters, correlated field evaporation and directional walk/migration of carbon atoms at the surface of the specimen tip during analysis. These phenomena impact the compositional and spatial accuracy of the atom probe measurement and thus require careful consideration for further cluster-finding analysis. © 2013 Elsevier B.V.

AUTHOR KEYWORDS: Atom probe; Carbon detection; Cluster-finding analysis; Fe-Mn-C TWIP steel; Short-range order
DOCUMENT TYPE: Article
SOURCE: Scopus

Raabe, D., Sandlöbes, S., Millán, J., Ponge, D., Assadi, H., Herbig, M., Choi, P.-P.
Segregation engineering enables nanoscale martensite to austenite phase transformation at grain boundaries: A pathway to ductile martensite
(2013) Acta Materialia, 61 (16), pp. 6132-6152. Cited 84 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84882842921&doi=10.1016%2fj.actamat.2013.06.055&partnerID=40&md5=a40a9549b8bc6079e82f07bb6ff019e3

DOI: 10.1016/j.actamat.2013.06.055
AFFILIATIONS: Department for Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany
ABSTRACT: In an Fe-9 at.% Mn maraging alloy annealed at 450 C reversed allotriomorphic austenite nanolayers appear on former Mn decorated lath martensite boundaries. The austenite films are 5-15 nm thick and form soft layers among the hard martensite crystals. We document the nanoscale segregation and associated martensite to austenite transformation mechanism using transmission electron microscopy and atom probe tomography. The phenomena are discussed in terms of the adsorption isotherm (interface segregation) in conjunction with classical heterogeneous nucleation theory (phase transformation) and a phase field model that predicts the kinetics of phase transformation at segregation decorated grain boundaries. The analysis shows that strong interface segregation of austenite stabilizing elements (here Mn) and the release of elastic stresses from the host martensite can generally promote phase transformation at martensite grain boundaries. The phenomenon enables the design of ductile and tough martensite.
AUTHOR KEYWORDS: Atom probe tomography; Austenite; Austenite reversion; Grain boundary segregation; Phase transformation
DOCUMENT TYPE: Article
SOURCE: Scopus

Li, Y.J., Choi, P., Goto, S., Borchers, C., Raabe, D., Kirchheim, R.
Atomic scale investigation of redistribution of alloying elements in pearlitic steel wires upon cold-drawing and annealing
(2013) Ultramicroscopy, 132, pp. 233-238. Cited 9 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84883780047&doi=10.1016%2fj.ultramic.2012.10.010&partnerID=40&md5=6ec0c1499cd9aa23150aac23cd666bb1

DOI: 10.1016/j.ultramic.2012.10.010
AFFILIATIONS: Institut für Materialphysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany;
Max-Planck Institut für Eisenforschung, Max-Planck-Str. 1, D-40237 Düsseldorf, Germany;
Department of Materials Science and Engineering, Faculty of Engineering and Resource Science, Akita University, Tegata Gakuencho, Akita 010-8502, Japan
ABSTRACT: A local electrode atom probe has been employed to analyze the redistribution of alloying elements including Si, Mn, and Cr in pearlitic steel wires upon cold-drawing and subsequent annealing. It has been found that the three elements undergo mechanical mixing upon cold-drawing at large strains, where Mn and Cr exhibit a nearly homogeneous distribution throughout both ferrite and cementite, whereas Si only dissolves slightly in cementite. Annealing at elevated temperatures leads to a reversion of the mechanical alloying. Si atoms mainly segregate at well-defined ferrite (sub)grain boundaries formed during annealing. Cr and Mn are strongly

concentrated in cementite adjacent to the ferrite/cementite interface due to their lower diffusivities in cementite than in ferrite. © 2012.
AUTHOR KEYWORDS: Annealing; Atom probe tomography; Cold-drawn pearlitic steel wire; Grain boundary segregation; Mechanical alloying; Partitioning
DOCUMENT TYPE: Article
SOURCE: Scopus

Kresse, T., Li, Y.J., Boll, T., Borchers, C., Choi, P., Al-Kassab, T., Raabe, D., Kirchheim, R.
Influence of supersaturated carbon on the diffusion of Ni in ferrite determined by atom probe tomography
(2013) Scripta Materialia, 69 (5), pp. 424-427. Cited 8 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84879886753&doi=10.1016%2fj.scriptamat.2013.05.039&partnerID=40&md5=515d50147958ce849a163868c8cb5a91

DOI: 10.1016/j.scriptamat.2013.05.039
AFFILIATIONS: Institut für Materialphysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany;
Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, D-40237 Düsseldorf, Germany;
Division of Physical Science and Engineering, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia;
International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, Japan
ABSTRACT: In patented and cold-drawn pearlitic steel wires dissociation of cementite occurs during mechanical deformation. In this study the influence of the carbon decomposition on the diffusion of nickel in ferrite is investigated by means of atom probe tomography. In the temperature range 423-523 K we observed a much smaller activation energy of Ni diffusion than for self-diffusion in body-centered cubic iron, indicating an increased vacancy density owing to enhanced formation of vacancy-carbon complexes. © 2013 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
AUTHOR KEYWORDS: Atom probe tomography; Body-centered cubic iron; Face-centered cubic iron; Ni diffusion; Self-diffusion; Vacancy-carbon complexes
DOCUMENT TYPE: Article
SOURCE: Scopus

Mandal, S., Chikkadi, V., Nienhuis, B., Raabe, D., Schall, P., Varnik, F.
Single-particle fluctuations and directional correlations in driven hard-sphere glasses
(2013) Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, 88 (2), art. no. 022129, . Cited 9 times.
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DOI: 10.1103/PhysRevE.88.022129
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck Strasse 1, 40237 Düsseldorf, Germany;
Institute of Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, Netherlands;
Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Stiepeler Strasse 129, 44801 Bochum, Germany
ABSTRACT: Via event-driven molecular dynamics simulations and experiments, we study the packing-fraction and shear-rate dependence of single-particle fluctuations and dynamic correlations in hard-sphere glasses under shear. At packing fractions above the glass transition, correlations increase as shear rate decreases: the exponential tail in the distribution of single-particle jumps broadens and dynamic four-point correlations increase. Interestingly, however, upon decreasing the packing fraction, a broadening

of the exponential tail is also observed, while dynamic heterogeneity is shown to decrease. An explanation for this behavior is proposed in terms of a competition between shear and thermal fluctuations. Building upon our previous studies, we further address the issue of anisotropy of the dynamic correlations. © 2013 American Physical Society.
DOCUMENT TYPE: Article
SOURCE: Scopus

Wu, X., Erbe, A., Raabe, D., Fabritius, H.-O.
Extreme optical properties tuned through phase substitution in a structurally optimized biological photonic polycrystal
(2013) Advanced Functional Materials, 23 (29), pp. 3615-3620. Cited 12 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84881191375&doi=10.1002%2fadfm.201203597&partnerID=40&md5=982ddcd475983522262d4ade66d5c385

DOI: 10.1002/adfm.201203597
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Department of Microstructure Physics and Alloy Design, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Department of Interface Chemistry and Surface Engineering, Max-Planck-Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: Biological photonic structures evolved by insects provide inspiring examples for the design and fabrication of synthetic photonic crystals. The small scales covering the beetle Entimus imperialis are subdivided into irregularly shaped domains that mostly show striking colors, yet some appear colorless. The colors originate from photonic crystals consisting of cuticular material and air, which are geometrically separated by a triply periodic D-surface (diamond). The structure and orientation of the photonic crystals are charactized and it is shown that in colorless domains SiO2 substitutes the air. The experimental results are incorporated into a precise D-surface structure model used to simulate the photonic band structure. The study shows that the structural parameters in colored domains are optimized for maximum reflectivity by maximizing the stop gap width. The colorless domains provide a biological example of how the optical appearance changes through alteration of the refractive index contrast between the constituting phases. The cuticular photonic polycrystals formed by the beetle Entimus imperialis are a perfect example of a natural diamond-type triply periodic bicontinuous cubic structure with structural parameters that are optimized to open up the largest possible photonic stop gaps. Depending on whether the cuticular network is complemented by air or SiO2, the optical properties of individual domains vary from bright coloration to no coloration and transparency. Copyright © 2013 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
AUTHOR KEYWORDS: cuticles; insects; photonic band-gap calculations; photonic polycrystals; SiO2
DOCUMENT TYPE: Article
SOURCE: Scopus

Sandlöbes, S., Friák, M., Neugebauer, J., Raabe, D.
Basal and non-basal dislocation slip in Mg-Y
(2013) Materials Science and Engineering A, 576, pp. 61-68. Cited 46 times.
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DOI: 10.1016/j.msea.2013.03.006
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Department for Microstructure Physics and Alloy Design, Max-Planck-Str. 1, Düsseldorf, Germany;

Max-Planck-Institut für Eisenforschung, Department for Computational Materials Design, Max-Planck-Str. 1, Düsseldorf, Germany
ABSTRACT: The activation of non-basal slip systems is of high importance for the ductility in hcp Mg and its alloys. In particular, for Mg–Y alloys where a higher activation of pyramidal dislocation slip causes an increased ductility detailed characterization of the activated slip systems is essential to understand and describe plasticity in these alloys. In this study a detailed analysis of the activated dislocations and slip systems via post-mortem TEM and SEM-EBSD based slip band analysis in 3% deformed Mg–3 wt% Y is presented. The analysis reveals a substantial activity of pyramidal <c+a> dislocations with different Burgers vectors. The obtained dislocation densities and active slip systems are discussed with respect to atomistic simulations of non-basal dislocations in hcp Mg. © 2013 Elsevier B.V.
AUTHOR KEYWORDS: Deformation; Dislocations; Mg alloys; Mg–Y; Transmission electron microscopy
DOCUMENT TYPE: Article
SOURCE: Scopus

Roters, F., Diehl, M., Eisenlohr, P., Raabe, D.
Crystal Plasticity Modeling
(2013) Microstructural Design of Advanced Engineering Materials, pp. 41-67. Cited 1 time.
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DOI: 10.1002/9783527652815.ch03
AFFILIATIONS: MPI für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany
DOCUMENT TYPE: Book Chapter
SOURCE: Scopus

Raabe, D., Ponge, D., Kirchheim, R., Assadi, H., Li, Y., Goto, S., Kostka, A., Herbig, M., Sandl, S., Kuzmina, M., Millán, J., Yuan, L., Choi, P.-P.
Interface Segregation in Advanced Steels Studied at the Atomic Scale
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DOI: 10.1002/9783527652815.ch11
AFFILIATIONS: MPI für Eisenforschung, Max-Planck-Str. 1, Düsseldorf, Germany
DOCUMENT TYPE: Book Chapter
SOURCE: Scopus

Gutierrez-Urrutia, I., Raabe, D.
Microbanding mechanism in an Fe-Mn-C high-Mn twinning-induced plasticity steel
(2013) Scripta Materialia, 69 (1), pp. 53-56. Cited 37 times.
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DOI: 10.1016/j.scriptamat.2013.03.010
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck Str. 1, D-40237 Düsseldorf, Germany
ABSTRACT: We study the microbanding mechanism in an Fe-22Mn-0.6C (wt.%) twinning-induced plasticity steel. Dislocation substructures were examined by electron channeling contrast imaging and electron backscatter diffraction. We observe a pronounced effect of the strain path on

microbanding, which is explained in terms of Schmid's law. Microbands created under shear loading have a non-crystallographic character. This is attributed to the microbanding mechanism and its relation with the dislocation substructure. Further insights into the dislocation configuration of microbands are provided.
AUTHOR KEYWORDS: Austenitic steels; Dislocation cell; Electron backscattering diffraction (EBSD); Electron channeling contrast imaging (ECCI); Plastic deformation
DOCUMENT TYPE: Article
SOURCE: Scopus

Koyama, M., Akiyama, E., Tsuzaki, K., Raabe, D.
Hydrogen-assisted failure in a twinning-induced plasticity steel studied under in situ hydrogen charging by electron channeling contrast imaging
(2013) Acta Materialia, 61 (12), pp. 4607-4618. Cited 65 times.
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DOI: 10.1016/j.actamat.2013.04.030
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strabe 1, 40237 Düsseldorf, Germany;
National Institute for Materials Science, 1-2-1, Sengen, Ibaraki 305-0047, Japan;
Department of Mechanical Engineering, Kyushu University, 744 Motooka, Nishi-ku, Fukuoka 819-0395, Japan
ABSTRACT: We investigated the hydrogen embrittlement of a Fe-18Mn-1.2%C (wt.%) twinning-induced plasticity steel, focusing on the influence of deformation twins on hydrogen-assisted cracking. A tensile test under ongoing hydrogen charging was performed at low strain rate (1.7 × 10-6 s -1) to observe hydrogen-assisted cracking and crack propagation. Hydrogen-stimulated cracks and deformation twins were observed by electron channeling contrast imaging. We made the surprising observation that hydrogen-assisted cracking was initiated both at grain boundaries and also at deformation twins. Also, crack propagation occurred along both types of interfaces. Deformation twins were shown to assist intergranular cracking and crack propagation. The stress concentration at the tip of the deformation twins is suggested to play an important role in the hydrogen embrittlement of the Fe-Mn-C twining-induced plasticity steel.
AUTHOR KEYWORDS: Crack propagation; Electron channeling contrast imaging; Hydrogen embrittlement; Mechanical properties; Twinning-induced plasticity (TWIP) steel
DOCUMENT TYPE: Article
SOURCE: Scopus

Jia, N., Roters, F., Eisenlohr, P., Raabe, D., Zhao, X.
Simulation of shear banding in heterophase co-deformation: Example of plane strain compressed Cu-Ag and Cu-Nb metal matrix composites
(2013) Acta Materialia, 61 (12), pp. 4591-4606. Cited 37 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84878550946&doi=10.1016%2fj.actamat.2013.04.029&partnerID=40&md5=c2db91f2b08450b708da9af508993125

DOI: 10.1016/j.actamat.2013.04.029
AFFILIATIONS: Key Laboratory for Anisotropy and Texture of Materials (MOE), Northeastern University, Shenyang 110819, China;
Max-Planck-Institut für Eisenforschung, D-40237 Düsseldorf, Germany
ABSTRACT: The co-deformation and shear localization in heterophase alloys is studied using two-dimensional crystal plasticity finite element simulations on plane strain compressed Cu-Ag and Cu-Nb metal matrix composites. The aim is to study the fundamentals of micromechanics, co-

deformation and shear banding in materials with heterophase interfaces. It is observed that, depending on the initial orientations of the crystals, co-deformation of the constituent heterophases often proceeds via collective mechanisms, i.e. by pronounced shear banding triggered by stress concentration at the interfaces. This phenomenon leads to highly localized strains within the bands, exceeding the average strain in part by two orders of magnitude. Shear band development is related to the inherent mechanical properties of each crystal and also to the properties of the abutting crystals. The predicted topology and nature of the cross-phase shear bands, i.e. the extreme local strains, significant bending of the interface regions, and sharp strain localization that propagates across the interfaces, agree well with experimental observations in cold-rolled composites. The simulations reveal that cross-phase shear banding leads to large and highly localized values of stress and strain at heterophase interfaces. Such information is essential for a better understanding of the micromechanical boundary conditions inside co-deformed composites and the associated shear-induced chemical mixing.
AUTHOR KEYWORDS: Crystal plasticity finite element analysis; Metal matrix composites; Shear band; Stress
DOCUMENT TYPE: Article
SOURCE: Scopus

Pradeep, K.G., Wanderka, N., Choi, P., Banhart, J., Murty, B.S., Raabe, D.
Atomic-scale compositional characterization of a nanocrystalline AlCrCuFeNiZn high-entropy alloy using atom probe tomography
(2013) Acta Materialia, 61 (12), pp. 4696-4706. Cited 54 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84878531094&doi=10.1016%2fj.actamat.2013.04.059&partnerID=40&md5=2754c7fc7bfb02b37fc6d20fe9565f1a

DOI: 10.1016/j.actamat.2013.04.059
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany;
Indian Institute of Technology - Madras, Chennai 600 036, India
ABSTRACT: We have studied a nanocrystalline AlCrCuFeNiZn high-entropy alloy synthesized by ball milling followed by hot compaction at 600 C for 15 min at 650 MPa. X-ray diffraction reveals that the mechanically alloyed powder consists of a solid-solution body-centered cubic (bcc) matrix containing 12 vol.% face-centered cubic (fcc) phase. After hot compaction, it consists of 60 vol.% bcc and 40 vol.% fcc. Composition analysis by atom probe tomography shows that the material is not a homogeneous fcc-bcc solid solution but instead a composite of bcc structured Ni-Al-, Cr-Fe- and Fe-Cr-based regions and of fcc Cu-Zn-based regions. The Cu-Zn-rich phase has 30 at.% Zn α-brass composition. It segregates predominantly along grain boundaries thereby stabilizing the nanocrystalline microstructure and preventing grain growth. The Cr- and Fe-rich bcc regions were presumably formed by spinodal decomposition of a Cr-Fe phase that was inherited from the hot compacted state. The Ni-Al phase remains stable even after hot compaction and forms the dominant bcc matrix phase. The crystallite sizes are in the range of 20-30 nm as determined by transmission electron microscopy. The hot compacted alloy exhibited very high hardness of 870 ± 10 HV. The results reveal that phase decomposition rather than homogeneous mixing is prevalent in this alloy. Hence, our current observations fail to justify the present high-entropy alloy design concept. Therefore, a strategy guided more by structure and thermodynamics for designing high-entropy alloys is encouraged as a pathway towards exploiting the solid-solution and stability idea inherent in this concept.
AUTHOR KEYWORDS: Atom probe tomography; High-entropy alloy; Mechanical alloying; Nanocrystalline; Solid solution

DOCUMENT TYPE: Article
SOURCE: Scopus

Hafez Haghighat, S.M., Eggeler, G., Raabe, D.
Effect of climb on dislocation mechanisms and creep rates in γ′-strengthened Ni base superalloy single crystals: A discrete dislocation dynamics study
(2013) Acta Materialia, 61 (10), pp. 3709-3723. Cited 37 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84876888304&doi=10.1016%2fj.actamat.2013.03.003&partnerID=40&md5=e42e11302899eb7459bf904431ddbd76

DOI: 10.1016/j.actamat.2013.03.003
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Institut für Werkstoffe, Ruhr-Universität Bochum, Universitätsstr. 150, 44780 Bochum, Germany
ABSTRACT: Creep of single-crystal superalloys is governed by dislocation glide, climb, reactions and annihilation. Discrete three-dimensional (3D) dislocation dynamics (DDD) simulations are used to study the evolution of the dislocation substructure in a γ/γ′ microstructure of a single-crystal superalloy for different climb rates and loading conditions. A hybrid mobility law for glide and climb is used to map the interactions of dislocations with γ′ cubes. The focus is on the early stages of creep, where dislocation plasticity is confined to narrow γ channels. With enhancing climb mobility, the creep strain increases, even if the applied resolved shear stress is below the critical stress required for squeezing dislocations into the γ channels. The simulated creep microstructure consists of long dislocations and a network near the corners of the γ′ precipitate in the low-stress regime. In the high-stress regime, dislocations squeeze into the γ channels, where they deposit dislocation segments at the γ/γ′ interfaces. These observations are in good agreement with experimentally observed dislocation structures that form during high-temperature and low-stress creep.
AUTHOR KEYWORDS: Creep; Dislocation dynamics; Simulation; Superalloys
DOCUMENT TYPE: Article
SOURCE: Scopus

Gross, M., Steinbach, I., Raabe, D., Varnik, F.
Viscous coalescence of droplets: A lattice Boltzmann study
(2013) Physics of Fluids, 25 (5), art. no. 052101, . Cited 12 times.
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DOI: 10.1063/1.4803178
AFFILIATIONS: Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Universitaetsstr. 90a, 44789 Bochum, Germany;
Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: The coalescence of two resting liquid droplets in a saturated vapor phase is investigated by Lattice Boltzmann simulations in two and three dimensions. We find that, in the viscous regime, the bridge radius obeys a t1/2-scaling law in time with the characteristic time scale given by the viscous time. Our results differ significantly from the predictions of existing analytical theories of viscous coalescence as well as from experimental observations. While the underlying reason for these deviations is presently unknown, a simple scaling argument is given that describes our results well.
DOCUMENT TYPE: Article
SOURCE: Scopus

Plancher, E., Tasan, C.C., Sandloebes, S., Raabe, D.
On dislocation involvement in Ti-Nb gum metal plasticity
(2013) Scripta Materialia, 68 (10), pp. 805-808. Cited 14 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84875229181&doi=10.1016%2fj.scriptamat.2013.01.034&partnerID=40&md5=5eb2aea0a95e82af6212516c9ed7f7bc

DOI: 10.1016/j.scriptamat.2013.01.034
AFFILIATIONS: Max-Planck-lnstitut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany
ABSTRACT: The excellent mechanical properties of the Ti-Nb-based gum metal were originally proposed to arise from a "dislocation-free" giant fault mechanism; however, the involvement of lattice dislocations in the process is still under debate. To address this issue, gum metal deformation mechanisms are investigated systematically on cast specimens, employing postmortem and in situ analysis techniques. The results demonstrate that a giant fault mechanism (which appears to be a phase-transformation-assisted nanotwinning mechanism) governs gum metal plasticity without direct assistance from dislocations during the process.
AUTHOR KEYWORDS: Beta titanium; Dislocation; Giant fault; Gum metal; In situ
DOCUMENT TYPE: Article
SOURCE: Scopus

Chen, Y.Z., Herz, A., Li, Y.J., Borchers, C., Choi, P., Raabe, D., Kirchheim, R.
Nanocrystalline Fe-C alloys produced by ball milling of iron and graphite
(2013) Acta Materialia, 61 (9), pp. 3172-3185. Cited 25 times.
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DOI: 10.1016/j.actamat.2013.02.006
AFFILIATIONS: State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, 710072 Xi'an, China;
Institut für Materialphysik, Universität Göttingen, 37077 Göttingen, Germany;
Max-Planck Institut für Eisenforschung GmbH, Department for Microstructure Physics, Max-Planck-Str.1, 40237 Düsseldorf, Germany;
Department of Materials for Electronics, Institute of Materials Engineering, Ilmenau University of Technology, 98684 Ilmenau, Germany;
International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, Japan
ABSTRACT: A series of nanocrystalline Fe-C alloys with different carbon concentrations (xtot) up to 19.4 at.% (4.90 wt.%) are prepared by ball milling. The microstructures of these alloys are characterized by transmission electron microscopy and X-ray diffraction, and partitioning of carbon between grain boundaries and grain interiors is determined by atom probe tomography. It is found that the segregation of carbon to grain boundaries of α-ferrite can significantly reduce its grain size to a few nanometers. When the grain boundaries of ferrite are saturated with carbon, a metastable thermodynamic equilibrium between the matrix and the grain boundaries is approached, inducing a decreasing grain size with increasing xtot. Eventually the size reaches a lower limit of about 6 nm in alloys with x tot > 6.19 at.% (1.40 wt.%); a further increase in xtot leads to the precipitation of carbon as Fe3C. The observed presence of an amorphous structure in 19.4 at.% C (4.90 wt.%) alloy is ascribed to a deformation-driven amorphization of Fe3C by severe plastic deformation. By measuring the temperature dependence of the grain size for an alloy with 1.77 at.% C additional evidence is provided for a metastable equilibrium reached in the

nanocrystalline alloy. © 2013 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
AUTHOR KEYWORDS: Fe-C alloy; Mechanical alloying; Nanocrystalline materials; Segregation; Thermodynamics
DOCUMENT TYPE: Article
SOURCE: Scopus

Sandim, M.J.R., Tytko, D., Kostka, A., Choi, P., Awaji, S., Watanabe, K., Raabe, D.
Grain boundary segregation in a bronze-route Nb3Sn superconducting wire studied by atom probe tomography
(2013) Superconductor Science and Technology, 26 (5), art. no. 055008, . Cited 8 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84876549154&doi=10.1088%2f0953-2048%2f26%2f5%2f055008&partnerID=40&md5=e390bf2e50895b22ed1f618bbe9748a8

DOI: 10.1088/0953-2048/26/5/055008
AFFILIATIONS: Escola de Engenharia de Lorena, USP, 12602-810, Lorena, Brazil;
Max-Planck-Institut für Eisenforschung, D-40237, Düsseldorf, Germany;
Institute of Materials Research, Tohoku University, 980-8577, Sendai, Japan
ABSTRACT: Atom probe tomography was used to characterize the A15 phase in a bronze-route Nb3Sn superconducting wire with a bronze matrix composition of Cu-8Sn-0.3Ti (in at.%). We observed depletion of niobium and segregation of Cu and Ti atoms at Nb3Sn grain boundaries. While the Nb depletion is about 15% relative to the grain interior, the average ratio between Cu and Ti excess values is 9 to 2. Segregation extends to a distance d ~ 9 Å from the point of maximum Cu and Ti concentrations. Such local variation in the stoichiometry at the grain boundary region can be an additional source of flux-pinning in the Nb3Sn phase. Other microstructural parameters, such as the grain size and chemical composition of the Nb 3Sn layer, were investigated by electron backscatter diffraction and transmission electron microscopy. © 2013 IOP Publishing Ltd.
DOCUMENT TYPE: Article
SOURCE: Scopus

de Oliveira, V.B., Padilha, A.F., Möslang, A., Raabe, D., Zschommler Sandim, H.R.
Abnormal grain growth in ferritic-martensitic Eurofer-97 steel
(2013) Materials Science Forum, 753, pp. 333-336. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84876524633&doi=10.4028%2fwww.scientific.net%2fMSF.753.333&partnerID=40&md5=3eadab1f757bbab5a908824ebde2f482

DOI: 10.4028/www.scientific.net/MSF.753.333
AFFILIATIONS: Escola de Engenharia de Lorena, Universidade de São Paulo, Lorena-SP, 12600-970, Brazil;
Escola Politécnica, Universidade de São Paulo, São Paulo-SP, 05508-900, Brazil;
Karlsruher Institute für Technologie, IMF I, Karlsruhe, D-72061, Germany;
Max-Planck-Institut für Eisenforschung, Düsseldorf, D-40237, Germany
ABSTRACT: Ferritic-martensitic steels like Eurofer-97 are candidate structural materials for future fusion reactors. In the tempered state, this steel contains fine particles dispersed in the ferritic matrix. The aim of this work is to investigate abnormal grain growth in Eurofer-97 steel. The microstructural evolution was followed by isothermal annealing between 200 and 800°C (ferritic phase field) after cold rolling to 70, 80, and 90% reductions. Representative samples were characterized by scanning electron microscopy in the backscattered electron mode. Microtexture was evaluated by electron backscattered diffraction. We propose a mechanism based on the size advantage acquired by nuclei with misorientation angles

above 45° relative to their nearest neighbors to explain abnormal grain growth. Abnormal grain growth textures have components belonging to the α- and γ-fibers with predominance of {111}<110>, {111}<112>, and {100}<110>. © (2013) Trans Tech Publications, Switzerland.
AUTHOR KEYWORDS: Abnormal grain growth; Eurofer-97 steel; Texture
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Friák, M., Raabe, D., Neugebauer, J.
Ab Initio Guided Design of Materials
(2013) Structural Materials and Processes in Transportation, pp. 481-495.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84886128098&doi=10.1002%2f9783527649846.ch15&partnerID=40&md5=6a17bda073fa1d43b6a7de12d0cd866d

DOI: 10.1002/9783527649846.ch15
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany
AUTHOR KEYWORDS: Body-centered cubic; Density-functional theory; Light-weight; Magnesium; Material science; Quantum-mechanical study
DOCUMENT TYPE: Book Chapter
SOURCE: Scopus

Ma, D., Friák, M., Pezold, J.V., Raabe, D., Neugebauer, J.
Ab initio identified design principles of solid-solution strengthening in Al
(2013) Science and Technology of Advanced Materials, 14 (2), art. no. 025001, . Cited 1 time.
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DOI: 10.1088/1468-6996/14/2/025001
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf D-40237, Germany
ABSTRACT: Solid-solution strengthening in six Al-X binary systems is investigated using first-principle methods. The volumetric mismatch parameter and the solubility enthalpy per solute were calculated. We derive three rules for designing solid-solution strengthened alloys: (i) the solubility enthalpy per solute is related to the volumetric mismatch by a power law; (ii) for each annealing temperature, there exists an optimal solute-volume mismatch to achieve maximum strength; and (iii) the strengthening potential of high volumetric mismatch solutes is severely limited by their low solubility. Our results thus show that the thermodynamic properties of the system (here Al-X alloys) set clear upper bounds to the achievable strengthening effects owing to the reduced solubility with increasing volume mismatch. © 2013 National Institute for Materials Science.
AUTHOR KEYWORDS: ab initio; Al alloys; alloy design; DFT; solid-solution strengthening; solubility
DOCUMENT TYPE: Article
SOURCE: Scopus

Mehrtens, T., Schowalter, M., Tytko, D., Choi, P., Raabe, D., Hoffmann, L., Jönen, H., Rossow, U., Hangleiter, A., Rosenauer, A.
Measurement of the indium concentration in high indium content InGaN layers by scanning transmission electron microscopy and atom probe tomography
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DOI: 10.1063/1.4799382
AFFILIATIONS: Insitut für Festkörperphysik, Universität Bremen, Otto-Hahn-Allee 1, D-28359 Bremen, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, D-40237 Düsseldorf, Germany;
Insitut für Angewandte Physik, TU Braunschweig, Mendelssohnstr. 2, D-38106 Braunschweig, Germany
ABSTRACT: A method for determining concentrations from high-angle annular dark field-scanning transmission electron microscopy images is presented. The method is applied to an InGaN/GaN multi-quantum well structure with high In content, as used for the fabrication of light emitting diodes and laser diodes emitting in the green spectral range. Information on specimen thickness and In concentration is extracted by comparison with multislice calculations. Resulting concentration profiles are in good agreement with a comparative atom probe tomography analysis. Indium concentrations in the quantum wells ranging from 26 at. to 33 at. are measured in both cases. © 2013 American Institute of Physics.
DOCUMENT TYPE: Article
SOURCE: Scopus

Pei, Z., Zhu, L.-F., Friák, M., Sandlöbes, S., Von Pezold, J., Sheng, H.W., Race, C.P., Zaefferer, S., Svendsen, B., Raabe, D., Neugebauer, J.
Ab initio and atomistic study of generalized stacking fault energies in Mg and Mg-Y alloys
(2013) New Journal of Physics, 15, art. no. 043020, . Cited 38 times.
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AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, D-40237 Düsseldorf, Germany;
Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Schinkelstraße 2, D-52062 Aachen, Germany;
School of Physics, Astronomy and Computational Sciences, George Mason University, Fairfax, VA 22030, United States;
Material Mechanics, Faculty of Georesources and Materials Engineering, RWTH Aachen University, Schinkelstraße 2, D-52062 Aachen, Germany
ABSTRACT: Magnesium-yttrium alloys show significantly improved room temperature ductility when compared with pure Mg. We study this interesting phenomenon theoretically at the atomic scale employing quantum-mechanical (so-called ab initio) and atomistic modeling methods. Specifically, we have calculated generalized stacking fault energies for five slip systems in both elemental magnesium (Mg) and Mg-Y alloys using (i) density functional theory and (ii) a set of embedded-atom-method (EAM) potentials. These calculations predict that the addition of yttrium results in a reduction in the unstable stacking fault energy of basal slip systems. Specifically in the case of an I2 stacking fault, the predicted reduction of the stacking fault energy due to Y atoms was verified by experimental measurements. We find a similar reduction for the stable stacking fault energy of the non-basal slip system. On the other hand, other energies along this particular γ-surface profile increase with the addition of Y. In parallel to our quantum-mechanical calculations, we have also developed a new EAM Mg-Y potential and thoroughly tested its performance. The comparison of quantum-mechanical and atomistic results indicates that the new potential is suitable for future large-scale atomistic simulations. © IOP Publishing and Deutsche Physikalische Gesellschaft.
DOCUMENT TYPE: Article
SOURCE: Scopus

Zhu, L.-F., Friák, M., Lymperakis, L., Titrian, H., Aydin, U., Janus, A.M., Fabritius, H.-O., Ziegler, A., Nikolov, S., Hemzalová, P., Raabe, D., Neugebauer, J.

Ab initio study of single-crystalline and polycrystalline elastic properties of Mg-substituted calcite crystals
(2013) Journal of the Mechanical Behavior of Biomedical Materials, 20, pp. 296-304. Cited 6 times.
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DOI: 10.1016/j.jmbbm.2013.01.030
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, Düsseldorf 40237, Germany;
University Duisburg-Essen, Germany;
Central Facility for Electron Microscopy, University of Ulm, Albert-Einstein-Allee 11, Ulm 89069, Germany;
Bulgarian Academy of Sciences, Institute of Mechanics, Acad. G. Bonchev Str. Bl. 4, 1113 Sofia, Bulgaria;
Masaryk University, Kotlářská 2, Brno 611 37, Czech Republic
ABSTRACT: We employ ab initio calculations and investigate the single-crystalline elastic properties of (Ca,Mg)CO3 crystals covering the whole range of concentrations from pure calcite CaCO3 to pure magnesite MgCO3. Studying different distributions of Ca and Mg atoms within 30-atom supercells, our theoretical results show that the energetically most favorable configurations are characterized by elastic constants that nearly monotonously increase with the Mg content. Based on the first principles-derived single-crystalline elastic anisotropy, the integral elastic response of (Ca,Mg)CO3 polycrystals is determined employing a mean-field self-consistent homogenization method. As in case of single-crystalline elastic properties, the computed polycrystalline elastic parameters sensitively depend on the chemical composition and show a significant stiffening impact of Mg atoms on calcite crystals in agreement with the experimental findings. Our analysis also shows that it is not advantageous to use a higher-scale two-phase mix of stoichiometric calcite and magnesite instead of substituting Ca atoms by Mg ones on the atomic scale. Such two-phase composites are not significantly thermodynamically favorable and do not provide any strong additional stiffening effect. © 2013 Elsevier Ltd.
AUTHOR KEYWORDS: Ab initio; Calcite; Elasticity; Mg-substitution; Stiffening
DOCUMENT TYPE: Article
SOURCE: Scopus

Mandal, S., Gross, M., Raabe, D., Varnik, F.
Flow heterogeneity and correlations in a sheared hard sphere glass: Insight from computer simulations
(2013) AIP Conference Proceedings, 1518, pp. 266-271.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84874683819&doi=10.1063%2f1.4794578&partnerID=40&md5=4c9479927cad77aab48cabe1a167dfbc

DOI: 10.1063/1.4794578
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, 40237 Düsseldorf, Germany;
Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Universitätstr. 150, 44780 Bochum, Germany
ABSTRACT: Understanding the origin of flow heterogeneity in glassy systems is of high interest both due to its importance from theoretical standpoint as well as due to its occurrence in a large number of practical situations such as the flow of the so-called soft-glassy materials (foams, colloidal suspensions, granular media, etc). Detailed experimental investigations do indeed confirm that the flow of driven amorphous solids is not homogeneous, even if the macroscopic stress is constant across the system. We study this issue via large scale event driven molecular dynamics simulations of a hard sphere glass. We observe significant fluctuations of the velocity profile with a time scale of the order of a few hundreds percent strain.

Furthermore, there appears to be a correlation between the fluctuations of the local volume fraction and the fluctuations of the local shear rate. The time scales of the fluctuations of density and shear rate are practically identical. These observations motivate an interpretation of our results via the shear concentration coupling (SCC) theory. A detailed comparison, however, reveals serious inconsistencies. In particular, the amplitude of the fluctuations of the shear rate seems to be decoupled from that of density, a feature which is rather unexpected within the SCC picture. An alternative interpretation of our observations is also discussed invoking dynamic heterogeneity. © 2013 American Institute of Physics.
AUTHOR KEYWORDS: colloidal glass; glass transition; jamming
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Siboni, N.H., Raabe, D., Varnik, F.
Maintaining the equipartition theorem in small heterogeneous molecular dynamics ensembles
(2013) Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, 87 (3), art. no. 030101, .
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84875336086&doi=10.1103%2fPhysRevE.87.030101&partnerID=40&md5=7475dc7fb5d6022d2c3ed1fc0d7066e0

DOI: 10.1103/PhysRevE.87.030101
AFFILIATIONS: Aachen Institute for Computational Engineering Sciences (AICES), RWTH-Aachen, Germany;
Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany;
Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany
ABSTRACT: It has been reported recently that the equipartition theorem is violated in molecular dynamics simulations with periodic boundary condition. This effect is associated with the conservation of the total momentum. Here, we propose a fluctuating center of mass molecular dynamics approach to solve this problem. Using the analogy to a system exchanging momentum with its surroundings, we work out - and validate via simulations - an expression for the rate at which fluctuations shall be added to the system. It is shown that the proposed method maintains equipartition both at equilibrium and beyond equilibrium in the linear response regime. © 2013 American Physical Society.
DOCUMENT TYPE: Article
SOURCE: Scopus

Gutierrez-Urrutia, I., Raabe, D.
Influence of Al content and precipitation state on the mechanical behavior of austenitic high-Mn low-density steels
(2013) Scripta Materialia, 68 (6), pp. 343-347. Cited 93 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84872136506&doi=10.1016%2fj.scriptamat.2012.08.038&partnerID=40&md5=36da74fd514e2b594290f34b087506e2

DOI: 10.1016/j.scriptamat.2012.08.038
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck Str. 1, D-40237 Düsseldorf, Germany
ABSTRACT: We investigate the strain hardening of two austenitic high-Mn low density steels, namely, Fe-30.5Mn-2.1Al-1.2C and Fe-30.5Mn-8.0Al-1.2C (wt.%), containing different precipitation states. The strain hardening of the alloy with low Al content is attributed to dislocation and twin substructures. The precipitation of intergranular M3C-type carbides strongly influences the fracture mode. We associate the strain hardening behavior of the alloy with high Al content to the precipitation of shearable nanosized κ-carbides and their role in the development of planar dislocation substructures.

AUTHOR KEYWORDS: Austenitic steels; Carbides; Dislocation structure; Electron diffraction; Work hardening
DOCUMENT TYPE: Article
SOURCE: Scopus

Nematollahi, G.A., Von Pezold, J., Neugebauer, J., Raabe, D.
Thermodynamics of carbon solubility in ferrite and vacancy formation in cementite in strained pearlite
(2013) Acta Materialia, 61 (5), pp. 1773-1784. Cited 17 times.
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DOI: 10.1016/j.actamat.2012.12.001
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, D-40237 Düsseldorf, Germany
ABSTRACT: In order to investigate the thermodynamic driving force for the experimentally observed accumulation of C in ferritic layers of severely plastically deformed pearlitic wires, the stabilities of C interstitials in ferrite and of C vacancies in cementite are investigated as a function of uniaxial stain, using density-functional theory. In the presence of an applied strain along [1 1 0] or [1 1 1], the C interstitial in ferrite is significantly stabilized, while the C vacancy in cementite is moderately destabilized by the corresponding strain states in cementite [1 0 0] and ([0 1 0]). The enhanced stabilization of the C interstitial gives rise to an increase in the C concentration within the ferritic layers by up to two orders of magnitude. Our results thus suggest that in addition to the generally assumed non-equilibrium, dislocation-based mechanism, there is also a strain-induced thermodynamic driving force for the experimentally observed accumulation of C in ferrite.
AUTHOR KEYWORDS: Carbon interstitial; Cementite; Density-functional theory; Ferrite; Vacancy formation energy
DOCUMENT TYPE: Article
SOURCE: Scopus

Ayodele, S.G., Raabe, D., Varnik, F.
Lattice Boltzmann modeling of advection-diffusion-reaction equations: Pattern formation under uniform differential advection
(2013) Communications in Computational Physics, 13 (3), pp. 741-756. Cited 3 times.
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DOI: 10.4208/cicp.441011.270112s
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck Straße 1, 40237, Düsseldorf, Germany;
Interdisciplinary Center for Advanced Materials Simulation, Ruhr University Bochum, Stiepeler Straße 129, 44780 Bochum, Germany
ABSTRACT: A lattice Boltzmann model for the study of advection-diffusion-reaction (ADR) problems is proposed. Via multiscale expansion analysis, we derive from the LB model the resulting macroscopic equations. It is shown that a linear equilibrium distribution is sufficient to produce ADR equations within error terms of the order of the Mach number squared. Furthermore, we study spatially varying structures arising fromthe interaction of advective transportwith a cubic autocatalytic reaction-diffusion process under an imposed uniform flow. While advecting all the present species leads to trivial translation of the Turing patterns, differential advection leads to flow induced instability characterized with traveling stripes with a velocity dependent wave vector parallel to the flow direction. Predictions from a linear stability analysis of the model

equations are found to be in line with these observations. © 2013 Global-Science Press.
AUTHOR KEYWORDS: Advective transport; Differential advection; Lattice Boltzmann; Linear stability; Turing patterns
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Seol, J.-B., Raabe, D., Choi, P., Park, H.-S., Kwak, J.-H., Park, C.-G.
Direct evidence for the formation of ordered carbides in a ferrite-based low-density Fe-Mn-Al-C alloy studied by transmission electron microscopy and atom probe tomography
(2013) Scripta Materialia, 68 (6), pp. 348-353. Cited 60 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84872154826&doi=10.1016%2fj.scriptamat.2012.08.013&partnerID=40&md5=5874aaf8390f482a3fe328d4d913cdfa

DOI: 10.1016/j.scriptamat.2012.08.013
AFFILIATIONS: Max-Planck-Insititut für Eisenforschung, Max-Planck-Str.1, 40237 Düsseldorf, Germany;
Materials Science and Engineering, POSTECH, Pohang 790-784, South Korea;
Automotive Steels Research Laboratories, POSCO, Gwangyang 545-711, South Korea
ABSTRACT: We study the structure and chemical composition of the κ-carbide formed as a result of isothermal transformation in an Fe-3.0Mn-5.5Al-0.3C alloy using transmission electron microscopy and atom probe tomography. Both methods reveal the evolution of κ-particle morphology as well as the partitioning of solutes. We propose that the κ-phase is formed by a eutectoid reaction associated with nucleation growth. The nucleation of κ-carbide is controlled by both the ordering of Al partitioned to austenite and the carbon diffusion at elevated temperatures.
AUTHOR KEYWORDS: Atom probe tomography; Decomposition; Lightweight steels; Ordered carbide
DOCUMENT TYPE: Article
SOURCE: Scopus

Schwarz, T., Cojocaru-Mirédin, O., Choi, P., Mousel, M., Redinger, A., Siebentritt, S., Raabe, D.
Atom probe study of Cu2ZnSnSe4 thin-films prepared by co-evaporation and post-deposition annealing
(2013) Applied Physics Letters, 102 (4), art. no. 042101, . Cited 38 times.
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DOI: 10.1063/1.4788815
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany;
Laboratory for Photovoltaics, University of Luxembourg, Belvaux, Luxembourg
ABSTRACT: We use atom probe tomography (APT) for resolving nanometer scale compositional fluctuations in Cu2ZnSnSe4 (CZTSe) thin-films prepared by co-evaporation and post-deposition annealing. We detect a complex, nanometer-sized network of CZTSe and ZnSe domains in these films. Some of the ZnSe domains contain precipitates having a Cu- and Sn-rich composition, where the composition cannot be assigned to any of the known equilibrium phases. Furthermore, Na impurities are found to be segregated at the CZTSe/ZnSe interface. The insights given by APT are essential for understanding the growth of CZTSe absorber layers for thin-film solar cells and for optimizing their optoelectronic properties.
DOCUMENT TYPE: Article
SOURCE: Scopus

Zheng, C., Raabe, D.
Interaction between recrystallization and phase transformation during intercritical annealing in a cold-rolled dual-phase steel: A cellular automaton model
(2013) Acta Materialia, 61 (14), pp. 5504-5517. Cited 53 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84882455232&doi=10.1016%2fj.actamat.2013.05.040&partnerID=40&md5=2d71aabe0de639785557088677ad5a6a

DOI: 10.1016/j.actamat.2013.05.040
AFFILIATIONS: Institute of Metal Research, Chinese Academy of Sciences, Wenhua Road 72, Shenyang 110016, China;
Max-Planck Institut für Eisenforschung, Max-Planck-Strabe 1, Düsseldorf 40237, Germany
ABSTRACT: The concurrent ferrite recrystallization and austenitic transformation during intercritical annealing of cold-rolled DP steels is investigated by cellular automaton (CA) modeling. The simulations provide insight into the microstructural phenomena that result from the interaction of primary recrystallization and phase transformation. We find that the interaction between ferrite recrystallization and austenite formation affects not only the transformation kinetics but also the morphology and spatial distribution of the austenite. From this we can interpret experimental data of the observed temperature-dependent hardness and its dependence on the two metallurgical processes. The influence of the initial heating rate on subsequent isothermal transformation kinetics and the microstructure evolution is also obtained by the model.
AUTHOR KEYWORDS: Austenitization; Cellular automaton; Ferrite recrystallization; Intercritical annealing; Mesoscopic modeling
DOCUMENT TYPE: Article
SOURCE: Scopus

De Siqueira, R.P., Sandim, H.R.Z., Raabe, D.
Particle stimulated nucleation in coarse-grained ferritic stainless steel
(2013) Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 44 (1), pp. 469-478. Cited 9 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84871969634&doi=10.1007%2fs11661-012-1408-x&partnerID=40&md5=6a8c683d33cc11467af1d94b0770bdec

DOI: 10.1007/s11661-012-1408-x
AFFILIATIONS: Departamento de Engenharia de Materiais, Escola de Engenharia de Lorena, University of Sao Paulo, Lorena SP 12600-970, Brazil;
Max-Planck Institut für Eisenforschung (MPIE), 40237 Düsseldorf, Germany
ABSTRACT: Particle-stimulated nucleation (PSN) is investigated in Nb-containing ferritic stainless steel. Coarse-grained sheets were cold rolled to 80 pct thickness reduction and annealed from 973 K to 998 K (700 C to 725 C) to obtain partially recrystallized microstructures. Electron backscatter diffraction was performed around coarse niobium carbonitride particles (larger than 1 μm) within coarse grains (~1 mm), with different host orientations in both deformed and annealed states. In the deformed state, the deformation zones around both spherical and rectangular particles were investigated. The local lattice rotations about the transverse direction necessary to accommodate the particle-matrix strain incompatibility were observed in all grains investigated. After annealing, recrystallization occurs preferentially around coarse particles at the initial stages of recrystallization. Based on a total number of 130 grains nucleated via PSN, we observe both, randomly oriented and minor {111}110 oriented texture components. The results also reveal that PSN in this material is not associated with a specific host orientation.
DOCUMENT TYPE: Article
SOURCE: Scopus

Shin, J., Yi, S., Pradeep, K.G., Choi, P.P., Raabe, D.
Spatial Distributions of Alloying Elements Obtained from Atom Probe Tomography of the Amorphous Ribbon Fe75C11Si2B8Cr4
(2013) Korean Journal of Materials Research, 23 (3), pp. 190-193.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84880841646&doi=10.3740%2fMRSK.2013.23.3.190&partnerID=40&md5=5c8624a87868ba760cefe811e6ed7002

DOI: 10.3740/MRSK.2013.23.3.190
AFFILIATIONS: Dept. of Materials Science and Metallurgical Engineering, Kyungpook National University, Daegu 702-701, South Korea;
Dept. of Microstructure Physics and Alloy Design, Max-Planck Institute for Iron Research GmbH, Duesseldorf 40237, Germany
ABSTRACT: Spatial distributions of alloying elements of an Fe-based amorphous ribbon with a nominal composition of Fe75C11Si2B8Cr4we re analyzed through the atom probe tomography method. The amorphous ribbon was prepared through the melt spinning method. The macroscopic amorphous natures were confirmed using an X-ray diffractometer (XRD) and a differential scanning calorimeter (DSC). Atom Probe (Cameca LEAP 3000X HR) analyses were carried out in pulsed voltage mode at a specimen base temperature of about 60 K, a pulse to base voltage ratio of 15 %, and a pulse frequency of 200 kHz. The target detection rate was set to 5 ions per 1000 pulses. Based on a statistical analyses of the data obtained from the volume of 59 x 59 x 33 nm3, homogeneous distributions of alloying elements in nano-scales were concluded. Even with high carbon and strong carbide forming element contents, nano-scale segregation zones of alloying elements were not detected within the Fe-based amorphous ribbon. However, the existence of small sub-nanometer scale clusters due to short range ordering cannot be completely excluded.
AUTHOR KEYWORDS: Alloy design; Amorphous alloy; Atom probe tomography; Carbide former.; Melt-spinning process
DOCUMENT TYPE: Article
SOURCE: Scopus

Cojocaru-Mirédin, O., Schwarz, T., Choi, P.-P., Herbig, M., Wuerz, R., Raabe, D.
Atom probe tomography studies on the Cu(In,ga)Se2 grain boundaries
(2013) Journal of visualized experiments : JoVE, (74), . Cited 3 times.
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DOI: 10.3791/50376
AFFILIATIONS: Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH
ABSTRACT: Compared with the existent techniques, atom probe tomography is a unique technique able to chemically characterize the internal interfaces at the nanoscale and in three dimensions. Indeed, APT possesses high sensitivity (in the order of ppm) and high spatial resolution (sub nm). Considerable efforts were done here to prepare an APT tip which contains the desired grain boundary with a known structure. Indeed, site-specific sample preparation using combined focused-ion-beam, electron backscatter diffraction, and transmission electron microscopy is presented in this work. This method allows selected grain boundaries with a known structure and location in Cu(In,Ga)Se2 thin-films to be studied by atom probe tomography. Finally, we discuss the advantages and drawbacks of using the atom probe tomography technique to study the grain boundaries in Cu(In,Ga)Se2 thin-film solar cells.
DOCUMENT TYPE: Article
SOURCE: Scopus

Titrian, H., Aydin, U., Friák, M., Ma, D., Raabe, D., Neugebauer, J.
Self-consistent scale-bridging approach to compute the elasticity of multi-phase polycrystalline materials
(2013) Materials Research Society Symposium Proceedings, 1524, pp. 17-23. Cited 6 times.
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DOI: 10.1557/opl.2013.41
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany;
University Duisburg-Essen, Germany
ABSTRACT: A necessary prerequisite for a successful theory-guided up-scale design of materials with application-driven elastic properties is the availability of reliable homogenization techniques. We report on a new software tool that enables us to probe and analyze scale-bridging structure-property relations in the elasticity of materials. The newly developed application, referred to as SC-EMA (Self-consistent Calculations of Elasticity of Multi-phase Aggregates) computes integral elastic response of randomly textured polycrystals. The application employs a Python modular library that uses single-crystalline elastic constants Cij as input parameters and calculates macroscopic elastic moduli (bulk, shear, and Young's) and Poisson ratio of both single-phase and multi-phase aggregates. Crystallites forming the aggregate can be of cubic, tetragonal, hexagonal, orthorhombic, or trigonal symmetry. For cubic polycrystals the method matches the Hershey homogenization scheme. In case of multi-phase polycrystalline composites, the shear moduli are computed as a function of volumetric fractions of phases present in aggregates. Elastic moduli calculated using the analytical self-consistent method are computed together with their bounds as determined by Reuss, Voigt and Hashin-Shtrikman homogenization schemes. The library can be used as (i) a toolkit for a forward prediction of macroscopic elastic properties based on known single-crystalline elastic characteristics, (ii) a sensitivity analysis of macro-scale output parameters as function of input parameters, and, in principle, also for (iii) an inverse materials-design search for unknown phases and/or their volumetric ratios.
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Steinmetz, D.R., Jäpel, T., Wietbrock, B., Eisenlohr, P., Gutierrez-Urrutia, I., Saeed-Akbari, A., Hickel, T., Roters, F., Raabe, D.
Revealing the strain-hardening behavior of twinning-induced plasticity steels: Theory, simulations, experiments
(2013) Acta Materialia, 61 (2), pp. 494-510. Cited 149 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84869509318&doi=10.1016%2fj.actamat.2012.09.064&partnerID=40&md5=45e3f5c273ef3508123d5315b6fff149

DOI: 10.1016/j.actamat.2012.09.064
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Institute of Metal Forming, RWTH Aachen University, Intzestrasse 10, 52056 Aachen, Germany;
Institute of Ferrous Metallurgy, RWTH Aachen University, Intzestrasse 1, 52056 Aachen, Germany
ABSTRACT: We present a multiscale dislocation density-based constitutive model for the strain-hardening behavior in twinning-induced plasticity (TWIP) steels. The approach is a physics-based strain rate- and temperature-sensitive model which reflects microstructural investigations of twins and dislocation structures in TWIP steels. One distinct advantage of the approach is that the model parameters, some of which are derived by ab initio predictions, are physics-based and known within an order of

magnitude. This allows more complex microstructural information to be included in the model without losing the ability to identify reasonable initial values and bounds for all parameters. Dislocation cells, grain size and twin volume fraction evolution are included. Particular attention is placed on the mechanism by which new deformation twins are nucleated, and a new formulation for the critical twinning stress is presented. Various temperatures were included in the parameter optimization process. Dissipative heating is also considered. The use of physically justified parameters enables the identification of a universal parameter set for the example of an Fe-22Mn-0.6C TWIP steel.
AUTHOR KEYWORDS: Constitutive modeling; Strain hardening; Twinning; TWIP steels
DOCUMENT TYPE: Article
SOURCE: Scopus

Duarte, M.J., Klemm, J., Klemm, S.O., Mayrhofer, K.J.J., Stratmann, M., Borodin, S., Romero, A.H., Madinehei, M., Crespo, D., Serrano, J., Gerstl, S.S.A., Choi, P.P., Raabe, D., Renner, F.U.
Element-resolved corrosion analysis of stainless-type glass-forming steels (2013) Science, 341 (6144), pp. 372-376. Cited 49 times.
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DOI: 10.1126/science.1230081
AFFILIATIONS: Department of Interface Chemistry and Surface Engineering, Max-Planck Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany;
Departamento de Materiales, Centro de Investigación y de Estudios Avanzados, Instituto Politécnico Nacional (CINVESTAV-IPN), 76230 Queretaro, Mexico;
Departament de Fisica Aplicada, Universitat Politècnica de Catalunya, 08860 Castelldefels, Spain;
Department of Microstructure Physics and Alloy Design, Max-Planck Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany;
Max-Planck Institut für Mikrostrukturphysik, 06120 Halle, Germany;
Institució Catalana de Recerca I Estudis Avançats (ICREA), Universitat Politècnica de Catalunya, 08860 Castelldefels, Spain;
Physics Department, West Virginia University, Morgantown, WV 26506-6315, United States;
Electron Microscopy of Eidgenössische Technische Hochschule Zurich (EMEZ), 8093 Zurich, Switzerland;
Instituut Voor Materiaalonderzoek, Universiteit Hasselt, 3590 Diepenbeek, Belgium
ABSTRACT: Ultrathin passive films effectively prevent the chemical attack of stainless steel grades in corrosive environments; their stability depends on the interplay between structure and chemistry of the constituents iron, chromium, and molybdenum (Fe-Cr-Mo). Carbon (C), and eventually boron (B), are also important constituents of steels, although in small quantities. In particular, nanoscale inhomogeneities along the surface can have an impact on material failure but are still poorly understood. Addressing a stainless-type glass-forming Fe50Cr15Mo14C15B 6 alloy and using a combination of complementary high-resolution analytical techniques, we relate near-atomistic insights into increasingly inhomogeneous nanostructures with time- and element-resolved dissolution behavior. The progressive elemental partitioning on the nanoscale determines the degree of passivation. A detrimental transition from Cr-controlled passivity to Mo-controlled breakdown is dissected atom by atom, demonstrating the importance of nanoscale knowledge for understanding corrosion.
DOCUMENT TYPE: Article
SOURCE: Scopus

Chikkadi, V., Mandal, S., Nienhuis, B., Raabe, D., Varnik, F., Schall, P.
Shear-induced anisotropic decay of correlations in hard-sphere colloidal glasses
(2012) EPL, 100 (5), art. no. 56001, . Cited 7 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84871302152&doi=10.1209%2f0295-5075%2f100%2f56001&partnerID=40&md5=96421e2bee023bd26c8006e28c2e82b4

DOI: 10.1209/0295-5075/100/56001
AFFILIATIONS: Institute of Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, Netherlands;
Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany;
Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Bochum, Germany
ABSTRACT: Spatial correlations of microscopic fluctuations are investigated via real-space experiments and computer simulations of colloidal glasses under steady shear. It is shown that while the distribution of one-particle fluctuations is always isotropic regardless of the relative importance of shear as compared to thermal fluctuations, their spatial correlations show a marked sensitivity to the competition between shear-induced and thermally activated relaxation. Correlations are isotropic in the thermally dominated regime, but develop strong anisotropy as shear dominates the dynamics of microscopic fluctuations. We discuss the relevance of this observation for a better understanding of flow heterogeneity in sheared amorphous solids.
DOCUMENT TYPE: Article
SOURCE: Scopus

Wu, W., Zhu, M.F., Sun, D.K., Dai, T., Han, Q.Y., Raabe, D.
Modelling of dendritic growth and bubble formation
(2012) IOP Conference Series: Materials Science and Engineering, 33 (1), art. no. 012103, . Cited 3 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84877905350&doi=10.1088%2f1757-899X%2f33%2f1%2f012103&partnerID=40&md5=deed3d1a4e3b477a7719aef94676be8f

DOI: 10.1088/1757-899X/33/1/012103
AFFILIATIONS: Jiangsu Key Lab for Advanced Metallic Materials, Southeast University, China;
Department of Mechanical Engineering Technology, Purdue University, United States;
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
ABSTRACT: A two-dimensional lattice Boltzmann method (LBM)-cellular automaton (CA) model is developed for the simulation of dendritic growth and bubble formation during alloy solidification. In the model, a kinetic LBM, which describes flow dynamics through the evolution of distribution functions of moving pseudo-particles, is adopted to numerically solve the gas-liquid two-phase flow based on the Shan-Chen multiphase scheme. The kinetics of dendritic growth is determined according to a local solute equilibrium approach. The present model takes into account the effect of liquid-solid phase transformation on the nucleation and growth of bubbles. The interaction mechanism between dendrites and bubbles is also embedded in the model. The wettability of a bubble on a smooth solid surface is simulated. The simulated contact angles with various interaction coefficients agree well with the data calculated from an empirical formula derived from the Young's equation. The proposed model is applied to simulate dendritic growth and bubble formation under directional solidification conditions. The simulated results are compared with those observed experimentally during solidification of a transparent organic material. The simulation results reveal some dynamic features of bubble nucleation, growth, and motion, as well as the interaction between the dendritic growth and bubble formation during solidification.

DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Friák, M., Counts, W.A., Ma, D., Sander, B., Holec, D., Raabe, D., Neugebauer, J.
Theory-guided materials design of multi-phase Ti-Nb alloys with bone-matching elastic properties
(2012) Materials, 5 (10), pp. 1853-1872. Cited 23 times.
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DOI: 10.3390/ma5101853
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany;
Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Franz-Josef-Strasse 18, A-8700 Leoben, Austria
ABSTRACT: We present a scale-bridging approach for modeling the integral elastic response of polycrystalline composite that is based on a multi-disciplinary combination of (i) parameter-free first-principles calculations of thermodynamic phase stability and single-crystal elastic stiffness; and (ii) homogenization schemes developed for polycrystalline aggregates and composites. The modeling is used as a theory-guided bottom-up materials design strategy and applied to Ti-Nb alloys as promising candidates for biomedical implant applications. The theoretical results (i) show an excellent agreement with experimental data and (ii) reveal a decisive influence of the multi-phase character of the polycrystalline composites on their integral elastic properties. The study shows that the results based on the density functional theory calculations at the atomistic level can be directly used for predictions at the macroscopic scale, effectively scale-jumping several orders of magnitude without using any empirical parameters.
AUTHOR KEYWORDS: Ab initio; Bio-materials; Biocompatibility; Finite element method; Multi-phase composites; Multi-scale; Ti alloys
DOCUMENT TYPE: Article
SOURCE: Scopus

Woldemedhin, M.T., Raabe, D., Hassel, A.W.
Characterization of thin anodic oxides of Ti-Nb alloys by electrochemical impedance spectroscopy
(2012) Electrochimica Acta, 82, pp. 324-332. Cited 33 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84866393228&doi=10.1016%2fj.electacta.2012.06.029&partnerID=40&md5=f0ac20102b139297e92dba5f0855ca21

DOI: 10.1016/j.electacta.2012.06.029
AFFILIATIONS: Max Planck Institut für Eisenforschung GmbH, Max Planck Str. 1, D-40237 Düsseldorf, Germany;
Johannes Kepler University, Institute for Chemical Technology of Inorganic Materials, Altenberger Str. 69, 4040 Linz, Austria
ABSTRACT: Electrochemical impedance spectroscopy was used to study the interface between the anodic oxide formed on Ti-Nb alloys with specific compositions of Ti-10 wt.% Nb and Ti-20 wt.% Nb and the electrolyte. The anodic oxides were grown in an acetate buffer of pH 6.0 by using cyclic voltammetry electrochemical technique in which the potential is scanned at a rate of 100 mV s -1. The potential applied starts from 0 V and increasing at steps of 1 V till 8 V which allows to study the mechanism and the kinetics involved during the oxide growth. The electrochemical impedance measurements were started prior to applying any potential so that the electronic properties of the native oxide on the Ti-Nb alloys can be determined. The electrochemical measurements were then carried out after each oxide growth so that the electronic properties of the previously grown

oxide can also be determined. The variation of the capacitance of the respective oxides determined from the impedance measurements with the applied potential enables the calculation of the relative permittivity of the respective oxides on the two alloys. Moreover the semiconducting properties of the oxides were determined by using Mott-Schottky analysis. The Mott-Schottky analysis involves electrochemical impedance measurements at fixed frequency with increasing applied bias potential so that the variation of the capacitance of the space charge region with the applied potential can be followed. The oxides from both alloys showed an n-type semiconducting property with 7.5 × 10 18 cm -3 and 2.4 × 10 19 cm -3 donor concentration for Ti-10 wt.% Nb and Ti-20 wt.% Nb alloys respectively. © 2012 Elsevier Ltd.
AUTHOR KEYWORDS: Anodic oxide; Electrochemical impedance spectroscopy; Mott-Schottky analysis
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Fabritius, H.-O., Karsten, E.S., Balasundaram, K., Hild, S., Huemer, K., Raabe, D.
Correlation of structure, composition and local mechanical properties in the dorsal carapace of the edible crab cancer pagurus
(2012) Zeitschrift fur Kristallographie, 227 (11), pp. 766-776. Cited 25 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84870901114&doi=10.1524%2fzkri.2012.1532&partnerID=40&md5=c723319372b36b35960b966d2b2ab2e8

DOI: 10.1524/zkri.2012.1532
AFFILIATIONS: Department Microstructure Physics and Alloy Design, Max-Planck-Institut Für Eisenforschung GmbH, 40237 Düsseldorf, Germany; Department of Polymer Science, Johannes Kepler University Linz (JKU), 4040 Linz, Austria
ABSTRACT: The exoskeleton of crustaceans is formed by the cuticle, a chitin-protein-based nano-composite with hierarchical organization over at least eight levels. On the molecular level, it consists of chitin associated with proteins forming fibres, which are organized in the form of twisted plywood. On the higher levels, the twisted plywood organization is modified and forms skeletal elements with elaborate functions. The load-bearing parts of crustacean cuticle are reinforced with both crystalline and amorphous biominerals. During evolution, all parts of the exoskeleton were optimized to fulfill different functions according to different ecophysiological strains faced by the animals. This is achieved by modifications in microstructure and chemical composition. In order to understand the relationship between structure, composition, mechanical properties and function we structurally characterized cuticle from the dorsal carapace of the edible crab Cancer pagurus using light and scanning electron microscopy (SEM). The local chemical composition was investigated using energy dispersive X-ray spectroscopy (EDX) and confocal m-Raman spectroscopy. Nanoindentation tests were performed to study the resulting local mechanical properties. The results show local differences in structure on several levels of the structural hierarchy in combination with a very heterogeneous mineralization. The distal exocuticle is mineralized with calcite, followed by a layer containing a magnesium, phosphate and carbonate rich phase and ACC in the proximal part. The endocuticle contains magnesian calcite and ACC in special regions below the exocuticle. Structure and mineral phase are reflected in the local stiffness and hardness of the respective cuticle regions. The heterogeneity of structural organization and mechanical properties suggests remarkable consequences for the mechanical behaviour of the bulk material.
AUTHOR KEYWORDS: Biomineralization; Crustacean cuticle; Structure-property relations
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Cojocaru-Mirédin, O., Choi, P., Wuerz, R., Raabe, D.
Exploring the p-n junction region in Cu(In,Ga)Se 2 thin-film solar cells at the nanometer-scale
(2012) Applied Physics Letters, 101 (18), art. no. 181603, . Cited 29 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84868651406&doi=10.1063%2f1.4764527&partnerID=40&md5=0523fee6adcbda21e3a8957d8a1e5469

DOI: 10.1063/1.4764527
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Strae 1, 40237 Düsseldorf, Germany;
Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, Stuttgart, Germany
ABSTRACT: In this work we study the CdS/Cu(In,Ga)Se 2 p-n junction region in Cu(In,Ga)Se 2 thin-film solar cells using atom probe tomography. A Cu-, Ga-depleted, and Cd-doped region of about 1 nm thickness is detected at the Cu(In,Ga)Se 2 side of the CdS/Cu(In,Ga)Se 2 interface. Furthermore, Cd is also found to be enriched at Cu(In,Ga)Se 2 grain boundaries connected to the CdS layer. Na and O impurities decorate the CdS/CIGS interface, where Na-rich clusters are preferentially located in CdS regions abutting to Cu(In,Ga)Se 2 grain boundaries. The experimental findings of this work demonstrate the capability of atom probe tomography in studying buried interfaces and yield vital information for understanding and modeling the p-n junction band structure in Cu(In,Ga)Se 2 solar cells. © 2012 American Institute of Physics.
DOCUMENT TYPE: Article
SOURCE: Scopus

Seol, J.-B., Raabe, D., Choi, P.-P., Im, Y.-R., Park, C.-G.
Atomic scale effects of alloying, partitioning, solute drag and austempering on the mechanical properties of high-carbon bainitic-austenitic TRIP steels
(2012) Acta Materialia, 60 (17), pp. 6183-6199. Cited 52 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84866734262&doi=10.1016%2fj.actamat.2012.07.064&partnerID=40&md5=a1967f59b53b74033c9eb6b9dee90ca2

DOI: 10.1016/j.actamat.2012.07.064
AFFILIATIONS: Max-Planck-Insititut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Technical Research Laboratories, POSCO, 790-785 Pohang, South Korea;
Department of Materials Science and Engineering, Pohang University of Science and Technology (POSTECH), 790-784 Pohang, South Korea
ABSTRACT: Understanding alloying and thermal processing at an atomic scale is essential for the optimal design of high-carbon (0.71 wt.%) bainitic-austenitic transformation-induced plasticity (TRIP) steels. We investigate the influence of the austempering temperature, chemical composition (especially the Si:Al ratio) and partitioning on the nanostructure and mechanical behavior of these steels by atom probe tomography. The effects of the austempering temperature and of Si and Al on the compositional gradients across the phase boundaries between retained austenite and bainitic ferrite are studied. We observe that controlling these parameters (i.e. Si, Al content and austempering temperature) can be used to tune the stability of the retained austenite and hence the mechanical behavior of these steels. We also study the atomic scale redistribution of Mn and Si at the bainitic ferrite/austenite interface. The observations suggest that either para-equilibrium or local equilibrium-negligible partitioning conditions prevail depending on the Si:Al ratio during bainite transformation.

AUTHOR KEYWORDS: Austempering; Bainite; High-carbon steels; Retained austenite; TRIP effect
DOCUMENT TYPE: Article
SOURCE: Scopus

Reeh, S., Music, D., Gebhardt, T., Kasprzak, M., Jäpel, T., Zaefferer, S., Raabe, D., Richter, S., Schwedt, A., Mayer, J., Wietbrock, B., Hirt, G., Schneider, J.M.
Elastic properties of face-centred cubic Fe-Mn-C studied by nanoindentation and ab initio calculations
(2012) Acta Materialia, 60 (17), pp. 6025-6032. Cited 24 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84866729410&doi=10.1016%2fj.actamat.2012.07.038&partnerID=40&md5=73b67a34b09306a97be5a897ceb44790

DOI: 10.1016/j.actamat.2012.07.038
AFFILIATIONS: Materials Chemistry, RWTH Aachen University, D-52056 Aachen, Germany;
Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany;
Central Facility for Electron Microscopy, RWTH Aachen University, D-52056 Aachen, Germany;
Institute of Metal Forming, RWTH Aachen University, D-52056 Aachen, Germany
ABSTRACT: We have studied experimentally and theoretically the influence of C and Mn content on the Young's modulus of Fe-Mn-C alloys. Combinatorial thin film and bulk samples were characterized regarding their structure, texture and Young's modulus. The following chemical composition range was investigated: 1.5-3.0 at.% C, 28.0-37.5 at.% Mn and 60.6-69.8 at.% Fe. The experimental lattice parameters change marginally within 3.597-3.614 Å with the addition of C and are consistent with ab initio calculations. The Young's modulus data are in the range of 185 ± 12-251 ± 59 GPa for the bulk samples and the thin film, respectively. C has no significant effect on the Young's modulus of these alloys within the composition range studied here. The ab initio calculations are 15-22% larger than the average Young's modulus values of the as-deposited and polished thin film at 3 at.% C. The comparison of thin film and bulk samples results reveals similar elastic properties for equivalent compositions, indicating that the applied research strategy consisting of the combinatorial thin film approach in conjunction with ab initio calculations is useful to study the composition dependence of the structure and elastic properties of Fe-Mn-C alloys. The very good agreement between the presented calculations and the experimentally determined lattice parameters and Young's modulus values implies that the here-adopted simulation strategy yields a reliable description of carbon in Fe-Mn alloys, important for future alloy design.
AUTHOR KEYWORDS: Ab initio electron theory; Elastic behaviour; Iron alloys; Nanoindentation; Sputtering
DOCUMENT TYPE: Article
SOURCE: Scopus

Gutierrez-Urrutia, I., Raabe, D.
Multistage strain hardening through dislocation substructure and twinning in a high strength and ductile weight-reduced Fe-Mn-Al-C steel
(2012) Acta Materialia, 60 (16), pp. 5791-5802. Cited 140 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84866105177&doi=10.1016%2fj.actamat.2012.07.018&partnerID=40&md5=f7f787dd40b4234b1134f1cba62ea7e9

DOI: 10.1016/j.actamat.2012.07.018
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck Str. 1, D-40237 Düsseldorf, Germany
ABSTRACT: We investigate the kinetics of the deformation structure evolution and its contribution to the strain hardening of a Fe-30.5Mn-2.1Al-1.2C (wt.%) steel during tensile deformation by means of transmission

electron microscopy and electron channeling contrast imaging combined with electron backscatter diffraction. The alloy exhibits a superior combination of strength and ductility (ultimate tensile strength of 1.6 GPa and elongation to failure of 55%) due to the multiple-stage strain hardening. We explain this behavior in terms of dislocation substructure refinement and subsequent activation of deformation twinning. The early hardening stage is fully determined by the size of the dislocation substructure, namely, Taylor lattices, cell blocks and dislocation cells. The high carbon content in solid solution has a pronounced effect on the evolving dislocation substructure. We attribute this effect to the reduction of the dislocation cross-slip frequency by solute carbon. With increasing applied stress, the cross-slip frequency increases. This results in a gradual transition from planar (Taylor lattices) to wavy (cells, cell blocks) dislocation configurations. The size of such dislocation substructures scales inversely with the applied resolved stress. We do not observe the so-called microband-induced plasticity effect. In the present case, due to texture effects, microbanding is not favored during tensile deformation and, hence, has no effect on strain hardening.
AUTHOR KEYWORDS: Austenitic steel; Deformation structures; Dislocation structures; Electron channeling contrast imaging; Strain hardening
DOCUMENT TYPE: Article
SOURCE: Scopus

Iwasa, N., Sakata, N., Takahashi, J., Raabe, D., Takemoto, Y., Senuma, T.
Precipitation behavior of v and/or cu bearing middle carbon steels
(2012) Tetsu-To-Hagane/Journal of the Iron and Steel Institute of Japan, 98 (8), pp. 434-441. Cited 2 times.
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DOI: 10.2355/tetsutohagane.98.434
AFFILIATIONS: School of Natural Science and Technology, Okayama University, 1-1-1 Tsushima-naka, Kita-ku Okayama 700-8530, Japan;
Advanced Technology Research Labs, Nippon Steel Corporation, Max-Planck-Institute for Iron Research, Japan
ABSTRACT: In this study, the precipitation behavior of middle carbon steels with single and multiple additions of 0.3mass%V and 2mass%Cu has been investigated. The precipitation treatment was carried out isothermally at 600°C.In the 0.3mass%V bearing steel, precipitates were observed in rows, indicating the occurrence of the interphase precipitation. On the other hand, precipitates observed in the 2mass%Cu bearing steel were randomly dispersed. In the V and Cu bearing steel, Cu precipitates were not randomly dispersed and mainly observed attached with VCN which were precipitated in rows. In the paper, the different precipitation behavior of the three steels is discussed in detail and is explained from a viewpoint of the thermodynamics and kinetics using a metallurgical model.
AUTHOR KEYWORDS: Hot forging; Interphase precipitation; Middle carbon steel; Precipitation
DOCUMENT TYPE: Article
SOURCE: Scopus

Liu, B., Eisenlohr, P., Roters, F., Raabe, D.
Simulation of dislocation penetration through a general low-angle grain boundary
(2012) Acta Materialia, 60 (13-14), pp. 5380-5390. Cited 30 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84864753557&doi=10.1016%2fj.actamat.2012.05.002&partnerID=40&md5=cffcdfcddb76ac81ec1f89e40cb771d8

DOI: 10.1016/j.actamat.2012.05.002

AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany
ABSTRACT: The interaction of dislocations with low-angle grain boundaries (LAGBs) is considered one important contribution to the mechanical strength of metals. Although LAGBs have been frequently observed in metals, little is known about how they interact with free dislocations that mainly carry the plastic deformation. Using discrete dislocation dynamics simulations, we are able to quantify the resistance of a LAGB - idealized as three sets of dislocations that form a hexagonal dislocation network - against lattice dislocation penetration, and examine the associated dislocation processes. Our results reveal that such a coherent internal boundary can massively obstruct and even terminate dislocation transmission and thus make a substantial contribution to material strength.
AUTHOR KEYWORDS: Dislocation dynamics; Dislocation processes; Hexagonal dislocation network; Low-angle grain boundary; Strength
DOCUMENT TYPE: Article
SOURCE: Scopus

He, D., Zhu, J.C., Zaefferer, S., Raabe, D., Liu, Y., Lai, Z.L., Yang, X.W.
Influences of deformation strain, strain rate and cooling rate on the Burgers orientation relationship and variants morphology during β→α phase transformation in a near α titanium alloy
(2012) Materials Science and Engineering A, 549, pp. 20-29. Cited 28 times.
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DOI: 10.1016/j.msea.2012.03.110
AFFILIATIONS: National Key Laboratory for Precision Hot Processing of Metals, Harbin Institute of Technology, Harbin 150001, China; Max-Planck-Institut für Eisenforschung, Abteilung Mikrostrukturphysik und Umformtechnik, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany
ABSTRACT: High temperature compression deformation studies of Ti-6Al-2Zr-1Mo-1V titanium alloy in full β phase region with different strains/strain rates and then with subsequent varied cooling rates were performed to understand the microstructure evolution. Crystal orientation information and microstructure morphology of all tested samples were investigated by electron backscatter diffraction (EBSD) measurements. The crystal orientations of prior high temperature β grains were estimated by reconstructing the retained β phase at room temperature. The theoretical crystal orientations of all possible α variants within an investigated prior β grain were calculated according to the Burgers orientation relationship (OR) between parent and product phase. The calculated and experimental results were then compared and analyzed. The influences of deformation strain, strain rate and cooling rate on the Burgers OR between prior β matrix and precipitated α phase were investigated. Full discussions have been conducted by combination of crystal plasticity finite element method (CP-FEM) grain-scale simulation results. The results indicate that external factors (such as deformation strain, strain rate and cooling rate) have a slight influence on the obeying of Burgers OR rule during β → α phase transformation. However, strain rate and cooling rate have a significant effect on the morphology of precipitated α phase.
AUTHOR KEYWORDS: Burgers orientation relationship; Cooling rate; Deformation strain; Strain rate; Variants morphology
DOCUMENT TYPE: Article
SOURCE: Scopus

Calcagnotto, M., Ponge, D., Raabe, D.
Microstructure control during fabrication of ultrafine grained dual-phase steel: Characterization and effect of intercritical annealing parameters
(2012) ISIJ International, 52 (5), pp. 874-883. Cited 25 times.

https://www.scopus.com/inward/record.uri?eid=2-s2.0-84863104781&partnerID=40&md5=7758e4588aca105b1af435cb5515f46b

AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf, 40237, Germany;
Salzgitter Mannesmann Forschung GmbH, Materials and Process Development, Eisenhüttenstraße 99, Salzgitter, 38239, Germany
ABSTRACT: An ultrafine grained (UFG) ferrite/cementite steel was subjected to intercritical annealing in order to obtain an UFG ferrite/martensite dual-phase (DP) steel. The intercritical annealing parameters, namely, holding temperature and time, heating rate, and cooling rate were varied independently by applying dilatometer experiments. Microstructure characterization was performed using scanning electron microscopy (SEM) and high-resolution electron backscatter diffraction (EBSD). An EBSD data post-processing routine is proposed that allows precise distinction between the ferrite and the martensite phase. The sensitivity of the microstructure to the different annealing conditions is identified. As in conventional DP steels, the martensite fraction and the ferrite grain size increase with intercritical annealing time and temperature. Furthermore, the variations of the microstructure are explained in terms of the changes in phase transformation kinetics due to grain refinement and the manganese enrichment in cementite during warm deformation. © 2012 ISIJ.
AUTHOR KEYWORDS: Dual-phase steel; EBSD; Grain refinement; Microstructure evolution; Ultrafine grains
DOCUMENT TYPE: Article
SOURCE: Scopus

Springer, H., Raabe, D.
Rapid alloy prototyping: Compositional and thermo-mechanical high throughput bulk combinatorial design of structural materials based on the example of 30Mn-1.2C-xAl triplex steels
(2012) Acta Materialia, 60 (12), pp. 4950-4959. Cited 50 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84862988454&doi=10.1016%2fj.actamat.2012.05.017&partnerID=40&md5=bfc8a336d8932a399a056359c684baa5

DOI: 10.1016/j.actamat.2012.05.017
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany
ABSTRACT: We introduce a new experimental approach to the compositional and thermo-mechanical design and rapid maturation of bulk structural materials. This method, termed rapid alloy prototyping (RAP), is based on semi-continuous high throughput bulk casting, rolling, heat treatment and sample preparation techniques. 45 Material conditions, i.e. 5 alloys with systematically varied compositions, each modified by 9 different ageing treatments, were produced and investigated within 35 h. This accelerated screening of the tensile, hardness and microstructural properties as a function of chemical and thermo-mechanical parameters allows the highly efficient and knowledge-based design of bulk structural alloys. The efficiency of the approach was demonstrated on a group of Fe-30Mn-1.2C-xAl steels which exhibit a wide spectrum of structural and mechanical characteristics, depending on the respective Al concentration. High amounts of Al addition (>8 wt.%) resulted in pronounced strengthening, while low concentrations (<2 wt.%) led to embrittlement of the material during ageing. © 2012 Acta Materialia Inc. Published by Elsevier Ltd.
AUTHOR KEYWORDS: Combinatorial alloy design; Fe-Mn-Al-C steel; Mechanical properties; Steels; Structural alloys
DOCUMENT TYPE: Article
SOURCE: Scopus

Zheng, C., Raabe, D., Li, D.
Prediction of post-dynamic austenite-to-ferrite transformation and reverse transformation in a low-carbon steel by cellular automaton modeling

(2012) Acta Materialia, 60 (12), pp. 4768-4779. Cited 29 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84862993802&doi=10.1016%2fj.actamat.2012.06.007&partnerID=40&md5=c205d43259ba8b39e29c291881c3ea6a

DOI: 10.1016/j.actamat.2012.06.007
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf 40237, Germany;
Institute of Metal Research, Chinese Academy of Sciences, Wenhua Road 72, Shenyang 110016, China
ABSTRACT: The post-dynamic transformation that takes place during the subsequent isothermal holding for the case when dynamic strain-induced transformation (DSIT) from austenite to ferrite occurs during hot deformation is investigated by cellular automaton modeling. The simulation provides a better understanding of carbon diffusion in retained austenite and the resulting microstructure evolution during the post-dynamic transformation. The predictions reveal that continuing transformation from retained austenite to ferrite and the reverse transformation can occur simultaneously in the same microstructure during post-deformation isothermal holding owing to the locally acting chemical equilibrium conditions. Competition between forward and reverse transformation exists during the early stage of post-dynamic heat treatment. It is also revealed that increasing the final strain of DSIT might promote the reverse transformation, whereas the continuous austenite-to-ferrite transformation yields a diminishing effect. The influence of the DSIT final strain on the grain size of ferrite and the characteristics of the resultant microstructure is also discussed. © 2012 Acta Materialia Inc. Published by Elsevier Ltd.
AUTHOR KEYWORDS: Cellular automaton; Low-carbon steel; Modeling; Post-dynamic transformation; Strain-induced transformation
DOCUMENT TYPE: Article
SOURCE: Scopus

Szczepaniak, A., Fan, J., Kostka, A., Raabe, D.
On the correlation between thermal cycle and formation of intermetallic phases at the interface of laser-welded aluminum-steel overlap joints
(2012) Advanced Engineering Materials, 14 (7), pp. 464-472. Cited 11 times.
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DOI: 10.1002/adem.201200075
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany;
BIAS-Bremer Institut für Angewandte Strahltechnik GmbH, 28359 Bremen, Germany
ABSTRACT: A laser beam welding process via heat conduction was applied to join DC01 steel with aluminum (Al) in overlap configuration without filler wire. The effect of the applied laser power (1.7, 1.8, 2.1, and 2.4 kW) on the formation and evolution of the interfaces between steel and Al was analyzed. Two intermetallic compounds were found at the interface, namely, one adjacent to the steel layer (Al 5Fe 2) and one close to the solidified Al (Al 13Fe 4). The thickness of the intermetallic reaction layer increases with laser power, while the morphology of its individual components evolves due to differences in accumulated thermal cycles. Correlations between simulations and measurements show that the peak temperature has significantly stronger influence on the thickness of the intermetallic reaction layer than cooling time and the integral of temperature over the time. Shear/tensile strength tests reveal that all the specimens fail in the Al heat affected zone. © 2012 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
DOCUMENT TYPE: Article
SOURCE: Scopus

Gutierrez-Urrutia, I., Raabe, D.
Grain size effect on strain hardening in twinning-induced plasticity steels
(2012) Scripta Materialia, 66 (12), pp. 992-996. Cited 83 times.
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DOI: 10.1016/j.scriptamat.2012.01.037
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck Str. 1, D-40237 Düsseldorf, Germany
ABSTRACT: We investigate the influence of grain size on the strain hardening of two Fe-22Mn-0.6C (wt.%) twinning-induced plasticity steels with average grain sizes of 3 and 50 μm, respectively. The grain size has a significant influence on the strain hardening through the underlying microstructure. The dislocation substructure formed in the early deformation stages determines the density of nucleation sites for twins per unit grain boundary area which controls the developing twin substructure.
AUTHOR KEYWORDS: Dislocation structure; Plastic deformation; Scanning electron microscopy (SEM); Twinning; TWIP steels
DOCUMENT TYPE: Article
SOURCE: Scopus

Enax, J., Prymak, O., Raabe, D., Epple, M.
Structure, composition, and mechanical properties of shark teeth
(2012) Journal of Structural Biology, 178 (3), pp. 290-299. Cited 47 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84861481135&doi=10.1016%2fj.jsb.2012.03.012&partnerID=40&md5=79aca9151bf36ad88b25638afb25ba9f

DOI: 10.1016/j.jsb.2012.03.012
AFFILIATIONS: Institute of Inorganic Chemistry and Center for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, Universitaetsstr. 5-7, 45117 Essen, Germany;
Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: The teeth of two different shark species (Isurus oxyrinchus and Galeocerdo cuvier) and a geological fluoroapatite single crystal were structurally and chemically characterized. In contrast to dentin, enameloid showed sharp diffraction peaks which indicated a high crystallinity of the enameloid. The lattice parameters of enameloid were close to those of the geological fluoroapatite single crystal. The inorganic part of shark teeth consisted of fluoroapatite with a fluoride content in the enameloid of 3.1 wt.%, i.e., close to the fluoride content of the geological fluoroapatite single crystal (3.64 wt.%). Scanning electron micrographs showed that the crystals in enameloid were highly ordered with a special topological orientation (perpendicular towards the outside surface and parallel towards the center). By thermogravimetry, water, organic matrix, and biomineral in dentin and enameloid of both shark species were determined. Dentin had a higher content of water, organic matrix, and carbonate than enameloid but contained less fluoride. Nanoindentation and Vicker's microhardness tests showed that the enameloid of the shark teeth was approximately six times harder than the dentin. The hardness of shark teeth and human teeth was comparable, both for dentin and enamel/enameloid. In contrast, the geological fluoroapatite single crystal was much harder than both kinds of teeth due to the absence of an organic matrix. In summary, the different biological functions of the shark teeth (" tearing" for Isurus and "cutting" for Galeocerdo) are controlled by the different geometry and not by the chemical or crystallographic composition.
AUTHOR KEYWORDS: Biomineralization; Calcium phosphate; Mechanical properties; Nanoindentation; Sharks; Teeth
DOCUMENT TYPE: Article

SOURCE: Scopus

Winning, M., Raabe, D.
Influence of grain boundary mobility on microstructure evolution during recrystallisation
(2012) Materials Science Forum, 715-716, pp. 191-196.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84860736026&doi=10.4028%2fwww.scientific.net%2fMSF.715-716.191&partnerID=40&md5=c870dfbe0fd6e5ab2ac43d263bef4de0

DOI: 10.4028/www.scientific.net/MSF.715-716.191
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Abteilung Mikrostrukturphysik und Umformtechnik, Max-Planck-Str. 1, Düsseldorf, 40237, Germany
ABSTRACT: The paper introduces first investigations on how low angle grain boundaries can influence the recrystallisation behaviour of crystalline metallic materials. For this purpose a threedimensional cellular automaton model was used. The approach in this study is to allow even low angle grain boundaries to move during recrystallisation. The effect of this non-zero mobility of low angle grain boundaries will be analysed for the recrystallisation of deformed Al single crystals with Cube orientation. It will be shown that low angle grain boundaries indeed influence the kinetics as well as the texture evolution of metallic materials during recrystallisation.
AUTHOR KEYWORDS: Cellular automaton; Grain boundary mobility; Recrystallisation; Simulation
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Peranio, N., Roters, F., Raabe, D.
Microstructure evolution during recrystallization in dual-phase steels
(2012) Materials Science Forum, 715-716, pp. 13-22. Cited 3 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84860782440&doi=10.4028%2fwww.scientific.net%2fMSF.715-716.13&partnerID=40&md5=0aa9d4d1c832ba19d0cae38dcc1f909e

DOI: 10.4028/www.scientific.net/MSF.715-716.13
AFFILIATIONS: Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen, Germany;
Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: The microstructure and texture of rolled and annealed dual-phase steels with 0.147 wt. % C, 1.868 wt. % Mn, and 0.403 wt. % Si were analyzed using SEM, EDX, and EBSD. Hot rolled sheets showed a ferritic-pearlitic microstructure with a pearlite volume fraction of about 40 % and ferrite grain size of about 6 μm. Ferrite and pearlite were heterogeneously distributed at the surface and distributed in bands at the center of the sheets. The hot rolled sheets revealed a throughthickness texture inhomogeneity with a plane-strain texture with strong α-fiber and γ-fiber at the center and a shear texture at the surface. After cold rolling, the ferrite grains showed elongated morphology and larger orientation gradients, the period of the ferrite-pearlite band structure at the center of the sheets was decreased, and the plane-strain texture components were strengthened in the entire sheet. Recrystallization, phase transformation, and the competition of both processes were of particular interest with respect to the annealing experiments. For this purpose, various annealing techniques were applied, i.e., annealing in salt bath, conductive annealing, and industrial hot-dip coating. The sheets were annealed in the ferritic, intercritical, and austenitic temperature regimes in a wide annealing time range including variation of heating and cooling rates.
AUTHOR KEYWORDS: Cold rolling; DP steel; EBSD; Hot rolling; Microstructure; Recrystallization; Texture

DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Ravi Kumar, B., Raabe, D.
Tensile deformation characteristics of bulk ultrafine-grained austenitic stainless steel produced by thermal cycling
(2012) Scripta Materialia, 66 (9), pp. 634-637. Cited 18 times.
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DOI: 10.1016/j.scriptamat.2012.01.052
AFFILIATIONS: MST Division, CSIR, National Metallurgical Laboratory, Jamshedpur, India;
Max-Planck-Institut für Eisenforschung, Max-Planck Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: Deformation microstructures of bulk ultrafine-grained austenitic AISI 304L stainless steels were analyzed by electron backscatter diffraction. Samples with grain sizes below 500 nm showed transition from grain-scale deformation to the collective phenomenon of shear banding. This was assisted by strain-induced grain rotation and coalescence. This phenomenon was suppressed in samples with a bimodal grain size distribution (maxima at ~650 and ~1400 nm) due to deformation-induced martensite formation, yielding high tensile strength and ductility (1348 MPa ultimate tensile strength at 0.36 max. true strain).
AUTHOR KEYWORDS: Deformation-induced martensite; Electron backscatter diffraction; Plastic deformation; Stainless steel; Ultrafine grain
DOCUMENT TYPE: Article
SOURCE: Scopus

Gutierrez-Urrutia, I., Raabe, D.
Erratum: Dislocation density measurement by electron channeling contrast imaging in a scanning electron microscope (Scripta Materialia (2012) 66 (343-346))
(2012) Scripta Materialia, 66 (9), p. 720. Cited 1 time.
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DOI: 10.1016/j.scriptamat.2012.02.001
AFFILIATIONS: Max-Planck-Institut fur Eisenforschung, Max-Planck Str. 1, D-40237 Dusseldorf, Germany
DOCUMENT TYPE: Erratum
SOURCE: Scopus

Eisenlohr, A., Gutierrez-Urrutia, I., Raabe, D.
Adiabatic temperature increase associated with deformation twinning and dislocation plasticity
(2012) Acta Materialia, 60 (9), pp. 3994-4004. Cited 27 times.
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DOI: 10.1016/j.actamat.2012.03.008
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany
ABSTRACT: We studied local deformation and temperature effects associated with mechanical twinning in Fe-3 wt.% Si at room temperature. During tensile testing, two large stress drops occurred. They were accompanied by local strain and temperature bursts, which we mapped via simultaneous displacement and temperature field characterization. To identify the

microstructural origin of these phenomena, we performed high resolution electron backscatter scanning diffraction and electron channeling contrast imaging measurements. The microstructure at the positions where strong adiabatic heating occurred was characterized by the formation of primary twins and high dislocation activity within a range of about 10 μm around the twin-matrix interface. We suggest that the local temperature and strain jumps result from the formation and dissipative motion of lattice dislocations that accommodate twinning.
AUTHOR KEYWORDS: Adiabatic; Dislocation; Plasticity; Steel; Twinning
DOCUMENT TYPE: Article
SOURCE: Scopus

Jia, N., Eisenlohr, P., Roters, F., Raabe, D., Zhao, X.
Orientation dependence of shear banding in face-centered-cubic single crystals
(2012) Acta Materialia, 60 (8), pp. 3415-3434. Cited 43 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84859387013&doi=10.1016%2fj.actamat.2012.03.005&partnerID=40&md5=826bf96d42a02f52a4d298c29b6e16d7

DOI: 10.1016/j.actamat.2012.03.005
AFFILIATIONS: Key Laboratory for Anisotropy and Texture of Materials (MOE), Northeastern University, Shenyang 110004, China;
Max-Planck-Institut für Eisenforschung, D-40237 Düsseldorf, Germany
ABSTRACT: We present crystal plasticity finite element simulations of plane strain compression of α-Brass single crystals with different initial orientations. The aim is to study the fundamentals of mesoscale structure and texture development in face-centered-cubic (fcc) metals with low stacking fault energy (SFE). Shear banding depends on the initial orientation of the crystals. In Copper and Brass-R-oriented crystals which show the largest tendency to form shear bands, an inhomogeneous texture distribution induced by shear banding is observed. To also understand the influence of the micromechanical boundary conditions on shear band formation, simulations on Copper-oriented single crystals with varying sample geometry and loading conditions are performed. We find that shear banding can be understood in terms of a mesoscopic softening mechanism. The predicted local textures and the shear banding patterns agree well with experimental observations in low SFE fcc crystals.
AUTHOR KEYWORDS: Crystal plasticity finite element analysis; Fcc material; Shear band; Texture
DOCUMENT TYPE: Article
SOURCE: Scopus

Li, Y.J., Choi, P., Goto, S., Borchers, C., Raabe, D., Kirchheim, R.
Evolution of strength and microstructure during annealing of heavily cold-drawn 6.3 GPa hypereutectoid pearlitic steel wire
(2012) Acta Materialia, 60 (9), pp. 4005-4016. Cited 81 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84860372977&doi=10.1016%2fj.actamat.2012.03.006&partnerID=40&md5=f7dd71b015eca8c61de58dfcc55c8fe8

DOI: 10.1016/j.actamat.2012.03.006
AFFILIATIONS: Institut für Materialphysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany;
Max-Planck Institut für Eisenforschung, Max-Planck-Str. 1, D-40237 Düsseldorf, Germany;
Department of Materials Science and Engineering, Faculty of Engineering and Resource Science, Akita University, Tegata Gakuencho, Akita 010-0852, Japan
ABSTRACT: Hypereutectoid steel wires with 6.35 GPa tensile strength after a cold-drawing true strain of 6.02 were annealed between 300 and 723 K. The ultrahigh strength remained upon annealing for 30 min up to a temperature

of 423 K but dramatically decreased with further increasing temperature. The reduction of tensile strength mainly occurred within the first 2-3 min of annealing. Atom probe tomography and transmission electron microscopy reveal that the lamellar structure remains up to 523 K. After annealing at 673 K for 30 min, coarse hexagonal ferrite (sub)grains with spheroidized cementite, preferentially located at triple junctions, were observed in transverse cross-sections. C and Si segregated at the (sub)grain boundaries, while Mn and Cr enriched at the ferrite/cementite phase boundaries due to their low mobility in cementite. No evidence of recrystallization was found even after annealing at 723 K for 30 min. The stability of the tensile strength for low-temperature annealing (<473 K) and its dramatic drop upon high-temperature annealing (>473 K) are discussed based on the nanostructural observations.
AUTHOR KEYWORDS: Annealing; Atom probe tomography; Grain boundary segregation; Pearlitic steel; Ultrahigh strength
DOCUMENT TYPE: Article
SOURCE: Scopus

Koyama, M., Akiyama, E., Sawaguchi, T., Raabe, D., Tsuzaki, K.
Hydrogen-induced cracking at grain and twin boundaries in an Fe-Mn-C austenitic steel
(2012) Scripta Materialia, 66 (7), pp. 459-462. Cited 70 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84857118154&doi=10.1016%2fj.scriptamat.2011.12.015&partnerID=40&md5=e379ec32f683ef9b9a72162ef0413a3c

DOI: 10.1016/j.scriptamat.2011.12.015
AFFILIATIONS: Doctoral Program in Materials Science and Engineering, University of Tsukuba, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan;
National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan;
Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, Düsseldorf 40237, Germany
ABSTRACT: Hydrogen embrittlement was observed in an Fe-18Mn-1.2C (wt.%) steel. The tensile ductility was drastically reduced by hydrogen charging during tensile testing. The fracture mode was mainly intergranular fracture, though transgranular fracture was also partially observed. The transgranular fracture occurred parallel to the primary and secondary deformation twin boundaries, as confirmed by electron backscattering diffraction analysis and orientation-optimized electron channeling contrast imaging. The microstructural observations indicate that cracks are initiated at grain boundaries and twin boundaries.
AUTHOR KEYWORDS: Austenitic steel; Electron backscattering; Hydrogen embrittlement; Tension test; Twinning
DOCUMENT TYPE: Article
SOURCE: Scopus

Yuan, L., Ponge, D., Wittig, J., Choi, P., Jiménez, J.A., Raabe, D.
Nanoscale austenite reversion through partitioning, segregation and kinetic freezing: Example of a ductile 2 GPa Fe-Cr-C steel
(2012) Acta Materialia, 60 (6-7), pp. 2790-2804. Cited 58 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84859101370&doi=10.1016%2fj.actamat.2012.01.045&partnerID=40&md5=71f9b64ec5e4115b6b956c3ea88deca4

DOI: 10.1016/j.actamat.2012.01.045
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Vanderbilt University, Nashville, TN 37235-1683, United States;
CENIM, CSIC, Avda. Gregorio del Amo 8, 28040 Madrid, Spain

ABSTRACT: Austenite reversion during tempering of a Fe-13.6 Cr-0.44 C (wt.%) martensite results in an ultra-high-strength ferritic stainless steel with excellent ductility. The austenite reversion mechanism is coupled to the kinetic freezing of carbon during low-temperature partitioning at the interfaces between martensite and retained austenite and to carbon segregation at martensite-martensite grain boundaries. An advantage of austenite reversion is its scalability, i.e. changing tempering time and temperature tailors the desired strength-ductility profiles (e.g. tempering at 400 °C for 1 min produces a 2 GPa ultimate tensile strength (UTS) and 14% elongation while 30 min at 400 °C results in a UTS of ~1.75 GPa with an elongation of 23%). The austenite reversion process, carbide precipitation and carbon segregation have been characterized by X-ray diffraction, electron back-scatter diffraction, transmission electron microscopy and atom probe tomography in order to develop the structure-property relationships that control the material's strength and ductility.
AUTHOR KEYWORDS: Austenite reversion; Diffusion; Ductility; Partitioning; Strength
DOCUMENT TYPE: Article
SOURCE: Scopus

Sandlöbes, S., Friák, M., Zaefferer, S., Dick, A., Yi, S., Letzig, D., Pei, Z., Zhu, L.-F., Neugebauer, J., Raabe, D.
The relation between ductility and stacking fault energies in Mg and Mg-Y alloys
(2012) Acta Materialia, 60 (6-7), pp. 3011-3021. Cited 144 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84859103664&doi=10.1016%2fj.actamat.2012.02.006&partnerID=40&md5=6251bc1441d759c2f33c8096fe07b775

DOI: 10.1016/j.actamat.2012.02.006
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Department for Microstructure Physics and Alloy Design, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Max-Planck-Institut für Eisenforschung, Department for Computational Materials Design, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Helmholtz-Zentrum Geesthacht, Magnesium Innovation Center, Max-Planck-Str. 1, 21502 Geesthacht, Germany
ABSTRACT: The underlying mechanisms that are responsible for the improved room-temperature ductility in Mg-Y alloys compared to pure Mg are investigated by transmission electron microscopy and density functional theory. Both methods show a significant decrease in the intrinsic stacking fault I 1 energy (I 1 SFE) with the addition of Y. The influence of the SFE on the relative activation of different competing deformation mechanisms (basal, prismatic, pyramidal slip) is discussed. From this analysis we suggest a key mechanism which explains the transition from primary basal slip in hexagonal close-packed Mg to basal plus pyramidal slip in solid solution Mg-Y alloys. This mechanism is characterized by enhanced nucleation of ⟨c + a⟩ dislocations where the intrinsic stacking fault I 1 (ISF 1) acts as heterogeneous source for ⟨c + a⟩ dislocations. Possible electronic and geometric reasons for the modification of the SFE by substitutional Y atoms are identified and discussed.
AUTHOR KEYWORDS: Density functional theory (DFT); Dislocation structure; Ductility; Magnesium alloys; Transmission electron microscopy (TEM)
DOCUMENT TYPE: Article
SOURCE: Scopus

Gutierrez-Urrutia, I., Raabe, D.
Dislocation density measurement by electron channeling contrast imaging in a scanning electron microscope

(2012) Scripta Materialia, 66 (6), pp. 343-346. Cited 43 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84855892091&doi=10.1016%2fj.scriptamat.2011.11.027&partnerID=40&md5=6f8181be24cfc2d5ace07d7a5bd4a53c

DOI: 10.1016/j.scriptamat.2011.11.027
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck Str. 1, D-40237 Düsseldorf, Germany
ABSTRACT: We have measured the average dislocation density by electron channeling contrast imaging (ECCI) in a scanning electron microscope under controlled diffraction conditions in a Fe-3 wt.% Si alloy tensile deformed to a macroscopic stress of 500 MPa. Under optimal diffraction conditions, ECCI provides an average dislocation density close to that obtained by bright-field transmission electron microscopy. This result confirms that ECCI is a powerful technique for determining dislocation densities in deformed bulk metals.
AUTHOR KEYWORDS: Dislocations; Electron diffraction; Ferritic steels; Low-temperature deformation; Scanning electron microscopy (SEM)
DOCUMENT TYPE: Article
SOURCE: Scopus

Mandal, S., Gross, M., Raabe, D., Varnik, F.
Heterogeneous shear in hard sphere glasses
(2012) Physical Review Letters, 108 (9), art. no. 098301, . Cited 15 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84857623748&doi=10.1103%2fPhysRevLett.108.098301&partnerID=40&md5=47ad03de1380a5dc97d72c25707bd126

DOI: 10.1103/PhysRevLett.108.098301
AFFILIATIONS: Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Stiepeler Strasse 129, 44801 Bochum, Germany;
Max-Planck Institut für Eisenforschung, Max-Planck Strasse 1, 40237 Düsseldorf, Germany
ABSTRACT: There is growing evidence that the flow of driven amorphous solids is not homogeneous, even if the macroscopic stress is constant across the system. Via event-driven molecular dynamics simulations of a hard sphere glass, we provide the first direct evidence for a correlation between the fluctuations of the local volume fraction and the fluctuations of the local shear rate. Higher shear rates do preferentially occur at regions of lower density and vice versa. The temporal behavior of fluctuations is governed by a characteristic time scale, which, when measured in units of strain, is independent of shear rate in the investigated range. Interestingly, the correlation volume is also roughly constant for the same range of shear rates. A possible connection between these two observations is discussed.
DOCUMENT TYPE: Article
SOURCE: Scopus

Cédat, D., Fandeur, O., Rey, C., Raabe, D.
Polycrystal model of the mechanical behavior of a Mo-TiC 30 vol.% metal-ceramic composite using a three-dimensional microstructure map obtained by dual beam focused ion beam scanning electron microscopy
(2012) Acta Materialia, 60 (4), pp. 1623-1632. Cited 11 times.
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DOI: 10.1016/j.actamat.2011.11.055
AFFILIATIONS: Departement Mechanical Soils, Structures and Materials, Ecole Centrale Paris, F-92295 Châtenay-Malabry, France;
CEA, DEN, DM2S, SEMT, LM2S, F-91191 Gif-sur-Yvette, France;

Department Microstructure Physics and Metal Forming, Max Planck Institut für Eisenforschung, Düsseldorf, Germany
ABSTRACT: The mechanical behavior of a Mo-TiC 30 vol.% ceramic-metal composite was investigated over a wide temperature range (25-700 °C). High-energy X-ray tomography was used to reveal percolation of the hard titanium carbide phase through the composite. Using a polycrystal approach for a two-phase material, finite-element simulations were performed on a real three-dimensional (3-D) aggregate of the material. The 3-D microstructure, used as the starting configuration for the predictions, was obtained by serial sectioning in a dual beam focused ion beam scanning electron microscope coupled to an electron backscattered diffraction system. The 3-D aggregate consists of a molybdenum matrix and a percolating TiC skeleton. As for most body-centered cubic (bcc) metals, the molybdenum matrix phase is characterized by a change in plasticity mechanism with temperature. We used a polycrystal model for bcc materials which was extended to two phases (TiC and Mo). The model parameters of the matrix were determined from experiments on pure molydenum. For all temperatures investigated the TiC particles were considered to be brittle. Gradual damage to the TiC particles was treated, based on an accumulative failure law that is approximated by evolution of the apparent particle elastic stiffness. The model enabled us to determine the evolution of the local mechanical fields with deformation and temperature. We showed that a 3-D aggregate representing the actual microstructure of the composite is required to understand the local and global mechanical properties of the composite studied.
AUTHOR KEYWORDS: Crystal plasticity; Damage; Metal-ceramic composite; Numerical simulation; Polycrystal modeling
DOCUMENT TYPE: Article
SOURCE: Scopus

Jia, N., Roters, F., Eisenlohr, P., Kords, C., Raabe, D.
Non-crystallographic shear banding in crystal plasticity FEM simulations: Example of texture evolution in α-brass
(2012) Acta Materialia, 60 (3), pp. 1099-1115. Cited 30 times.
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DOI: 10.1016/j.actamat.2011.10.047
AFFILIATIONS: Key Laboratory for Anisotropy and Texture of Materials (MOE), Northeastern University, Shenyang 110004, China;
Max-Planck-Institut für Eisenforschung, D-40237 Düsseldorf, Germany
ABSTRACT: We present crystal plasticity finite element simulations of the texture evolution in α-brass polycrystals under plane strain compression. The novelty is a non-crystallographic shear band mechanism [Anand L, Su C. J Mech Phys Solids 2005;53:1362] that is incorporated into the constitutive model in addition to dislocation and twinning. Non-crystallographic deformation associated with shear banding leads to weaker copper and S texture components and to a stronger brass texture compared to simulations enabling slip and twinning only. The lattice rotation rates are reduced when shear banding occurs. This effect leads to a weaker copper component. Also, the initiation of shear banding promotes brass-type components. In summary the occurrence of non-crystallographic deformation through shear bands shifts face-centered-cubic deformation textures from the copper type to the brass type.
AUTHOR KEYWORDS: Finite element analysis; Shear bands; Texture
DOCUMENT TYPE: Article
SOURCE: Scopus

Tytko, D., Choi, P.-P., Klöwer, J., Kostka, A., Inden, G., Raabe, D.

Microstructural evolution of a Ni-based superalloy (617B) at 700 °c studied by electron microscopy and atom probe tomography
(2012) Acta Materialia, 60 (4), pp. 1731-1740. Cited 82 times.
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DOI: 10.1016/j.actamat.2011.11.020
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Department for Microstructure Physics and Metal Forming, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
ThyssenKrupp VDM GmbH, Kleffstrasse 23, 58762 Altena, Germany
ABSTRACT: We report on the microstructural evolution of a polycrystalline Ni-based superalloy (Alloy 617B) for power plant applications at a service temperature of 700 °C. The formation of secondary M 23C 6-carbides close to grain boundaries (GBs) and around primary Ti(C,N) particles is observed upon annealing at 700 °C, where γ′ is found to nucleate heterogeneously at M 23C 6 carbides. Using atom probe tomography, elemental partitioning to the phases and composition profiles across phase and grain boundaries are determined. Enrichments of B at γ/M 23C 6 and γ′/M 23C 6 interfaces as well as at grain boundaries are detected, while no B enrichment is found at γ/γ′ interfaces. It is suggested that segregation of B in conjunction with γ′ formation stabilizes a network of secondary M 23C 6 precipitates near GBs and thus increases the creep rupture life of Alloy 617B. Calculations of the equilibrium phase compositions by Thermo-Calc confirm the chemical compositions measured by atom probe tomography.
AUTHOR KEYWORDS: Alloy 617B; Atom probe tomography; Boron enrichment; M 23C 6; Ni-based superalloy
DOCUMENT TYPE: Article
SOURCE: Scopus

Sandim, H.R.Z., Renzetti, R.A., Padilha, A.F., Möslang, A., Lindau, R., Raabe, D.
Annealing behavior of RAFM ODS-Eurofer steel
(2012) Fusion Science and Technology, 61 (2), pp. 136-140.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84858219025&partnerID=40&md5=14b5658472cacc1255f354bfcbe3bf7f

AFFILIATIONS: Universidade de São Paulo, Escola de Engenharia de Lorena, Lorena-SP, 12600-970, Brazil;
Universidade de São Paulo, Escola Politécnica, São Paulo-SP, 05508-900, Brazil;
Karlsruher Institut für Technologie, KIT, IMF I, Karlsruhe, D-72061, Germany;
Max Planck Institut für Eisenforschung, Düsseldorf, D-40237, Germany
ABSTRACT: Oxide-dispersion-strengthened (ODS) ferriticmartensitic steels are candidates for applications infusion power plants where microstructural long-term stability at temperatures of ~650°C to 700°C are required. The microstructural stability of 80% cold-rolled reduced-activation ferritic-martensitic 9% Cr ODS-Eurofer steel was investigated within a wide range of temperatures (300°C to 1350°C). Fine oxide dispersion is very effective to prevent recrystallization in the ferritic phase field. The low recrystallized volume fraction (<0.1) found in samples annealed at 800°C is associated with the nuclei found at prior grain boundaries and around coarse M 23C 6 particles. The combination of retarding effects such as Zener drag and concurrent recovery decrease the local stored energy and impede further growth of the recrystallization nuclei. Above 900°C, martensitic transformation takes place with consequent coarsening. Significant changes in crystallographic texture are also reported.
AUTHOR KEYWORDS: ODS-Eurofer steel; Recovery; Recrystallization
DOCUMENT TYPE: Article

SOURCE: Scopus

Zheng, C., Raabe, D., Li, D.
Numerical simulation of dynamic strain-induced austenite-ferrite transformation and post-dynamic kinetics in a low carbon steel
(2012) Materials Science Forum, 706-709, pp. 1592-1597. Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84862931614&doi=10.4028%2fwww.scientific.net%2fMSF.706-709.1592&partnerID=40&md5=a35abf68e492afdf7cca5f7488fb4c0c

DOI: 10.4028/www.scientific.net/MSF.706-709.1592
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf 40237, Germany;
Division of Materials Processing Modeling, Institute of Metal Research, CAS, Wenhua Road 72, Shenyang 110016, China
ABSTRACT: 2-D cellular automaton model was developed to simulate the dynamic strain-induced transformation (DSIT) from austenite (?) to ferrite (a) and the post-dynamic kinetic behavior in a low carbon steel with the purpose of developing a methodology of mesoscopic computer simulation for an improved understanding of the formation of ultra-fine ferrite (UFF) in DSIT and the conservation of this microstructure during the post-deformation period. The predicted microstructure obtained after DSIT was compared with a quenched dual-phase steel. Its microstructure, consisting of fine-grained ferrite and fine islands of retained austenite dispersed in the matrix, were found to be in good agreement with the predictions. The simulated results indicate that the refinement of ferrite grains produced via DSIT can be interpreted in terms of unsaturated nucleation and limited growth mechanisms. It is also revealed that continuing transformation from retained austenite to ferrite and the reverse transformation both could take place simultaneously during the post-deformation isothermal holding. A competition between them exists at the early stage of the post-dynamic transformation. © 2012 Trans Tech Publications, Switzerland.
AUTHOR KEYWORDS: Cellular automaton; Dynamic strain-induced transformation; Ferrite refinement; Low carbon steel; Mesoscopic modeling; Post-dynamic behaviors
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Zambaldi, C., Yang, Y., Bieler, T.R., Raabe, D.
Orientation informed nanoindentation of α-titanium: Indentation pileup in hexagonal metals deforming by prismatic slip
(2012) Journal of Materials Research, 27 (1), pp. 356-367. Cited 51 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84862920166&doi=10.1557%2fjmr.2011.334&partnerID=40&md5=6fc9f1e7576e64884d85473513c29ff2

DOI: 10.1557/jmr.2011.334
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany;
Department of Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI 48824-1226, United States
ABSTRACT: This study reports on the anisotropic indentation response of α-titanium. Coarse-grained titanium was characterized by electron backscatter diffraction. Sphero-conical nanoindentation was performed for a number of different crystallographic orientations. The grain size was much larger than the size of the indents to ensure quasi-single-crystal indentation. The hexagonal c-axis was determined to be the hardest direction. Surface topographies of several indents were measured by atomic force microscopy. Analysis of the indent surfaces, following Zambaldi and Raabe (Acta Mater. 58(9), 3516-3530), revealed the orientation-dependent pileup behavior of α-titanium during axisymmetric indentation. Corresponding crystal plasticity finite element (CPFE) simulations predicted the pileup patterns with good accuracy. The constitutive parameters of the CPFE model were identified by

a nonlinear optimization procedure, and reproducibly converged toward easy activation of prismatic glide systems. The calculated critical resolved shear stresses were 150 ± 4, 349 ± 10, and 1107 ± 39 MPa for prismatic and basal «a»-glide and pyramidal «c + a»-glide, respectively. © 2011 Materials Research Society.
AUTHOR KEYWORDS: Dislocations; Nanoindentation; Ti
DOCUMENT TYPE: Article
SOURCE: Scopus

Gutierrez-Urrutia, I., Raabe, D.
Study of deformation twinning and planar slip in a TWIP steel by electron channeling contrast imaging in a SEM
(2012) Materials Science Forum, 702-703, pp. 523-529. Cited 11 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84855366181&doi=10.4028%2fwww.scientific.net%2fMSF.702-703.523&partnerID=40&md5=d3686883a0122081267bec0817de0963

DOI: 10.4028/www.scientific.net/MSF.702-703.523
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany
ABSTRACT: We study the dislocation and twin substructures in a high manganese twinning-induced-plasticity steel (TWIP) by means of electron channeling contrast imaging. At low strain (true strain below 0.1) the dislocation substructure shows strong orientation dependence. It consists of dislocation cells and planar dislocation arrangements. This dislocation substructure is replaced by a complex dislocation/twin substructure at high strain (true strain of 0.3-0.4). The twin substructure also shows strong orientation dependence. We identify three types of dislocation/twin substructures. Two of these substructures, those which are highly favorable or unfavorable oriented for twinning, exhibit a Schmid behavior. The other twin substructure does not fulfill Schmid's law. © (2012) Trans Tech Publications, Switzerland.
AUTHOR KEYWORDS: Dislocation substructure; EBSD; Electron channeling contrast imaging; Twin substructure; TWIP steel
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Konijnenberg, P.J., Zaefferer, S., Lee, S.-B., Rollett, A.D., Rohrer, G.S., Raabe, D.
Advanced methods and tools for reconstruction and analysis of grain boundaries from 3D-EBSD data sets
(2012) Materials Science Forum, 702-703, pp. 475-478. Cited 5 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84855397444&doi=10.4028%2fwww.scientific.net%2fMSF.702-703.475&partnerID=40&md5=d9d56305576ee3f2132100f407359361

DOI: 10.4028/www.scientific.net/MSF.702-703.475
AFFILIATIONS: Max-Planck-Inst. for Iron Research, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Carnegie Mellon University, 5000 Forbes Avenue, Pittsburgh, PA 15213, United States
ABSTRACT: We report the recent development of a 3D orientation data post-processing software, which we refer to as QUBE. Amongst other functionalities, it offers the possibility to specify the spatial and orientational distribution of boundary normals. We describe a method to reconstruct a voxel-accurate and smooth 3D boundary triangle mesh by algorithmic means. A proof of concept is given by a benchmark on a generic dataset and we demonstrate a first result with the description of selected grain boundaries in an Fe-28%Ni sample. © (2012) Trans Tech Publications, Switzerland.
AUTHOR KEYWORDS: 3D-EBSD; Boundary surface reconstruction; Marching tetrahedra; Vertex model; Voxel cloud
DOCUMENT TYPE: Conference Paper

SOURCE: Scopus

Gutierrez-Urrutia, I., Raabe, D.
New insights on quantitative microstructure characterization by electron channeling contrast imaging under controlled diffraction conditions in SEM
(2012) Microscopy and Microanalysis, 18, pp. 686-687. Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-85007995751&doi=10.1017%2fS1431927612005284&partnerID=40&md5=a60abbbe5416b81a6416cbfb5b8e2c1b

DOI: 10.1017/S1431927612005284
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
DOCUMENT TYPE: Article
SOURCE: Scopus

Calcagnotto, M., Ponge, D., Raabe, D.
On the effect of manganese on grain size stability and hardenability in ultrafine-grained ferrite/martensite dual-phase steels
(2012) Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 43 (1), pp. 37-46. Cited 53 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84855777371&doi=10.1007%2fs11661-011-0828-3&partnerID=40&md5=6e2acd1b65f8572a2f4a36885cf6d826

DOI: 10.1007/s11661-011-0828-3
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf 40237, Germany;
Salzgitter Mannesmann Forschung GmbH, Salzgitter 38239, Germany
ABSTRACT: Two plain carbon steels with varying manganese content (0.87 wt pct and 1.63 wt pct) were refined to approximately 1 μm by large strain warm deformation and subsequently subjected to intercritical annealing to produce an ultrafine grained ferrite/martensite dual-phase steel. The influence of the Mn content on microstructure evolution is studied by scanning electron microscopy (SEM). The Mn distribution in ferrite and martensite is analyzed by high-resolution electron backscatter diffraction (EBSD) combined with energy dispersive X-ray spectroscopy (EDX). The experimental findings are supported by the calculated phase diagrams, equilibrium phase compositions, and the estimated diffusion distances using Thermo-Calc (Thermo-Calc Software, McMurray, PA) and Dictra (Thermo-Calc Software). Mn substantially enhances the grain size stability during intercritical annealing and the ability of austenite to undergo martensitic phase transformation. The first observation is explained in terms of the alteration of the phase transformation temperatures and the grain boundary mobility, while the second is a result of the Mn enrichment in cementite during large strain warm deformation, which is inherited by the newly formed austenite and increases its hardenability. The latter is the main reason why the ultrafine-grained material exhibits a hardenability that is comparable with the hardenability of the coarse-grained reference material.

DOCUMENT TYPE: Article
SOURCE: Scopus

Maniruzzaman, M., Rahman, M.A., Gafur, M.A., Fabritius, H., Raabe, D.
Modification of pineapple leaf fibers and graft copolymerization of acrylonitrile onto modified fibers
(2012) Journal of Composite Materials, 46 (1), pp. 79-90. Cited 4 times.
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DOI: 10.1177/0021998311410486
AFFILIATIONS: Department of Applied Chemistry and Chemical Technology, Islamic University, Kushtia 7003, Bangladesh;

PPandPD, Bangladesh Council of Scientific and Industrial Research (BCSIR), Dhaka, Bangladesh;
Department of Microstructure Physics and Metal Forming, Max-Planck-Institut für Eisenforschung, Dusseldorf, Germany
ABSTRACT: Raw pineapple leaf fibers (PALFs) were chemically modified by scouring, NaOH treatment, and bleaching (NaClO2). The graft copolymerization of synthetic acrylonitrile monomer onto bleached PALFs was carried out in aqueous medium using potassium persulfate (K2S2O8/FeSO4) as a redox initiator. The maximum grafting level at optimum conditions, namely, monomer concentration, initiator concentration, catalyst concentration, reaction time, and temperature have been determined. The main objective of this study is to decrease the amorphous region of lignocellulose in PALFs and improve its hydrophobic nature by incorporation of synthetic polymer of polyacrylonitrile and mechanical properties. The modified and grafted fibers were characterized by Fourier transform infrared spectroscopy, scanning electron microscope, thermogravimetric analysis, and X-ray diffraction study techniques. The moisture content and tensile strength properties were also evaluated for their environmental and mechanical performances.
AUTHOR KEYWORDS: acrylonitrile monomer; chemical modification; graft copolymerization; Pineapple leaf fibers; tensile strength
DOCUMENT TYPE: Article
SOURCE: Scopus

Roters, F., Eisenlohr, P., Kords, C., Tjahjanto, D.D., Diehl, M., Raabe, D.
DAMASK: The d¨usseldorf advanced material simulation kit for studying crystal plasticity using an fe based or a spectral numerical solver
(2012) Procedia IUTAM, 3, pp. 3-10. Cited 45 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84867356417&doi=10.1016%2fj.piutam.2012.03.001&partnerID=40&md5=a71c71f3c424d0462e7fd851be5e8b58

DOI: 10.1016/j.piutam.2012.03.001
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, Düsseldorf, Germany;
IMDEA Materials Institute, C/ Profesor Aranguren s/n, 28040 Madrid, Spain
ABSTRACT: The solution of a continuum mechanical boundary value problem requires a constitutive response that connects deformation and stress at each material point. Such connection can be regarded as three separate hierarchical problems. At the top-most level, partitioning of the (mean) boundary values of the material point among its microstructural constituents and the associated homogenization of their response is required, provided there is more than one constituent present. Second, based on an elastoplastic decomposition of (finite strain) deformation, these responses follow from explicit or implicit time integration of the plastic deformation rate per constituent. Third, to establish the latter, a state variable-based constitutive law needs to be interrogated and its state updated. The D¨usseldorf Advanced MAterial Simulation Kit (DAMASK) reflects this hierarchy as it is built in a strictly modular way. This modular structure makes it easy to add additional constitutive models as well as homogenization schemes. Moreover it interfaces with a number of FE solvers as well as a spectral solver using an FFT. We demonstrate the versatility of such a modular framework by considering three scenarios: Selective refinement of the constitutive material description within a single geometry, component-scale forming simulations comparing different homogenization schemes, and comparison of representative volume element simulations based on the FEM and the spectral solver.
AUTHOR KEYWORDS: Constitutive model; CPFEM; FFT; Spectral method
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Sandim, M.J.R., Stamopoulos, D., Aristomenopoulou, E., Zaefferer, S., Raabe, D., Awaji, S., Watanabe, K.
Grain structure and irreversibility line of a bronze route CuNb reinforced NbNb3Sn multifilamentary wire
(2012) Physics Procedia, 36, pp. 1504-1509. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84960373900&doi=10.1016%2fj.phpro.2012.06.122&partnerID=40&md5=05a02970428c930260dc797010076bf2

DOI: 10.1016/j.phpro.2012.06.122
AFFILIATIONS: Escola de Engenharia de Lorena - USP, Lorena, Brazil;
Institute of Materials Science, NCSR Demokritos, Athens, Greece;
Max-Planck-Institut Für Eisenforshung, Düsseldorf, Germany;
Institute of Materials Research, Tohoku University, Sendai, Japan
ABSTRACT: High-resolution electron backscatter diffraction (EBSD) technique and DC magnetization were used to characterize a Cu-Nb reinforced bronze route Nb3Sn superconducting multifilamentary wire. The results of DC-magnetization show an extended regime of magnetic reversibility in the operational magnetic field-temperature phase diagram. This observation is discussed in terms of microstructure characteristics of the A15 phase such as grain size, grain boundary misorientation angle distribution, tin gradient across the filaments and residual strain, in connection to the literature. © 2012 Published by Elsevier B.V. Selection and/or peer-review under responsibility of the Guest Editors.
AUTHOR KEYWORDS: DC magnetization; Electron backscatter diffraction; Grain structure; Irreversibility line; Nb3sn
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Mehrtens, T., Schowalter, M., Tytko, D., Choi, P.-P., Raabe, D., Hoffmann, L., Hangleiter, A., Rosenauer, A.
Temperature dependence of Z-Contrast for InGaN
(2012) Microscopy and Microanalysis, 18, pp. 1818-1819.
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DOI: 10.1017/S143192761201094X
AFFILIATIONS: Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany;
Max-Planck-Institut fur Eisenforschung GmbH, Max-Plack-Str. 1, 40237 Düsseldorf, Germany;
Institute of Applied Physics, TU Braunschweig, Mendelssohnstr. 2, 38106 Braunschweig, Germany
DOCUMENT TYPE: Article
SOURCE: Scopus

Choi, P.-P., Cojocaru-Mirédin, O., Wuerz, R., Raabe, D.
Comparative atom probe study of Cu(In,Ga)Se 2 thin-film solar cells deposited on soda-lime glass and mild steel substrates
(2011) Journal of Applied Physics, 110 (12), art. no. 124513, . Cited 26 times.
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DOI: 10.1063/1.3665723
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Zentrum für Sonnenenergie-und Wasserstoff-Forschung Baden-Württemberg, Industriestrasse 6, 70565 Stuttgart, Germany
ABSTRACT: We report on a comparative study of Cu(In,Ga)Se 2 solar cells deposited on soda-lime glass and mild steel substrates, using atom probe

tomography in conjunction with secondary ion mass spectrometry, x-ray fluorescence, current density-voltage, and external quantum efficiency measurements. Cu(In,Ga)Se 2 films deposited on soda-lime glass substrates and on steel substrates with a NaF precursor layer on top of the Mo back contact contain a significant amount of Na impurities and yield an enhanced open circuit voltage and fill factor. Using atom probe tomography, Na atoms are found to be segregated at grain boundaries and clustered in both bulk and grain boundaries. The atom probe data indicate that Na Cu point defects are most likely formed at grain boundaries, reducing the number of compensating In Cu point defects and thus contributing to an enhanced cell efficiency. However, for steel substrates the positive effect of Na on the cell performance is counterbalanced by the incorporation of Fe impurities into the Cu(In,Ga)Se 2 film. Fe atoms are homogeneously distributed inside the grains suggesting that Fe introduces point defects in the bulk © 2011 American Institute of Physics.
DOCUMENT TYPE: Article
SOURCE: Scopus

Mehrtens, T., Bley, S., Schowalter, M., Sebald, K., Seyfried, M., Gutowski, J., Gerstl, S.S.A., Choi, P.-P., Raabe, D., Rosenauer, A.
A (S)TEM and atom probe tomography study of InGaN
(2011) Journal of Physics: Conference Series, 326 (1), art. no. 012029, .
Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-82955171594&doi=10.1088%2f1742-6596%2f326%2f1%2f012029&partnerID=40&md5=61c4387366daa444f2fd7b20ec5c9774

DOI: 10.1088/1742-6596/326/1/012029
AFFILIATIONS: Institute of Solid State Physics, University of Bremen, Bremen 28359, Germany;
Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany
ABSTRACT: In this work we show how the indium concentration in high indium content InxGa1-xN quantum wells, as they are commonly used in blue and green light emitting diodes, can be deduced from high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) images. This method bases on introducing normalized intensities which can be compared with multislice simulations to determine the specimen thickness or the indium concentration. The evaluated concentrations are compared with atom probe tomography measurements. It is also demonstrated how the quality of focused ion beam prepared TEM-lamellas can be improved by an additional etching with low energy ions.
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Choi, P., Li, Y.J., Kirchheim, R., Raabe, D.
Deformation-induced cementite decomposition in pearlitic steel wires studied by atom probe tomography
(2011) ICCM International Conferences on Composite Materials, 4 p.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-84875959752&partnerID=40&md5=7452d69e0e47750f84cdb7fe2a9b1516

AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck-Str.1, 40237 Düsseldorf, Germany;
Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany
AUTHOR KEYWORDS: Atom probe tomography; Cementite decomposition; Cold-drawing; Pearlitic steel
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Brands, D., Balzani, D., Schröder, J., Raabe, D.
Simulation of DP-steels based on statistically similar representative volume elements and 3D EBSD data

(2011) Computational Plasticity XI - Fundamentals and Applications, COMPLAS XI, pp. 1552-1563. Cited 2 times.
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AFFILIATIONS: Department of Civil Engineering, Institute of Mechanics, University of Duisburg-Essen, Universitätsstraße 15, 45141 Essen, Germany; Max-Planck-Institut für Eisenforschung GmbH, Dept. Microstructure Physics and Metal Forming, Max-Planck-Straße 1, 40237 Düsseldorf, Germany
ABSTRACT: Micrographs of a dual-phase steel obtained from a EBSD-FIB imaging are analyzed with respect to a set of statistical measures. Then the applicability of this data to the construction of statistically similar representative volume elements (SSRVEs) is discussed. These SSRVEs are obtained by minimizing a least-square functional taking into account differences of statistical measures computed for a given reference microstructure and the SSRVE, cf. [11]. For an analysis of the mechanical response the FE2-method is used and a series of virtual experiments shows the accordance of the response of the SSRVE to the one of the reference microstructure. In order to demonstrate the performance of the proposed procedure some representative numerical examples are given.
AUTHOR KEYWORDS: EBSD; Finite plasticity; Homogenization; Material properties; Microstructures; Multiscale problems; Statistically similar RVE
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Cojocaru-Mirédin, O., Choi, P.-P., Abou-Ras, D., Schmidt, S.S., Caballero, R., Raabe, D.
Characterization of grain boundaries in Cu(In,Ga)Se 2 films using atom-probe tomography
(2011) IEEE Journal of Photovoltaics, 1 (2), art. no. 6064862, pp. 207-212. Cited 37 times.
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DOI: 10.1109/JPHOTOV.2011.2170447
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany;
Helmholtz-Zentrum Berlin für Materialien und Energie, Institute of Technology, D-14109 Berlin, Germany
ABSTRACT: This paper discusses the advantages of pulsed laser atom-probe tomography (APT) to analyze Cu(In,Ga)Se 2-based solar cells. Electron backscatter diffraction (EBSD) was exploited for site-specific preparation of APT samples at selected Cu(In,Ga)Se 2 grain boundaries. This approach is very helpful not only to determine the location of grain boundaries but also to classify them as well. We demonstrate that correlative transmission electron microscopy (TEM) analyses on atom-probe specimens enable the atom-probe datasets to be reconstructed with high accuracy. Moreover, EBSD and TEM can be very useful to obtain complementary information about the crystal structure in addition to the compositional analyses. The local chemical compositions at grain boundaries of a solar grade Cu(In,Ga)Se 2 film are presented here. Na, K, and O impurities are found to be segregated at grain boundaries. These impurities most likely diffuse from the soda lime glass substrate into the absorber layer during cell fabrication and processing. Based on the experimental results, we propose that Na, K, and O play an important role in the electrical properties of grain boundaries in Cu(In,Ga)Se 2 thin films for solar cells. © 2011 IEEE.
AUTHOR KEYWORDS: Atom-probe tomography (APT); copper indium gallium diselenide (CIGS); Cu(In,Ga)Se 2; grain boundary segregation; sodium and oxygen diffusion; thin-film solar cells
DOCUMENT TYPE: Article
SOURCE: Scopus

Liu, B., Raabe, D., Eisenlohr, P., Roters, F., Arsenlis, A., Hommes, G.
Dislocation interactions and low-angle grain boundary strengthening
(2011) Acta Materialia, 59 (19), pp. 7125-7134. Cited 39 times.
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DOI: 10.1016/j.actamat.2011.07.067
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany;
Lawrence Livermore National Laboratory, University of California, Livermore, CA 94550, United States
ABSTRACT: The transmission of an incoming dislocation through a symmetrical low-angle tilt grain boundary (GB) is studied for {1 1 0}⟨1 1 1⟩ slip systems in body-centered cubic metals using discrete dislocation dynamics (DD) simulations. The transmission resistance is quantified in terms of the different types of interactions between the incoming and GB dislocations. Five different dislocation interaction types are considered: collinear, mixed-symmetrical junction, mixed-asymmetrical junction, edge junction, and coplanar. Mixed-symmetrical junction formation events are found not only to cause a strong resistance against the incident dislocation penetration, but also to transform the symmetrical low-angle tilt GB into a hexagonal network (a general low-angle GB). The interactions between the incident dislocation and the GB dislocations can form an array of ⟨1 0 0⟩ dislocations (binary junctions) in non-coplanar interactions, or a single ⟨1 0 0⟩ dislocation in coplanar interaction. We study how the transmission resistance depends on the mobility of ⟨1 0 0⟩ dislocations. ⟨1 0 0⟩ dislocations have usually been treated as immobile in DD simulations. In this work, we discuss and implement the mobility law for ⟨1 0 0⟩ dislocations. As an example, we report how the mobility of ⟨1 0 0⟩ dislocations affects the equilibrium configuration of a ternary dislocation interaction.
AUTHOR KEYWORDS: Dislocation dynamics; Dislocation interactions; Dislocation reactions; Low-angle grain boundary; Strength
DOCUMENT TYPE: Article
SOURCE: Scopus

Raabe, D.
Automotive lightweight construction (1): Steel research secures competitiveness of the industry. Application-oriented basic research paves the way for automotive lightweight construction [Automobiler Leichtbau (1): Stahlforschung sichert Wettbewerbsfähigkeit der Industrie: Anwendungsorientierte Grundlagenforschung bereitet automobilem Leichtbau den Weg]
(2011) Stahl und Eisen, 131 (10), pp. 88-90.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-80755155941&partnerID=40&md5=e967bbbae4a799a04dfeb52e82825c04

DOCUMENT TYPE: Article
SOURCE: Scopus

Yeap, K.B., Hangen, U.D., Raabe, D., Zschech, E.
Nanoindentation study of elastic anisotropy of Cu single crystals and grains in TSVs
(2011) AIP Conference Proceedings, 1378, pp. 121-128. Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-80053626170&doi=10.1063%2f1.3615699&partnerID=40&md5=d49ad14f7f5c581e8654d517462f9980

DOI: 10.1063/1.3615699

AFFILIATIONS: Fraunhofer Institute for Non-Destructive Testing, 01109 Dresden, Germany;
Hysitron Incoporation, Technologiezentrum Am Europaplatz, 52068 Aachen, Germany;
Max-Planck-Institute for Iron Research, 40237 Düsseldorf, Germany
ABSTRACT: This paper presents the results of nanoindentation experiments on Cu single crystals and Cu grains in through silicon via (TSV) structures used for 3D integrated circuit (IC) stacking, at sub-10nm and several-10nm penetration depths. The reduced moduli for Cu single crystals change from an average value to the uni-directional values, as the penetration depths decrease from several-10nm to sub-10nm. At sub-10nm deformation, about one third of the indentations on Cu(111) and Cu(110) show fully elastic behavior, while all indentations on Cu(100) shows elastic-plastic behavior. The reduced modulus values extracted from indents on Cu(111) and Cu(110) with fully elastic behavior are about 195GPa and 145GPa, respectively. For penetration depths of several-10nm up to 50nm, the reduced modulus for Cu(100) varies between 50GPa to 100GPa. The averaged reduced moduli determined at relatively large penetration depths are explained with lattice rotation beneath the indentations. Since the activation of multiple slip systems is required for lattice rotation, the transition of the unidirectional reduced modulus to the averaged value with increasing penetration depths occurs differently for Cu(111) and Cu(100). Similar to the results from Cu single crystals, unidirectional reduced moduli are obtained for the Cu grains in TSV structures at sub-10nm penetration depths.
AUTHOR KEYWORDS: Copper microstructure; Elastic modulus; Nanoindentation
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Alankar, A., Eisenlohr, P., Raabe, D.
A dislocation density-based crystal plasticity constitutive model for prismatic slip in α-titanium
(2011) Acta Materialia, 59 (18), pp. 7003-7009. Cited 28 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-80052951039&doi=10.1016%2fj.actamat.2011.07.053&partnerID=40&md5=7eb09cc0a1398e923ccc9f03b2a8e64a

DOI: 10.1016/j.actamat.2011.07.053
AFFILIATIONS: Materials Science Division, Los Alamos National Laboratory, MS-G755, Los Alamos, NM 87545, United States;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany
ABSTRACT: A new constitutive plasticity model for prismatic slip in hexagonal α-titanium is developed. In the concept pure edge and screw dislocation densities evolve on the $\{10\bar{1}0\}\langle 1\bar{2}10\rangle$ slip systems. The model considers that the screw dislocation segments have a spread out core, leading to a much higher velocity of edge compared with screw dislocations. This enables the model to describe the observed transition in strain hardening from stage I to stage II in single crystals oriented for prismatic slip. Good agreement is found between the experimentally observed and simulated stress-strain behavior.
AUTHOR KEYWORDS: Crystal plasticity; Dislocations; Single crystal; Titanium
DOCUMENT TYPE: Article
SOURCE: Scopus

Kundin, J., Raabe, D., Emmerich, H.
A phase-field model for incoherent martensitic transformations including plastic accommodation processes in the austenite
(2011) Journal of the Mechanics and Physics of Solids, 59 (10), pp. 2082-2102. Cited 42 times.

https://www.scopus.com/inward/record.uri?eid=2-s2.0-80052312438&doi=10.1016%2fj.jmps.2011.07.001&partnerID=40&md5=7d5dde92cebb1b905617e71a8a4401a3

DOI: 10.1016/j.jmps.2011.07.001
AFFILIATIONS: Material and Process Simulation (MPS), University Bayreuth, 95448 Bayreuth, Germany;
Microstructure Physics and Metal Forming, Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany
ABSTRACT: If alloys undergo an incoherent martensitic transformation, then plastic accommodation and relaxation accompany the transformation. To capture these mechanisms we develop an improved 3D microelasticplastic phase-field model. It is based on the classical concepts of phase-field modeling of microelastic problems (Chen, L.Q.; Wang Y.; Khachaturyan, A.G.; 1992. Philos. Mag. Lett. 65, 1523). In addition to these it takes into account the incoherent formation of accommodation dislocations in the austenitic matrix, as well as their inheritance into the martensitic plates based on the crystallography of the martensitic transformation. We apply this new phase-field approach to the butterfly-type martensitic transformation in a Fe30 wt%Ni alloy in direct comparison to recent experimental data (Sato, H.; Zaefferer, S.; 2009. Acta Mater. 57, 19311937). It is shown that the therein proposed mechanisms of plastic accommodation during the transformation can indeed explain the experimentally observed morphology of the martensitic plates as well as the orientation between martensitic plates and the austenitic matrix. The developed phase-field model constitutes a general simulations approach for different kinds of phase transformation phenomena that inherently include dislocation based accommodation processes. The approach does not only predict the final equilibrium topology, misfit, size, crystallography, and aspect ratio of martensiteaustenite ensembles resulting from a transformation, but it also resolves the associated dislocation dynamics and the distribution, and the size of the crystals itself. © 2011 Elsevier Ltd.
AUTHOR KEYWORDS: Martensitic transformation; Phase field modeling; Plastic accommodation
DOCUMENT TYPE: Article
SOURCE: Scopus

Voß, S., Palm, M., Stein, F., Raabe, D.
Compositional dependence of the compressive yield strength of Fe-Nb(-Al) and Co-Nb Laves phases
(2011) Materials Research Society Symposium Proceedings, 1295, pp. 311-316. Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-80053192287&doi=10.1557%2fopl.2011.459&partnerID=40&md5=47b21eb5836b319875fb5c7907161243

DOI: 10.1557/opl.2011.459
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, D-40237 Düsseldorf, Germany
ABSTRACT: Large, defect-free single-phase samples of the hexagonal C14 NbFe2 and Nb(Fe,Al)2, and the cubic C15 NbCo2 Laves phases have been produced by a modified levitation melting technique. The compressive strength of NbFe2 and NbCo2 has been determined in dependence on the Nb content, that of Nb(Fe,Al)2 in dependence on the Al content. The binary phases did not show either a maximum (defect softening) or minimum (defect hardening) in strength when the Nb content was varied. Instead, for both phases an increase of the compressive strength with increasing Nb content is observed. © 2011 Materials Research Society.
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Gutierrez-Urrutia, I., Raabe, D.

Dislocation and twin substructure evolution during strain hardening of an Fe-22 wt.% Mn-0.6 wt.% C TWIP steel observed by electron channeling contrast imaging
(2011) Acta Materialia, 59 (16), pp. 6449-6462. Cited 235 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-80051802106&doi=10.1016%2fj.actamat.2011.07.009&partnerID=40&md5=a7859d067448c95a0bdca3d6d5874b40

DOI: 10.1016/j.actamat.2011.07.009
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck Str. 1, D-40237 Düsseldorf, Germany
ABSTRACT: We study the kinetics of the substructure evolution and its correspondence to the strain hardening evolution of an Fe-22 wt.% Mn-0.6 wt.% C TWIP steel during tensile deformation by means of electron channeling contrast imaging (ECCI) combined with electron backscatter diffraction (EBSD). The contribution of twin and dislocation substructures to strain hardening is evaluated in terms of a dislocation mean free path approach involving several microstructure parameters, such as the characteristic average twin spacing and the dislocation substructure size. The analysis reveals that at the early stages of deformation (strain below 0.1 true strain) the dislocation substructure provides a high strain hardening rate with hardening coefficients of about G/40 (G is the shear modulus). At intermediate strains (below 0.3 true strain), the dislocation mean free path refinement due to deformation twinning results in a high strain rate with a hardening coefficient of about G/30. Finally, at high strains (above 0.4 true strain), the limited further refinement of the dislocation and twin substructures reduces the capability for trapping more dislocations inside the microstructure and, hence, the strain hardening decreases. Grains forming dislocation cells develop a self-organized and dynamically refined dislocation cell structure which follows the similitude principle but with a smaller similitude constant than that found in medium to high stacking fault energy alloys. We attribute this difference to the influence of the stacking fault energy on the mechanism of cell formation.

AUTHOR KEYWORDS: Austenitic steel; Deformation twinning; Dislocation structures; Electron channeling contrast imaging; Strain hardening
DOCUMENT TYPE: Article
SOURCE: Scopus

Helm, D., Butz, A., Raabe, D., Gumbsch, P.
Microstructure-based description of the deformation of metals: Theory and application
(2011) Proceedings of the 1st World Congress on Integrated Computational Materials Engineering, ICME, pp. 89-98. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-80051700780&partnerID=40&md5=8e90d631b9646af2075d9a73bf256c60

AFFILIATIONS: Fraunhofer Institute for Mechanics of Materials IWM, 79108 Freiburg, Germany;
Max-Planck-Institute for Iron Research, 40237 Düsseldorf, Germany;
Institute for Applied Materials IAM, Karlsruhe Institute of Technology K1T, 76131 Karlsruhe, Germany
ABSTRACT: Aiming for an integrated approach to computational materials engineering in an industrial context poses big challenges on the development of suitable materials descriptions for the different steps along the processing chain. The first key component is to correctly describe the microstructural changes during the thermal and mechanical processing of the base material into a semi-finished product. Explicit representations of the microstructure are most suitable there. The final processing steps and particularly component assessment then has to describe the entire component which requires homogenized continuum mechanical representations. One of the main challenges is the step in between, the determination of the (macroscopic) materials descriptions from microscopic

structures, which can be seen as a virtual testing laboratory. In the first part this manuscript gives a short overview of the different methods to include microstructure into descriptions of the deformation of metals. In the second part it demonstrates the central steps of the simulation along the processing chain of an automotive component manufactured from a dual phase steel. The simulation of the cold rolling of the steel sheet provides the morphology, texture and deformation history of the individual grains in a representative microstructure, which is then evolved in a virtual thermal treatment into the dual phase ferritic-martensitic structure from which the anisotropic yield surface of the sheet can be calculated. The simulations are compared to dedicated experiments performed at each step. The results demonstrate the enormous potential of such a systematic computational approach.
AUTHOR KEYWORDS: Crystal plasticity; Homogenization; Process chain; Sheet metal forming
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Zhang, H., Bai, B., Raabe, D.
Superplastic martensitic Mn-Si-Cr-C steel with 900% elongation
(2011) Acta Materialia, 59 (14), pp. 5787-5802. Cited 13 times.
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DOI: 10.1016/j.actamat.2011.05.055
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck Str 1, 40237 Düsseldorf, Germany;
Key Laboratory for Advanced Materials, Department of Materials Science and Engineering, Tsinghua University, 100084 Beijing, China
ABSTRACT: High-strength (1.2-1.5)C-(2-2.5)Mn-(1.5-2)Si-(0.8-1.5)Cr steels (mass%) consisting of martensite and carbides exhibit excellent superplastic properties (e.g. strain rate sensitivity m ≈ 0.5, elongation ≈900% at 1023 K). A homogeneous martensitic starting microstructure is obtained through thermomechanical processing (austenitization plus 1.2 true strain, followed by quenching). Superplastic forming leads to a duplex structure consisting of ferrite and spherical micro-carbides. Through 1.5-2% Si alloying, carbides precipitate at hetero-phase interfaces and martensite blocks at the beginning of superplastic forming. Via Ostwald ripening, these interface carbides grow at the expense of carbides precipitating at martensite laths, thereby promoting ferrite dynamic recrystallization. Simultaneously, carbides at ferrite grain boundaries retard the growth of recrystallized ferrite grains. Due to 2-2.5% Mn and 0.8-1.5% Cr alloying, carbide coarsening is suppressed owing to the slow diffusion of these elements. As a result, fine and homogeneous ferrite plus spherical carbide duplex microstructures with a ferrite grain size of ~1.5 μm are obtained after superplastic forming.
AUTHOR KEYWORDS: Carbide; Martensite; Steel; Superplasticity; Thermomechanical processing
DOCUMENT TYPE: Article
SOURCE: Scopus

Sun, D.-K., Zhu, M.-F., Dai, T., Cao, W.-S., Chen, S.-L., Raabe, D., Hong, C.-P.
Modelling of dendritic growth in ternary alloy solidification with melt convection
(2011) International Journal of Cast Metals Research, 24 (3-4), pp. 177-183. Cited 6 times.
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DOI: 10.1179/136404611X13001912813988
AFFILIATIONS: Jiangsu Key Laboratory for Advanced Metallic Materials, School of Materials Science and Engineering, Southeast University, Nanjing 211189, China;
CompuTherm LLC, 437 S. Yellowstone Dr, Suite 217, Madison, WI 53719, United States;
Max-Planck-Institut fur Eisenforschung, Düsseldorf 40237, Germany;
Center for Computer-Aided Materials Processing (CAMP), Department of Metallurgical Engineering, Yonsei University, Seoul 120749, South Korea
ABSTRACT: A two-dimensional lattice Boltzmann-cellular automaton model is coupled with the CALPHAD (Calculation of Phase Diagrams) method for simulating dendritic growth during ternary alloy solidification with convection. In the model, the kinetics of dendritic growth is determined by the difference between the equilibrium liquidus temperature and the actual temperature at the solid/liquid interface, incorporating the effects of the interface curvature and the preferred dendritic growth orientation. The lattice Boltzmann method is used for evaluating the local liquid compositions of the two solutes impacted by diffusion and convection. Based on the local liquid compositions, the equilibrium liquidus temperature and the solid concentrations of the two solutes are obtained by the CALPHAD method. The model is applied to simulate dendritic growth of an Al-4?0 wt-%Cu-1?0 wt-%Mg ternary alloy with melt convection. The results demonstrate the high numerical convergence and stability, as well as computational efficiency, of the proposed model. Melt convection is found to influence the dendritic morphologies and microsegregation patterns in the solidification of ternary alloys. © 2011 W. S. Maney & Son Ltd.
AUTHOR KEYWORDS: Cellular automaton; Convection; Dendritic growth; Lattice boltzmann method; Modelling; Ternary alloy
DOCUMENT TYPE: Article
SOURCE: Scopus

Sandlöbes, S., Schestakow, I., Yi, S., Zaefferer, S., Chen, J., Friák, M., Neugebauer, J., Raabe, D.
The relation between shear banding, microstructure and mechanical properties in Mg and Mg-Y alloys
(2011) Materials Science Forum, 690, pp. 202-205. Cited 5 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-79960396968&doi=10.4028%2fwww.scientific.net%2fMSF.690.202&partnerID=40&md5=2ee44aa3a6e13748db71ebdf395a2e7b

DOI: 10.4028/www.scientific.net/MSF.690.202
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Helmholtz Centre Geesthacht, Magnesium Innovation Center (MagIC), Max-Planck-Str. Geb. 47, 21502 Geesthacht, Germany
ABSTRACT: The formation of deformation-induced shear bands plays an important role for the room temperature deformation of both, Mg and Mg-Y alloys, but the formation and structure of shear bands is distinctively different in the two materials. Due to limited deformation modes in pure Mg, the strain is localized in few shear bands leading to an early failure of the material during cold deformation. Contrarily, Mg-RE (RE: rare earth) alloys exhibit a high density of homogeneously distributed local shear bands during deformation at room temperature. A study of the microstructure of the shear bands by electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM) at different strains was performed. These investigations give insight into the formation of shear bands and their effects on the mechanical behaviour of pure Mg and Mg-3Y. Since in pure Mg mainly extension twinning and basal <a> dislocation slip are active, high stress fields at grain resp. twin boundaries in shear bands effect fast growth of the shear bands. In Mg-RE alloys additionally contraction and secondary twinning and pyramidal <c+a> dislocation slip are active leading to the formation of microscopic shear bands which are

limited to the boundary between two grains. The effects of shear bands on the mechanical behaviour of pure Mg and Mg-RE alloys are discussed with respect to their formation and growth. © (2011) Trans Tech Publications.
AUTHOR KEYWORDS: Deformation; EBSD; Mg-RE alloys; Shear banding; TEM
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Renzetti, R.A., Sandim, H.R.Z., Padilha, A.F., Raabe, D., Lindau, R., Möslang, A.
Annealing effects on the microstructure of ferritic-martensitic ODS-Eurofer steel
(2011) Fusion Science and Technology, 60 (1 T), pp. 22-26. Cited 1 time.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-80051962568&partnerID=40&md5=59fa63291e48ae5f9cf8c3b69b037ec4

AFFILIATIONS: Escola de Engenharia de Lorena, University of São Paulo, 12600-970, Lorena, Brazil;
Escola Politécnica, University of Sao Paulo, 05508-900, São Paulo, Brazil;
Max-Planck-Institut für Eisenforschung, D-40237 Düsseldorf, Germany;
Karlsruher Institut für Technologie (KIT), IMF I, P.O. Box, 3640 72061 Karlsruhe, Germany
ABSTRACT: Oxide dispersion strengthened (ODS) ferritic/martensitic (FM) steels are promising candidates for structural applications in future fusion power reactors. In order to evaluate the thermal stability of 80% cold-rolled ODSEUROFER, samples were annealed for 1 h at temperatures up to about 0.9 T m where Tm is the absolute melting point. The characterization of the annealed samples was performed using transmission electron microscopy and electron backscatter diffraction. Results show that static recovery is the main softening mechanism of this steel when annealed below 800°C. The volume fraction of recrystallized grains is quite small (below 0.10). Above 900°C, martensitic transformation takes place causing pronounced hardening. Large M23C6 particles are found at the grain boundaries after tempering at 750°Cfor 2 h.
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Krüger, T., Varnik, F., Raabe, D.
Particle stress in suspensions of soft objects
(2011) Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, 369 (1945), pp. 2414-2421. Cited 10 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-79959855911&doi=10.1098%2frsta.2011.0090&partnerID=40&md5=89c3c0ba6d008aa31bef4d7dde60ca28

DOI: 10.1098/rsta.2011.0090
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany;
Interdisciplinary Centre for Advanced Materials Simulation, Stiepeler Strasse 129, 44780 Bochum, Germany
ABSTRACT: In a suspension of extended objects such as colloidal particles, capsules or vesicles, the contribution of particles to the stress is usually evaluated by first determining the stress originating from a single particle (e.g. via integrating the fluid stress over the surface of a particle) and then adding up the contributions of individual particles. While adequate for a computation of the average stress over the entire system, this approach fails to correctly reproduce the local stress. In this work, we propose and validate a variant of the method of planes which overcomes this problem. The method is particularly suited for many-body interactions arising from, for example, shear and bending rigidity of red blood cells. © 2011 The Royal Society.
AUTHOR KEYWORDS: Apparent viscosity; Haemorheology; Immersed boundary method; Lattice Boltzmann method; Method of planes; Particle stress

DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Woldemedhin, M.T., Raabe, D., Hassel, A.W.
Grain boundary electrochemistry of β-type Nb-Ti alloy using a scanning droplet cell
(2011) Physica Status Solidi (A) Applications and Materials Science, 208 (6), pp. 1246-1251. Cited 10 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-79959251788&doi=10.1002%2fpssa.201000991&partnerID=40&md5=04a1160f7f52ee5563da1446b61591e1

DOI: 10.1002/pssa.201000991
AFFILIATIONS: Institute for Chemical Technology of Inorganic Materials, Johannes Kepler University, Altenberger Str. 69, 4040 Linz, Austria; Max-Planck-Institut für Eisenforschung GmbH, Max Planck Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: Localized oxide spots were grown at the grain boundaries of a technically relevant 30at.% Nb-Ti β-type titanium alloy to study the local electrochemical response. The grain boundaries selected were combinations of grains having different orientations and grain boundary angle. Crystallographic information of the grains and boundary angles were revealed by electron back scattering diffraction (EBSD) technique. Cyclic voltammetry is the electrochemical technique used to grow the oxides starting from 0V and increasing the potential in steps of 1V till 8V at a scan rate of 100mVs -1 in an acetate buffer of pH 6.0. Electrochemical impedance spectroscopy was used to investigate the electrical properties of the oxide/electrolyte interface in the frequency range between 100kHz and 100mHz. Important oxide parameters such as formation factor and dielectric number were determined from these measurements. Significant differences were observed for different grain boundaries. The semiconducting properties of the oxides at the grain boundaries were assessed by using Mott-Schottky analysis on a potentiostatically grown oxide. All the oxides showed n-type semiconducting properties where the donor concentration varies with the grain boundaries mentioned above. A flat band potential -0.25 ±0.02V versus standard hydrogen electrode is more or less the same for all the boundaries studied.
AUTHOR KEYWORDS: anodic oxides; biomaterials; cyclic voltammetry; grain boundary; Mott-Schottky analysis
DOCUMENT TYPE: Article
SOURCE: Scopus

Krüger, T., Varnik, F., Raabe, D.
Efficient and accurate simulations of deformable particles immersed in a fluid using a combined immersed boundary lattice Boltzmann finite element method
(2011) Computers and Mathematics with Applications, 61 (12), pp. 3485-3505. Cited 76 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-79958799444&doi=10.1016%2fj.camwa.2010.03.057&partnerID=40&md5=d4c13dc7ea9939fcb77c28db4b49a129

DOI: 10.1016/j.camwa.2010.03.057
AFFILIATIONS: Max-Planck-Institut Fr Eisenforschung (MPIE), Max-Planck-Straße 1, D-40237 Dsseldorf, Germany;
Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Stiepeler Straße 129, D-44801 Bochum, Germany
ABSTRACT: The deformation of an initially spherical capsule, freely suspended in simple shear flow, can be computed analytically in the limit of small deformations [D. Barths-Biesel, J.M. Rallison, The time-dependent deformation of a capsule freely suspended in a linear shear flow, J. Fluid Mech. 113 (1981) 251267]. Those analytic approximations are used to study the influence of the mesh tessellation method, the spatial resolution, and

the discrete delta function of the immersed boundary method on the numerical results obtained by a coupled immersed boundary lattice Boltzmann finite element method. For the description of the capsule membrane, a finite element method and the Skalak constitutive model [R. Skalak, A. Tozeren, R.P. Zarda, S. Chien, Strain energy function of red blood cell membranes, Biophys. J. 13 (1973) 245264] have been employed. Our primary goal is the investigation of the presented model for small resolutions to provide a sound basis for efficient but accurate simulations of multiple deformable particles immersed in a fluid. We come to the conclusion that details of the membrane mesh, as tessellation method and resolution, play only a minor role. The hydrodynamic resolution, i.e., the width of the discrete delta function, can significantly influence the accuracy of the simulations. The discretization of the delta function introduces an artificial length scale, which effectively changes the radius and the deformability of the capsule. We discuss possibilities of reducing the computing time of simulations of deformable objects immersed in a fluid while maintaining high accuracy.
AUTHOR KEYWORDS: Capsule; Finite element method; Immersed boundary method; Lattice Boltzmann method; Simple shear flow; Small deformations
DOCUMENT TYPE: Article
SOURCE: Scopus

Zambaldi, C., Roters, F., Raabe, D.
Analysis of the plastic anisotropy and pre-yielding of (γ/ α2)-phase titanium aluminide microstructures by crystal plasticity simulation
(2011) Intermetallics, 19 (6), pp. 820-827. Cited 11 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-79954618302&doi=10.1016%2fj.intermet.2011.01.012&partnerID=40&md5=761723723368adf2fe4af21dc69af50d

DOI: 10.1016/j.intermet.2011.01.012
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, Düsseldorf, Germany
ABSTRACT: The plastic deformation of lamellar microstructures composed of the two phases γ-TiAl and α2-Ti3Al is highly orientation dependent. In this paper we present a homogenized model that takes into account the micromechanical effect of the plate-like morphologies that are often observed in two-phase titanium aluminide alloys. The model is based on crystal elasto-viscoplasticity and 18 deformation systems were implemented that have been identified to govern the plastic flow of the lamellar microstructures. The model is validated against experiments on polysynthetically twinned (PST) crystals and shows good agreement with the data. On a larger length scale, the model is applied to a 64-grain aggregate to investigate the mechanical response of two different kinds of microstructures. Different magnitudes of the kinematic constraints exerted by the densely spaced and highly aligned interfaces are shown to affect the macroscopic flow behavior of the microstructures. The phenomenon of pronounced microplasticity of fully lamellar material as well as the stress variation inside two-phase microstructures are studied quantitatively.
AUTHOR KEYWORDS: A. Titanium aluminides, based on TiAl; B. Brittleness and ductility; B. Mechanical properties at ambient temperature; B. Plastic deformation mechanisms; E. Mechanical properties, theory
DOCUMENT TYPE: Article
SOURCE: Scopus

Herrera, C., Ponge, D., Raabe, D.
Design of a novel Mn-based 1 GPa duplex stainless TRIP steel with 60% ductility by a reduction of austenite stability
(2011) Acta Materialia, 59 (11), pp. 4653-4664. Cited 140 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-79956028411&doi=10.1016%2fj.actamat.2011.04.011&partnerID=40&md5=b19f87d0bee6725cbb5ec562c0970a9b

DOI: 10.1016/j.actamat.2011.04.011
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany
ABSTRACT: We report on the microstructure, texture and deformation mechanisms of a novel ductile lean duplex stainless steel (Fe-19.9Cr-0.42Ni-0.16N-4.79Mn-0.11C- 0.46Cu-0.35Si, wt.%). The austenite is stabilized by Mn, C, and N (instead of Ni). The microstructure is characterized by electron channeling contrast imaging (ECCI) for dislocation mapping and electron backscattering diffraction (EBSD) for texture and phase mapping. The material has 1 GPa ultimate tensile strength and an elongation to fracture of above 60%. The mechanical behavior is interpreted in terms of the strength of both the starting phases, austenite and ferrite, and the amount, dispersion, and transformation kinetics of the mechanically induced martensite (TRIP effect). Transformation proceeds from austenite to hexagonal martensite to near cubic martensite (γ → → α′). The -martensite forms in the austenite with an orientation relationship close to Shoji-Nishiyama. The α′-martensite nucleates at the intersections of deformation bands, especially -bands, with Kurdjumov-Sachs and Nishiyama-Wassermann relationships. The ferrite deforms by dislocation slip and contains cell substructures.
AUTHOR KEYWORDS: EBSD; High strength; Microstructure; Stainless steels; Texture
DOCUMENT TYPE: Article
SOURCE: Scopus

Sun, D.K., Zhu, M.F., Pan, S.Y., Yang, C.R., Raabe, D.
Lattice Boltzmann modeling of dendritic growth in forced and natural convection
(2011) Computers and Mathematics with Applications, 61 (12), pp. 3585-3592. Cited 26 times.
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DOI: 10.1016/j.camwa.2010.11.001
AFFILIATIONS: Jiangsu Key Laboratory for Advanced Metallic Materials, Southeast University, Jiangning District, Nanjing, 211189, China; Dept. Microstructure Physics and Metal Forming, Max-Planck-Institut Fr Eisenforschung GmbH, Max-Planck-Str.1, D-40237 Dsseldorf, Germany
ABSTRACT: A two-dimensional (2D) coupled model is developed for the simulation of dendritic growth during alloy solidification in the presence of forced and natural convection. Instead of conventional continuum-based NavierStokes (NS) solvers, the present model adopts a kinetic-based lattice Boltzmann method (LBM), which describes flow dynamics by the evolution of distribution functions of moving pseudo-particles, for the numerical computations of flow dynamics as well as thermal and solutal transport. The dendritic growth is modeled using a solutal equilibrium approach previously proposed by Zhu and Stefanescu (ZS), in which the evolution of the solid/liquid interface is driven by the difference between the local equilibrium composition and the local actual liquid composition. The local equilibrium composition is calculated from the local temperature and curvature. The local temperature and actual liquid composition, controlled by both diffusion and convection, are obtained by solving the LB equations using the lattice BhatnagarGrossKrook (LBGK) scheme. Detailed model validation is performed by comparing the simulations with analytical predictions, which demonstrates the quantitative capability of the proposed model. Furthermore, the convective dendritic growth features predicted by the present model are compared with those obtained from the ZhuStefanescu and NavierStokes (ZSNS) model, in which the fluid flow is calculated using an NS solver. It is found that the evolution of the solid fraction of dendritic growth calculated by both models coincides well. However, the

present model has the significant advantages of numerical stability and computational efficiency for the simulation of dendritic growth with melt convection.
AUTHOR KEYWORDS: Dendritic growth; Lattice Boltzmann method; Melt convection; Microstructure modeling
DOCUMENT TYPE: Article
SOURCE: Scopus

Kadkhodapour, J., Schmauder, S., Raabe, D., Ziaei-Rad, S., Weber, U., Calcagnotto, M.
Experimental and numerical study on geometrically necessary dislocations and non-homogeneous mechanical properties of the ferrite phase in dual phase steels
(2011) Acta Materialia, 59 (11), pp. 4387-4394. Cited 118 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-79956000943&doi=10.1016%2fj.actamat.2011.03.062&partnerID=40&md5=b3bc6a404d53ab78fd4cd3a97130f156

DOI: 10.1016/j.actamat.2011.03.062
AFFILIATIONS: Department of Mechanical Engineering, Isfahan University of Technology, Isfahan 84156-83111, Iran;
Institute for Materials Testing, Materials Science and Strength of Materials, University of Stuttgart, Stuttgart, Germany;
Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
ABSTRACT: The microstructure of dual phase steels can be compared with a composite composed of a matrix of ferrite reinforced by small islands of martensite. This assumption has been used in several attempts to model the mechanical properties of dual phase steels. However, recent measurements show that the properties of the ferrite phase change with distance from the martensite grains. These measurements showed that the grains of the ferrite phase are harder in the vicinity of martensite grains. As a consequence of this local hardening effect, the ferrite phase has to be considered as an inhomogeneous matrix in modeling dual phase steels. This experiment inspired the idea that local hardening is caused by geometrically necessary dislocations. The idea is investigated experimentally and numerically in the present analysis, which for the first time leads to good agreement with experimental observations of the mechanical stress-strain behavior.
AUTHOR KEYWORDS: Dual phase steels; Geometrically necessary dislocations; Local hardening; Micromechanical model; Nano hardness test
DOCUMENT TYPE: Article
SOURCE: Scopus

Li, Y.J., Choi, P., Borchers, C., Westerkamp, S., Goto, S., Raabe, D., Kirchheim, R.
Atomic-scale mechanisms of deformation-induced cementite decomposition in pearlite
(2011) Acta Materialia, 59 (10), pp. 3965-3977. Cited 117 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-79955562592&doi=10.1016%2fj.actamat.2011.03.022&partnerID=40&md5=a946109171d4e9f7f4bdbb980a9a25cf

DOI: 10.1016/j.actamat.2011.03.022
AFFILIATIONS: Institut für Materialphysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany;
Max-Planck Institut für Eisenforschung, Max-Planck-Str. 1, D-40237 Düsseldorf, Germany;
Department of Materials Science and Engineering, Faculty of Engineering and Resource Science, Akita University, Tegata Gakuencho, Akita 010-0852, Japan
ABSTRACT: Pearlitic steel can exhibit tensile strengths higher than 5 GPa after severe plastic deformation, where the deformation promotes a refinement of the lamellar structure and cementite decomposition. However, a convincing correlation between deformation and cementite decomposition in

pearlite is still absent. In the present work, a local electrode atom probe was used to characterize the microstructural evolution of pearlitic steel, cold-drawn with progressive strains up to 5.4. Transmission electron microscopy was also employed to perform complementary analyses of the microstructure. Both methods yielded consistent results. The overall carbon content in the detected volumes as well as the carbon concentrations in ferrite and cementite were measured by atom probe. In addition, the thickness of the cementite filaments was determined. In ferrite, we found a correlation of carbon concentration with the strain, and in cementite, we found a correlation of carbon concentration with the lamella thickness. Direct evidence for the formation of cell/subgrain boundaries in ferrite and segregation of carbon atoms at these defects was found. Based on these findings, the mechanisms of cementite decomposition are discussed in terms of carbon-dislocation interaction.
AUTHOR KEYWORDS: Atom probe tomography; Cementite decomposition; Cold-drawn pearlitic steel wire; Dislocations; Grain boundaries
DOCUMENT TYPE: Article
SOURCE: Scopus

Springer, H., Kostka, A., dos Santos, J.F., Raabe, D.
Influence of intermetallic phases and Kirkendall-porosity on the mechanical properties of joints between steel and aluminium alloys
(2011) Materials Science and Engineering A, 528 (13-14), pp. 4630-4642.
Cited 67 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-79953277446&doi=10.1016%2fj.msea.2011.02.057&partnerID=40&md5=6d7478b2784bb4e2c233f5e896b3fd0a

DOI: 10.1016/j.msea.2011.02.057
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany;
Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Materials Mechanics, Solid-State Joining Processes, 21502 Geesthacht, Germany
ABSTRACT: The formation of intermetallic reaction layers and their influence on mechanical properties was investigated in friction stir welded joints between a low C steel and both pure Al (99.5wt.%) and Al-5wt.% Si. Characterisation of the steel/Al interface, tensile tests and fractography analysis were performed on samples in the as-welded state and after annealing in the range of 200-600°C for 9-64min. Annealing was performed to obtain reaction layers of distinct thickness and composition. For both Al alloys, the reaction layers grew with parabolic kinetics with the η phase (Al5Fe2) as the dominant component after annealing at 450°C and above. In joints with pure Al, the tensile strength is governed by the formation of Kirkendall-porosity at the reaction layer/Al interface. The tensile strength of joints with Al-5wt.% Si is controlled by the thickness of the η phase (Al5Fe2) layer. The pre-deformation of the base materials, induced by the friction stir welding procedure, was found to have a pronounced effect on the composition and growth kinetics of the reaction layers.
AUTHOR KEYWORDS: Aluminium; Friction stir welding; Interdiffusion; Intermetallic phases; Steel
DOCUMENT TYPE: Article
SOURCE: Scopus

Varnik, F., Gross, M., Moradi, N., Zikos, G., Uhlmann, P., Müller-Buschbaum, P., Magerl, D., Raabe, D., Steinbach, I., Stamm, M.
Stability and dynamics of droplets on patterned substrates: Insights from experiments and lattice Boltzmann simulations
(2011) Journal of Physics Condensed Matter, 23 (18), art. no. 184112, .
Cited 17 times.

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DOI: 10.1088/0953-8984/23/18/184112
AFFILIATIONS: Interdisciplinary Center for Advanced Materials Simulation (ICAMS), Ruhr University Bochum, Stiepeler Straße 129, 44780 Bochum, Germany;
Max-Planck-Institut für Eisenforschung, Max-Planck Straße 1, 40237 Düsseldorf, Germany;
Leibniz-Institut für Polymerforschung Dresden E.V., Hohe Straße 6, 01069 Dresden, Germany;
Physik-Department, Technische Universität München, LS E13, James-Franck-Straße 1, 85748 Garching, Germany
ABSTRACT: The stability and dynamics of droplets on solid substrates are studied both theoretically and via experiments. Focusing on our recent achievements within the DFG-priority program 1164 (Nano-and Microfluidics), we first consider the case of (large) droplets on the so-called gradient substrates. Here the term gradient refers to both a change of wettability (chemical gradient) or topography (roughness gradient). While the motion of a droplet on a perfectly flat substrate upon the action of a chemical gradient appears to be a natural consequence of the considered situation, we show that the behavior of a droplet on a gradient of topography is less obvious. Nevertheless, if care is taken in the choice of the topographic patterns (in order to reduce hysteresis effects), a motion may be observed. Interestingly, in this case, simple scaling arguments adequately account for the dependence of the droplet velocity on the roughness gradient (Moradi et al 2010 Europhys. Lett. 8926006). Another issue addressed in this paper is the behavior of droplets on hydrophobic substrates with a periodic arrangement of square shaped pillars. Here, it is possible to propose an analytically solvable model for the case where the droplet size becomes comparable to the roughness scale (Gross et al 2009 Europhys. Lett. 8826002). Two important predictions of the model are highlighted here. (i)There exists a state with a finite penetration depth, distinct from the full wetting (Wenzel) and suspended (Cassie-Baxter, CB) states. (ii)Upon quasi-static evaporation, a droplet initially on the top of the pillars (CB state) undergoes a transition to this new state with a finite penetration depth but then (upon further evaporation) climbs up the pillars and goes back to the CB state again. These predictions are confirmed via independent numerical simulations. Moreover, we also address the fundamental issue of the internal droplet dynamics and the terminal center of mass velocity on a flat substrate. © 2011 IOP Publishing Ltd.
DOCUMENT TYPE: Article
SOURCE: Scopus

Goetz, A.J., Steinmetz, D.R., Griesshaber, E., Zaefferer, S., Raabe, D., Kelm, K., Irsen, S., Sehrbrock, A., Schmahl, W.W.
Interdigitating biocalcite dendrites form a 3-D jigsaw structure in brachiopod shells
(2011) Acta Biomaterialia, 7 (5), pp. 2237-2243. Cited 33 times.
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DOI: 10.1016/j.actbio.2011.01.035
AFFILIATIONS: Department für Geo-und Umweltwissenschaften, LMU, Theresienstr. 41, D-80333 München, Germany;
Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, D-40237 Düsseldorf, Germany;
German Aerospace Center (DLR), Institute for Materials Research, Linder Höhe, D-51147 Köln, Germany;
Forschungszentrum CAESAR, Ludwig-Erhard-Alle 2, D-53175 Bonn, Germany

ABSTRACT: We report a newly discovered dense microstructure of dendrite-like biocalcite that is formed by marine organisms. High spatial resolution electron backscatter diffraction (EBSD) was carried out under specific analytical conditions (15 and 10 kV) on the primary layer of the modern brachiopod Gryphus vitreus. The primary layer of modern brachiopods, previously termed nanocrystalline, is formed by an array of concave/convex calcite grains with interdigitated recesses and protrusions of abutting crystals without any cavities in or between the dendrites. The interface topology of this structure ranges from a few tens of nanometres to tens of micrometres, giving a nanoscale structure to the material fabric. The dendritic grains show a spread of crystallographic orientation of several degrees and can thus be referred to as mesocrystals. Individual dendritic mesocrystals reach sizes in one dimension larger than 20 μm. The preferred crystallographic orientation is similar in the primary and adjacent fibrous shell layers, even though these two layers show completely different crystal morphologies and grain boundary topologies. This observation indicates that two separate control mechanisms are active when the primary and the fibrous shell layers are formed. We propose a growth model for the interdigitated dendritic calcite grain structure based on a precursor of vesicles filled with amorphous calcium carbonate (ACC).
AUTHOR KEYWORDS: Brachiopod primary layer texture; High-resolution EBSD; Hybrid composite biomateria; Interdigitated/ interlinked dendritic microstructure; Nacre
DOCUMENT TYPE: Article
SOURCE: Scopus

Siqueira, R.P., Sandim, H.R.Z., Oliveira, T.R., Raabe, D.
Composition and orientation effects on the final recrystallization texture of coarse-grained Nb-containing AISI 430 ferritic stainless steels
(2011) Materials Science and Engineering A, 528 (9), pp. 3513-3519. Cited 24 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-79951671298&doi=10.1016%2fj.msea.2011.01.007&partnerID=40&md5=5c5f7a27a1b311121b7736aaca612dea

DOI: 10.1016/j.msea.2011.01.007
AFFILIATIONS: Departamento de Engenharia de Materiais, Escola de Engenharia de Lorena, University of Sao Paulo, 12600-970, Lorena-SP, Brazil;
Centro de Pesquisa da ArcelorMittal Inox Brasil S.A., 35180-000, Timóteo-MG, Brazil;
Max-Planck Institut für Eisenforschung, D-40237, Düsseldorf, Germany
ABSTRACT: Composition and orientation effects on the final recrystallization texture of three coarse-grained Nb-containing AISI 430 ferritic stainless steels (FSSs) were investigated. Hot-bands of steels containing distinct amounts of niobium, carbon and nitrogen were annealed at 1250 °C for 2. h to promote grain growth. In particular, the amounts of Nb in solid solution vary from one grade to another. For purposes of comparison, the texture evolution of a hot-band sheet annealed at 1030 °C for 1. min (finer grain structure) was also investigated. Subsequently, the four sheets were cold rolled up to 80% reduction and then annealed at 800 °C for 15. min. Texture was determined using X-ray diffraction and electron backscatter diffraction (EBSD). Noticeable differences regarding the final recrystallization texture and microstructure were observed in the four investigated grades. Results suggest that distinct nucleation mechanisms take place within these large grains leading to the development of different final recrystallization textures.
AUTHOR KEYWORDS: Coarse grain; Composition effects; Ferritic stainless steel; Hot-band; Recrystallization; Texture
DOCUMENT TYPE: Article
SOURCE: Scopus

Vob, S., Palm, M., Stein, F., Raabe, D.

Phase equilibria in the Fe-Nb system
(2011) Journal of Phase Equilibria and Diffusion, 32 (2), pp. 97-104. Cited 12 times.
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DOI: 10.1007/s11669-010-9808-3
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: A review of the literature revealed that recently published phase diagrams of the Fe-Nb system show considerable discrepancies regarding phase equilibria with the melt and the homogeneity ranges of the intermetallic phases, specifically of the Laves phase Fe 2Nb. Therefore the system has been reinvestigated by metallography, electron probe microanalysis (EPMA), and differential thermal analysis (DTA). Temperatures of invariant reactions were determined and the homogeneity ranges of the two intermetallic phases, Fe 2Nb Laves phase and Fe 7Nb 6 μ phase, which both exist within a wide composition range, were established. © ASM International.
AUTHOR KEYWORDS: Binary system; Experimental study; Intermetallics; Phase diagram
DOCUMENT TYPE: Review
SOURCE: Scopus

Khorashadizadeh, A., Raabe, D., Winning, M., Pippan, R.
Recrystallization and grain growth in ultrafine-grained materials produced by high pressure torsion
(2011) Advanced Engineering Materials, 13 (4), pp. 245-250. Cited 4 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-79953174618&doi=10.1002%2fadem.201000253&partnerID=40&md5=78223606dec54b56148773e035528858

DOI: 10.1002/adem.201000253
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Department Microstructure Physics and Metal Forming, Düsseldorf, Germany;
Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Department Material Physics, Leoben, Austria
ABSTRACT: Ultrafine-grained (UFG) materials processed by severe plastic deformation are known to exhibit good mechanical properties. Much about the annealing behavior of such materials is still unknown, and this work aims to provide a better understanding of the thermal properties of UFG materials. For this purpose a Cu-0.17 wt%Zr alloy was subjected to high pressure torsion (HPT) with a maximal pressure of 4.8GPa at room temperature. The microstructures of the specimens were characterized using electron back scatter (EBSD) measurements, transmission electron microscopy (TEM), and hardness measurements. During annealing of the samples, dispersoids were formed which improved the thermal stability of the alloy. At higher strain levels the fraction of high angle grain boundaries (HAGBs) increased above 70% of the total grain boundaries. Ultrafine-grained materials processed by severe plastic deformation are known to exhibit good mechanical properties. Much about the annealing behavior of such materials is still unknown, and this work aims to provide a better understanding of the thermal properties of such materials. For this purpose a Cu-0.17 wt%Zr alloy was subjected to high pressure torsion. The microstructures of the specimens were characterized in the deformed state as well as after annealing using EBSD and hardness measurements. Copyright © 2011 WILEY-VCH Verlag GmbH & Co. KGaA.
DOCUMENT TYPE: Article
SOURCE: Scopus

Helm, D., Butz, A., Raabe, D., Gumbsch, P.

Microstructure-based description of the deformation of metals: Theory and application
(2011) JOM, 63 (4), pp. 26-33. Cited 26 times.
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DOI: 10.1007/s11837-011-0056-8
AFFILIATIONS: Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, Freiburg 79108, Germany;
Max-Planck-Institute for Iron Research, Max-Planck-Str. 1, Düsseldorf 40237, Germany;
Institute for Applied Materials IAM, Karlsruhe Institute of Technology KIT, Kaiserstrae 12, Karlsruhe 6131, Germany
ABSTRACT: Aiming for an integrated approach to computational materials engineering in an industrial context poses big challenges in the development of suitable materials descriptions for the different steps along the processing chain. The first key component is to correctly describe the microstructural changes during the thermal and mechanical processing of the base material into a semi-finished product. Explicit representations of the microstructure are most suitable there. The final processing steps and particularly component assessment then has to describe the entire component which requires homogenized continuum mechanical representations. A key challenge is the step in between, the determination of the (macroscopic) materials descriptions from microscopic structures. This article describes methods to include microstructure into descriptions of the deformation of metal, and demonstrates the central steps of the simulation along the processing chain of an automotive component manufactured from a dual phase steel. © 2011 TMS.
DOCUMENT TYPE: Review
SOURCE: Scopus

Khorashadizadeh, A., Raabe, D., Zaefferer, S., Rohrer, G.S., Rollett, A.D., Winning, M.
Five-parameter grain boundary analysis by 3D EBSD of an ultra fine grained CuZr alloy processed by equal channel angular pressing
(2011) Advanced Engineering Materials, 13 (4), pp. 237-244. Cited 21 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-79953165004&doi=10.1002%2fadem.201000259&partnerID=40&md5=8bd2253bf401b1e9d51b46dfcdcfcc4d

DOI: 10.1002/adem.201000259
AFFILIATIONS: Department Microstructure Physics and Metal Forming, Max-Planck-Institute für Eisenforschung, Düsseldorf, Germany;
Department Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, United States
ABSTRACT: The 3D grain boundary character distribution (GBCD) of a sample subjected to equal channel angular pressing (ECAP) after eight passes and successive annealing at 650°C for about 10min is analyzed. The experiments are conducted using a dual beam system, which is a combination of a focused ion beam and a scanning electron microscope to collect a series of electron backscatter diffraction (EBSD) maps of the microstructure (3D EBSD). The data set was aligned and reconstructed to a 3D microstructure. The crystallographic character of the grain boundary planes was determined using three different methods, namely, the line segment method, the stereological method, and the triangular surface mesh method. The line segment and triangular surface mesh methods produce consistent data sets, both yielding approximately a 7% area fraction of coherent twins. These results starkly contrast that of the statistical stereological method, which produced a 44% area fraction of coherent twins. The 3D grain boundary character distribution (GBCD) of a sample subjected to equal channel angular pressing (ECAP) after eight passes and successive annealing at 650°C for about 10min is analyzed. The crystallographic character of the

grain boundary planes was determined using three different methods, namely, the line segment method, the stereological method, and the triangular surface mesh method. The line segment and triangular surface mesh methods produce consistent results. These results starkly contrast that of the statistical stereological method.
DOCUMENT TYPE: Article
SOURCE: Scopus

Song, J., Kostka, A., Veehmayer, M., Raabe, D.
Hierarchical microstructure of explosive joints: Example of titanium to steel cladding
(2011) Materials Science and Engineering A, 528 (6), pp. 2641-2647. Cited 89 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-79151470947&doi=10.1016%2fj.msea.2010.11.092&partnerID=40&md5=52b40b7d6fea638f8f137793c4b478a5

DOI: 10.1016/j.msea.2010.11.092
AFFILIATIONS: Max-Planck Institut für Eisenforschung GmbH, Max-Planck Str. 1, 40237 Düsseldorf, Germany;
Dynamic Materials Corporation GmbH, Dr. Hermann-Fleck-Allee 8, 57299 Burbach, Germany
ABSTRACT: The microstructure of explosive cladding joints formed among parallel Ti and steel plates was examined by electron microscopy. The bonding interface and the bulk materials around it form pronounced hierarchical microstructures. This hierarchy is characterized by the following features: at the mesoscopic scale of the hierarchy a wavy course of the interface characterizes the interface zone. This microstructure level is formed by heavy plastic shear waves (wavelength≈0.5mm) which expand within the two metal plates during the explosion parallel to the bonding interface. At the micro-scale range, intermetallic inclusions (size≈100-200μm) are formed just behind the wave crests on the steel side as a result of partial melting. Electron diffraction revealed FeTi and metastable Fe9.64Ti0.36. Most of the observed phases do not appear in the equilibrium Fe-Ti phase diagram. These intermetallic inclusions are often accompanied by micro-cracks of similar dimension. At the smallest hierarchy level we observe a reaction layer of about 100-300nm thickness consisting of nano-sized grains formed along the entire bonding interface. Within that complex hierarchical micro- and nanostructure, the mesoscopic regime, more precisely the type and brittleness of the intermetallic zones, seems to play the dominant role for the mechanical behavior of the entire compound. © 2010 Elsevier B.V.
AUTHOR KEYWORDS: Electron microscopy; Explosive welding; Interfaces; Steel; Titanium
DOCUMENT TYPE: Article
SOURCE: Scopus

Cojocaru-Miŕdin, O., Choi, P., Wuerz, R., Raabe, D.
Atomic-scale characterization of the CdS/CuInSe2 interface in thin-film solar cells
(2011) Applied Physics Letters, 98 (10), art. no. 103504, . Cited 35 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-79952653344&doi=10.1063%2f1.3560308&partnerID=40&md5=e2c201ccecd1c8b91255b83e649463f8

DOI: 10.1063/1.3560308
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Zentrum für Sonnenenergie-und Wasserstoff-Forschung Baden-Württemberg, Industriestr. 6, 70565 Stuttgart, Germany
ABSTRACT: Elemental mixing at the CdS/ CuInSe2 interface of a thin-film solar cell was studied by means of atom probe tomography. A Cu-depleted and

Cd-doped region (~2 nm in width) was detected at the CuInSe2 surface, proving the existence of a buried p-n homojunction within the CuInSe2 absorber layer. Furthermore, CdS was found to infiltrate open pores existing in CuInSe2 during the chemical bath deposition. This could explain why chemical bath deposition of CdS leads to higher solar cell efficiencies compared to physical vapor deposition of CdS. © 2011 American Institute of Physics.
DOCUMENT TYPE: Article
SOURCE: Scopus

Millán, J., Ponge, D., Raabe, D., Choi, P., Dmitrieva, O.
Characterization of nano-sized precipitates in a Mn-based lean maraging steel by atom probe tomography
(2011) Steel Research International, 82 (2), pp. 137-145. Cited 7 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-79251513971&doi=10.1002%2fsrin.201000274&partnerID=40&md5=20f058bbfeaaec5a84a605965b5141e8

DOI: 10.1002/srin.201000274
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: We present atom probe tomography results of a precipitation-hardened Mn-based maraging steel (9 Mn, 1.9 Ni, 0.6 Mo, 1.1 Ti, 0.33 Al; in at.%). The alloy is characterized by the surprising effect that both, strength and total elongation increase upon aging. The material reveals a high ultimate tensile strength (UTS) up to 1GPa and good ductility (total elongation (TE) of up to 15% in a tensile test) depending on aging conditions. We map the evolution of the precipitates after 450°C aging treatment using atom probe tomography in terms of chemical composition and size distribution. Copyright © 2011 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim.
AUTHOR KEYWORDS: aging; atom probe tomography; high strength steels; precipitation hardening
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Springer, H., Kostka, A., Payton, E.J., Raabe, D., Kaysser-Pyzalla, A., Eggeler, G.
On the formation and growth of intermetallic phases during interdiffusion between low-carbon steel and aluminum alloys
(2011) Acta Materialia, 59 (4), pp. 1586-1600. Cited 117 times.
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DOI: 10.1016/j.actamat.2010.11.023
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany;
Institut für Werkstoffe, Ruhr-Universität Bochum, 44801 Bochum, Germany;
Helmholtz-Zentrum für Materialien und Energie GmbH, 14109 Berlin, Germany
ABSTRACT: The formation of intermetallic reaction layers was investigated for interdiffusion between a low-carbon steel and commercially pure aluminum (99.99%) and between a low-carbon steel and an aluminum-silicon alloy (Al-5 wt.% Si). Solid/solid, solid/semi-solid and solid/liquid diffusion couples were produced at both 600 and 675 °C. The total width of the reaction layer is governed mainly by the parabolic diffusion-controlled growth of the η phase (Al_5Fe_2), which exhibits orientation-dependent growth kinetics. The addition of Si to Al, which is known to decelerate reaction layer growth in interdiffusion experiments with Al melts, was found to accelerate the reaction layer growth in solid/semi-solid interdiffusion experiments. This phenomenon is discussed in light of previous atomistic explanations and the apparent activation energy calculated for the growth

of the η phase (Al 5Fe2). © 2010 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
AUTHOR KEYWORDS: Aluminum; Interdiffusion; Intermetallic phases; Joining; Steel
DOCUMENT TYPE: Article
SOURCE: Scopus

Nikolov, S., Fabritius, H., Petrov, M., Friák, M., Lymperakis, L., Sachs, C., Raabe, D., Neugebauer, J.
Robustness and optimal use of design principles of arthropod exoskeletons studied by ab initio-based multiscale simulations
(2011) Journal of the Mechanical Behavior of Biomedical Materials, 4 (2), pp. 129-145. Cited 56 times.
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DOI: 10.1016/j.jmbbm.2010.09.015
AFFILIATIONS: Bulgarian Academy of Sciences, Institute of Mechanics, Acad. G. Bonchev Str. Bl. 4, 1113 Sofia, Bulgaria;
Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Massachusetts Institute of Technology, 77 Massachusetts Avenue, Building 35-135A, Cambridge, MA 02139-4307, United States
ABSTRACT: Recently, we proposed a hierarchical model for the elastic properties of mineralized lobster cuticle using (i) ab initio calculations for the chitin properties and (ii) hierarchical homogenization performed in a bottom-up order through all length scales. It has been found that the cuticle possesses nearly extremal, excellent mechanical properties in terms of stiffness that strongly depend on the overall mineral content and the specific microstructure of the mineral-protein matrix. In this study, we investigated how the overall cuticle properties changed when there are significant variations in the properties of the constituents (chitin, amorphous calcium carbonate (ACC), proteins), and the volume fractions of key structural elements such as chitin-protein fibers. It was found that the cuticle performance is very robust with respect to variations in the elastic properties of chitin and fiber proteins at a lower hierarchy level. At higher structural levels, variations of design parameters such as the volume fraction of the chitin-protein fibers have a significant influence on the cuticle performance. Furthermore, we observed that among the possible variations in the cuticle ingredients and volume fractions, the experimental data reflect an optimal use of the structural variations regarding the best possible performance for a given composition due to the smart hierarchical organization of the cuticle design. © 2010 Elsevier Ltd.
AUTHOR KEYWORDS: Ab initio method; Biominerals; Chitin; Elastic properties; Homogenization
DOCUMENT TYPE: Article
SOURCE: Scopus

Friák, M., Hickel, T., Körmann, F., Udyansky, A., Dick, A., Von Pezold, J., Ma, D., Kim, O., Counts, W.A., Šob, M., Gebhardt, T., Music, D., Schneider, J., Raabe, D., Neugebauer, J.
Determining the elasticity of materials employing quantum-mechanical approaches from the electronic ground state to the limits of materials stability
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DOI: 10.1002/srin.201000264
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, D-40237, Düsseldorf, Germany;

Department of Chemistry, Faculty of Science, Masaryk University, Kotlářská 2, 61137 Brno, Czech Republic;
Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Žižkova 22, 61662 Brno, Czech Republic;
Materials Chemistry, RWTH Aachen University, D-52056 Aachen, Germany
ABSTRACT: Quantum-mechanical (so-called ab initio) calculations have achieved considerable reliability in predicting physical and chemical properties and phenomena. Due to their reliability they are becoming increasingly useful when designing new alloys or revealing the origin of phenomena in existing materials, also because these calculations are able to accurately predict basic material properties without experimental input. Due to the universal validity of fundamental quantum mechanics, not only ground-state properties, but also materials responses to external parameters can reliably be determined. The focus of the present paper is on ab initio approaches to the elasticity of materials. First, the methodology to determine single-crystalline elastic constants and polycrystalline moduli of ordered compounds as well as disordered alloys is introduced. In a second part, the methodology is applied on α-Fe, with a main focus on (i) investigating the influence of magnetism on its elasticity and phase stability and (ii) simulating extreme loading conditions that go up to the theoretical tensile strength limits and beyond.
AUTHOR KEYWORDS: ab initio; elasticity; magnetism; stability; strength
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Ayodele, S.G., Varnik, F., Raabe, D.
Lattice Boltzmann study of pattern formation in reaction-diffusion systems (2011) Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, 83 (1), art. no. 016702, . Cited 16 times.
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DOI: 10.1103/PhysRevE.83.016702
AFFILIATIONS: Max-Planck Institut für Eisenforschung, Max-Planck Straße 1, D-40237 Düsseldorf, Germany;
Interdisciplinary Center for Advanced Materials Simulation, Ruhr University Bochum, Stiepeler Straße 129, D-44780 Bochum, Germany
ABSTRACT: Pattern formation in reaction-diffusion systems is of great importance in surface micropatterning, self-organization of cellular micro-organisms, and in developmental biology. In this work, we apply the lattice Boltzmann method to study pattern formation in reaction-diffusion systems. As a first methodological step, we consider the case of a single species undergoing transformation reaction and diffusion. In this case, we perform a third-order Chapman-Enskog multiscale expansion and study the dependence of the lattice Boltzmann truncation error on the diffusion coefficient and the reaction rate. These findings are in good agreement with numerical simulations. Furthermore, taking the Gray-Scott model as a prominent example, we provide evidence for the maturity of the lattice Boltzmann method in studying pattern formation in nonlinear reaction-diffusion systems. For this purpose, we perform linear stability analysis of the Gray-Scott model and determine the relevant parameter range for pattern formation. Lattice Boltzmann simulations allow us not only to test the validity of the linear stability phase diagram including Turing and Hopf instabilities, but also permit going beyond the linear stability regime, where large perturbations give rise to interesting dynamical behavior such as the so-called self-replicating spots. We also show that the length scale of the patterns may be tuned by rescaling all relevant diffusion coefficients in the system with the same factor while leaving all the reaction constants unchanged.
DOCUMENT TYPE: Article
SOURCE: Scopus

Renzetti, R.A., Sandim, H.R.Z., Sandim, M.J.R., Santos, A.D., Möslang, A., Raabe, D.
Annealing effects on microstructure and coercive field of ferritic-martensitic ODS Eurofer steel
(2011) Materials Science and Engineering A, 528 (3), pp. 1442-1447. Cited 14 times.
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DOI: 10.1016/j.msea.2010.10.051
AFFILIATIONS: Escola de Engenharia de Lorena - USP, 12600-970 Lorena, SP, Brazil;
Instituto de Física - USP, 05314-970 São Paulo, SP, Brazil;
Karlsruher Institut für Technologie (KIT), IMF I, D-72061 Karlsruhe, Germany;
Max-Planck Institut für Eisenforschung (MPI-E), D-40237 Düsseldorf, Germany
ABSTRACT: Oxide dispersion strengthened reduced-activation ferritic-martensitic steels are promising candidates for applications in future fusion power plants. Samples of a reduced activation ferritic-martensitic 9wt.%Cr-oxide dispersion strengthened Eurofer steel were cold rolled to 80% reduction in thickness and annealed in vacuum for 1h from 200 to 1350°C to evaluate its thermal stability. Vickers microhardness testing and electron backscatter diffraction (EBSD) were used to characterize the microstructure. The microstructural changes were also followed by magnetic measurements, in particular the corresponding variation of the coercive field (Hc), as a function of the annealing treatment. Results show that magnetic measurements were sensitive to detect the changes, in particular the martensitic transformation, in samples annealed above 850°C (austenitic regime). © 2010 Elsevier B.V.
AUTHOR KEYWORDS: Coercive field; EBSD; Magnetic measurements; ODS; Recrystallization; Steel
DOCUMENT TYPE: Article
SOURCE: Scopus

Calcagnotto, M., Adachi, Y., Ponge, D., Raabe, D.
Deformation and fracture mechanisms in fine- and ultrafine-grained ferrite/martensite dual-phase steels and the effect of aging
(2011) Acta Materialia, 59 (2), pp. 658-670. Cited 237 times.
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DOI: 10.1016/j.actamat.2010.10.002
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany;
National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan
ABSTRACT: Three ferrite/martensite dual-phase steels varying in the ferrite grain size (12.4, 2.4 and 1.2 μm) but with the same martensite content (~30 vol.%) were produced by large-strain warm deformation at different deformation temperatures, followed by intercritical annealing. Their mechanical properties were compared, and the response of the ultrafine-grained steel (1.2 μm) to aging at 170 °C was investigated. The deformation and fracture mechanisms were studied based on microstructure observations using scanning electron microscopy and electron backscatter diffraction. Grain refinement leads to an increase in both yield strength and tensile strength, whereas uniform elongation and total elongation are less affected. This can be partly explained by the increase in the initial strain-hardening rate. Moreover, the stress/strain partitioning characteristics between ferrite and martensite change due to grain

refinement, leading to enhanced martensite plasticity and better interface cohesion. Grain refinement further promotes ductile fracture mechanisms, which is a result of the improved fracture toughness of martensite. The aging treatment leads to a strong increase in yield strength and improves the uniform and total elongation. These effects are attributed to dislocation locking due to the formation of Cottrell atmospheres and relaxation of internal stresses, as well as to the reduction in the interstitial carbon content in ferrite and tempering effects in martensite.

AUTHOR KEYWORDS: Aging; Deformation mechanisms; Dual-phase steel; Fracture mechanisms; Ultrafine grains
DOCUMENT TYPE: Article
SOURCE: Scopus

Jia, J., Mao, W., Raabe, D.
Plastic deformation mechanisms of isotactic polypropylene during rolling
(2011) Gaofenzi Cailiao Kexue Yu Gongcheng/Polymeric Materials Science and Engineering, 27 (1), pp. 116-119.
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AFFILIATIONS: Key Laboratory for Ferrous Metallurgy and Resources Utilization of Ministry of Education, Wuhan University of Science and Technology, Wuhan 430081, China;
School of Material Science and Engineering, Beijing University of Science and Technology, Beijing 100083, China;
Max-Planck-Institut Für Eisenforschung, Düsseldorf 40237, Germany
ABSTRACT: The wide angle X-ray diffractormeter with an area detector was used to measure the crystallographic texture of the isotactic polypropylene (iPP) during rolling deformation. Pole figures of the rolled iPP were obtained, from which the orientation distribution functions were calculated. The deformation mechanism of the material was analyzed. The results show that the main deformation mechanism is crystallographic chain slip during rolling. It is found that the first active slip system is (010) [001] and the second is (100) [001]. The action of the (110) [001] slip system does not be found in this work. The final texture of the rolled iPP is the [001]//RD fiber texture, which includes several (hk0) [001] texture components. The macromolecular chains parallel to the rolling direction in the rolled iPP.
AUTHOR KEYWORDS: Isotactic polypropylene; Orientation distribution functions; Texture
DOCUMENT TYPE: Article
SOURCE: Scopus

Cojocaru-Miredin, O., Choi, P., Wuerz, R., Raabe, D.
Atomic-scale distribution of impurities in cuinse2-based thin-film solar cells
(2011) Ultramicroscopy, 111 (6), pp. 552-556. Cited 21 times.
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DOI: 10.1016/j.ultramic.2010.12.034
AFFILIATIONS: Max-Planck-Institut fur Eisenforschung, Max-Planck-Straße 1, 40237 Dusseldorf, Germany;
Zentrum fur Sonnenenergie- und Wasserstoff-Forschung Baden-Wurttemberg, Industriestraße 6, 70565 Stuttgart, Germany
ABSTRACT: Atom Probe Tomography was employed to investigate the distribution of impurities, in particular sodium and oxygen, in a cuinse2-based thin-film solar cell. It could be shown that sodium, oxygen, and silicon diffuse from the soda lime glass substrate into the cuinse2 film and accumulate at the grain boundaries. Highly dilute concentrations of sodium and oxygen were measured in the bulk. Selenium was found to be

depleted at the grain boundaries. These observations could be confirmed by complementary energy dispersive X-ray spectroscopy studies. Our results support the model proposed by Kronik et al. (1998) [1], which explains the enhanced photovoltaic efficiency of sodium containing cuinse2 solar cells by the passivation of selenium vacancies at grain boundaries. © 2011 Elsevier B.V.
AUTHOR KEYWORDS: Grain boundary segregation; Photovoltaic; Pulsed laser atom probe; Sodium diffusion; Thin-film solar cells; Transmission electron microscopy
DOCUMENT TYPE: Article
SOURCE: Scopus

Dmitrieva, O., Choi, P., Gerstl, S.S.A., Ponge, D., Raabe, D.
Pulsed-laser atom probe studies of a precipitation hardened maraging TRIP steel
(2011) Ultramicroscopy, 111 (6), pp. 623-627. Cited 15 times.
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DOI: 10.1016/j.ultramic.2010.12.007
AFFILIATIONS: Max-Planck-Institute for Iron Research, Max-Planck-Str. 1, 40237 Dusseldorf, Germany;
Imago Scientific Instruments, Madison, WI 53711, United States
ABSTRACT: A precipitation hardened maraging TRIP steel was analyzed using a pulsed laser atom probe. The laser pulse energy was varied from 0.3 to 1.9 nJ to study its effect on the measured chemical compositions and spatial resolution. Compositional analyses using proximity histograms did not show any significant variations in the average matrix and precipitate compositions. The only remarkable change in the atom probe data was a decrease in the++/+ charge state ratios of the elements. The values of the evaporation field used for the reconstructions exhibit a linear dependence on the laser pulse energy. The adjustment of the evaporation fields used in the reconstructions for different laser pulse energies was based on the correlation of the obtained cluster shapes to the TEM observations. No influence of laser pulse energy on chemical composition of the precipitates and on the chemical sharpness of their interfaces was detected. © 2010 Elsevier B.V.
AUTHOR KEYWORDS: Field evaporation; Local electrode atom probe; Microanalysis; Precipitation hardened steels; Pulsed-laser atom probe tomography; Solute clustering
DOCUMENT TYPE: Article
SOURCE: Scopus

Choi, P.-P., Povstugar, I., Ahn, J.-P., Kostka, A., Raabe, D.
Thermal stability of TiAlN/CrN multilayer coatings studied by atom probe tomography
(2011) Ultramicroscopy, 111 (6), pp. 518-523. Cited 13 times.
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DOI: 10.1016/j.ultramic.2010.11.012
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Department for Microstructure Physics and Metal Forming, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany;
Korea Institute of Science and Technology, Advanced Analysis Center, P.O. Box 131, Cheongryang, 130-650 Seoul, South Korea
ABSTRACT: This study is about the microstructural evolution of TiAlN/CrN multilayers (with a Ti:Al ratio of 0.75:0.25 and average bilayer period of 9 nm) upon thermal treatment. Pulsed laser atom probe analyses were performed in conjunction with transmission electron microscopy and X-ray diffraction. The layers are found to be thermally stable up to 600 °C. At

700 °C TiAlN layers begin to decompose into Ti- and Al-rich nitride layers in the out-of-plane direction. Further increase in temperature to 1000 °C leads to a strong decomposition of the multilayer structure as well as grain coarsening. Layer dissolution and grain coarsening appear to begin at the surface. Domains of AlN and TiCrN larger than 100 nm are found, together with smaller nano-sized AlN precipitates within the TiCrN matrix. Fe and V impurities are detected in the multilayers as well, which diffuse from the steel substrate into the coating along columnar grain boundaries.
AUTHOR KEYWORDS: Atom probe tomography; Hardcoatings; Multilayers; Thermal stability
DOCUMENT TYPE: Article
SOURCE: Scopus

Dmitrieva, O., Ponge, D., Inden, G., Millán, J., Choi, P., Sietsma, J., Raabe, D.
Chemical gradients across phase boundaries between martensite and austenite in steel studied by atom probe tomography and simulation
(2011) Acta Materialia, 59 (1), pp. 364-374. Cited 100 times.
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DOI: 10.1016/j.actamat.2010.09.042
AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany;
Delft University of Technology, Faculty 3mE, Dept. MSE, 2628 CD Delft, Netherlands
ABSTRACT: Partitioning at phase boundaries of complex steels is important for their properties. We present atom probe tomography results across martensite/austenite interfaces in a precipitation-hardened maraging-TRIP steel (12.2 Mn, 1.9 Ni, 0.6 Mo, 1.2 Ti, 0.3 Al; at.%). The system reveals compositional changes at the phase boundaries: Mn and Ni are enriched while Ti, Al, Mo and Fe are depleted. More specific, we observe up to 27 at.% Mn in a 20 nm layer at the phase boundary. This is explained by the large difference in diffusivity between martensite and austenite. The high diffusivity in martensite leads to a Mn flux towards the retained austenite. The low diffusivity in the austenite does not allow accommodation of this flux. Consequently, the austenite grows with a Mn composition given by local equilibrium. The interpretation is based on DICTRA and mixed-mode diffusion calculations (using a finite interface mobility).
AUTHOR KEYWORDS: Aging; Atom probe tomography; High-strength steels; Precipitation hardening; TRIP
DOCUMENT TYPE: Article
SOURCE: Scopus

Lia, Y.J., Choi, P., Borchers, C., Chen, Y.Z., Goto, S., Raabe, D., Kirchheim, R.
Atom probe tomography characterization of heavily cold drawn pearlitic steel wire
(2011) Ultramicroscopy, 111 (6), pp. 628-632. Cited 29 times.
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DOI: 10.1016/j.ultramic.2010.11.010
AFFILIATIONS: Institutfur Materialphysik, Georg-August-Universitat Gottingen, Friedrich-Hund-Platz 1, D-37077 Gottingen, Germany;
Max-Planck Institut fur Eisenforschung, Max-Planck-Str. 1, D-40237Diisseldorf, Germany;

Department of Materials Science and Engineering, Faculty of Engineering and Resource Science, Akita University, Tegata Gakuencho, Akita 010-0852, Japan
ABSTRACT: Atom Probe Tomography (APT) was used to analyze the carbon distribution in a heavily cold drawn pearlitic steel wire with a true strain of 6.02. The carbon concentrations in cementite and ferrite were separately measured by a sub-volume method and compared with the literature data. It is found that the carbon concentration in ferrite saturates with strain. The carbon concentration in cementite decreases with the lamellar thickness, while the carbon atoms segregate at dislocations or cell/grain boundaries in ferrite. The mechanism of cementite decomposition is discussed in terms of the evolution of dislocation structure during severe plastic deformation. © 2010 Elsevier B.V.
AUTHOR KEYWORDS: Atom probetomography; Cell boundaries; Cementite decomposition; Dislocations; Pearlitic steelwire; Severe plasticdeformation
DOCUMENT TYPE: Article
SOURCE: Scopus

Friák, M., Hickel, T., Grabowski, B., Lymperakis, L., Udyansky, A., Dick, A., Ma, D., Roters, F., Zhu, L.-F., Schlieter, A., Kühn, U., Ebrahimi, Z., Lebensohn, R.A., Holec, D., Eckert, J., Emmerich, H., Raabe, D., Neugebauer, J.
Methodological challenges in combining quantum-mechanical and continuum approaches for materials science applications
(2011) European Physical Journal Plus, 126 (10), art. no. 101, pp. 1-22. Cited 16 times.
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DOI: 10.1140/epjp/i2011-11101-2
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, D-40237, Düsseldorf, Germany;
IFW Dresden, Institute for Complex Materials, Helmholtzstr. 20, D-01069 Dresden, Germany;
Dresden University of Technology, Institute of Materials Science, D-01062 Dresden, Germany;
AICES Graduate School, RWTH Aachen, D-52056 Aachen, Germany;
Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87845, United States;
Montanuniversität Leoben, Franz-Josef-Straße 18, A-8700 Leoben, Austria;
University Bayreuth, Universitätsstrasse 30, 95440 Bayreuth, Germany
ABSTRACT: Multi-methodological approaches combining quantum-mechanical and/or atomistic simulations with continuum methods have become increasingly important when addressing multi-scale phenomena in computational materials science. A crucial aspect when applying these strategies is to carefully check, and if possible to control, a variety of intrinsic errors and their propagation through a particular multimethodological scheme. The first part of our paper critically reviews a few selected sources of errors frequently occurring in quantum-mechanical approaches to materials science and their multi-scale propagation when describing properties of multi-component and multi-phase polycrystalline metallic alloys. Our analysis is illustrated in particular on the determination of i) thermodynamic materials properties at finite temperatures and ii) integral elastic responses. The second part addresses methodological challenges emerging at interfaces between electronic structure and/or atomistic modeling on the one side and selected continuum methods, such as crystal elasticity and crystal plasticity finite element method (CEFEM and CPFEM), new fast Fourier transforms (FFT) approach, and phase-field modeling, on the other side. © Società Italiana di Fisica / Springer-Verlag 2011.
DOCUMENT TYPE: Review
SOURCE: Scopus

Zambaldi, C., Raabe, D.
Crystal plasticity modelling and experiments for deriving microstructure-property relationships in γ-TiAl based alloys
(2010) Journal of Physics: Conference Series, 240, art. no. 012140, . Cited 2 times.
https://www.scopus.com/inward/record.uri?eid=2-s2.0-78651078989&doi=10.1088%2f1742-6596%2f240%2f1%2f012140&partnerID=40&md5=11367d41e665023aafd97c195b5fdc8f

DOI: 10.1088/1742-6596/240/1/012140
AFFILIATIONS: Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: Single-crystals of γ-TiAl cannot be grown for the compositions present inside the two-phase γ/α 2-microstructures that show good mechanical properties. Therefore the single crystal constitutive behaviour of γ-TiAl was studied by nanoindentation experiments in single phase regions of these microstructures. The experiments were extensively characterized by a combined experimental approach to clarify the orientation dependent mechanical response during nanoindentation. They further were analyzed by a three-dimensional crystal plasticity finite element model that incorporated the deformation behaviour of γ-TiAl. The spatially resolved activation of competing deformation mechanisms during indentation was used to assess their relative strengths. On the length-scale of multi-grain aggregates two kinds of microstructures were investigated. The lamellar microstructure was analyzed in terms of kinematic constraints perpendicular to densely spaced lamellar boundaries which lead to pronounced plastic anisotropy. Secondly, the mechanical behaviour of massively transformed microstructures was modelled by assuming a lower degree of kinematic constraints. This resulted in less plastic anisotropy on a single grain scale and lower compatibility stresses in a 64-grain aggregate. On the macroscopic length scale, the results could possibly explain the pre-yielding of lamellar microstructures.
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Winning, M., Raabe, D.
Fast, physically-based algorithms for online calculations of texture and anisotropy during fabrication of steel sheets
(2010) Advanced Engineering Materials, 12 (12), pp. 1206-1211. Cited 1 time.
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DOI: 10.1002/adem.201000206
AFFILIATIONS: Max-Planck Institut für Eisenforschung GmbH, Düsseldorf, Germany
ABSTRACT: Because of the complex microstructures of crystalline materials exposed to commercial manufacturing processes it is up to now not possible to obtain fast and on-line simulations of crystallographic texture and anisotropy in the course of multiple deformation- and heat treatment procedures. In the present paper a hybrid approach for the on-line texture and anisotropy prediction will be developed for the fabrication of low alloyed ferritic steel sheets during cold rolling and subsequent annealing procedures. Our approach is based on two consecutive models: The first one is an artificial neuronal network (ANN) for the description of the rolling texture evolution. The second one is an analytical, Avrami-based texture component approach for the recrystallization. First results on low carbon steels will be presented.
DOCUMENT TYPE: Conference Paper
SOURCE: Scopus

Kobayashi, S., Zambaldi, C., Raabe, D.
Orientation dependence of local lattice rotations at precipitates: Example of κ-Fe3AlC carbides in a Fe3Al-based alloy
(2010) Acta Materialia, 58 (20), pp. 6672-6684. Cited 7 times.
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AFFILIATIONS: Osaka Center for Industrial Materials Research, Institute for Materials Research, Tohoku University, 1-1 Gakuen-cho, Naka-ku, Sakai, Osaka 599-8531, Japan;
Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany
ABSTRACT: Local lattice rotations and in-grain orientation gradients at κ precipitates in matrix grains with orientations near the 45° rotated cube {0 0 1} ⟨1 1 0⟩ (RC) and the γ-fiber components {1 1 1} ⟨1 1 2⟩ were investigated in a Fe3Al alloy warm-rolled to reductions of between 10% and 60%. Near-RC grains showed larger local lattice rotations at precipitates than γ-fiber grains. In RC-oriented grains the local lattice rotations about the transverse direction (TD) were dominant at low reductions, but rotations about the rolling direction (RD) also occurred at higher strains. In the γ-fiber grains the axes of the in-grain lattice rotations were scattered between TD and RD. The rotations around the particles and their orientation dependence were analyzed using 3-D crystal plasticity finite-element simulations of a spherical inclusion in a plane strain deformed matrix of different orientations, namely RC, {1 1 1} ⟨1 1 2⟩ and {1 1 1} ⟨0 1 1⟩ .
AUTHOR KEYWORDS: Deformation structure; EBSD; Iron aluminides; Texture
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AFFILIATIONS: Max-Planck-Institut für Eisenforschung, Max-Planck Str. 1, Düsseldorf 40237, Germany
ABSTRACT: Recent Bauschinger-type tests conducted on a twinning-induced plasticity (TWIP) steel highlights the important contribution of internal stresses to work hardening [1]. Along this line we present Bauschinger experiments in a Fe-22Mn wt%-0.6C wt% TWIP steel. The mechanical behavior upon load reversal shows transient and permanent softening effects. Determination of the internal stress from the magnitude of the permanent softening yields a contribution to work hardening of the order of 20%. Analysis of the transient softening, during strain reversal, indicates that internal stress is consistent with reported data on high carbon spheroidized steels.
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