RAP - Rapid Alloy Prototyping: Compositional and Thermomechanical Bulk Combinatorial Design of Alloys

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shortened version

Overview

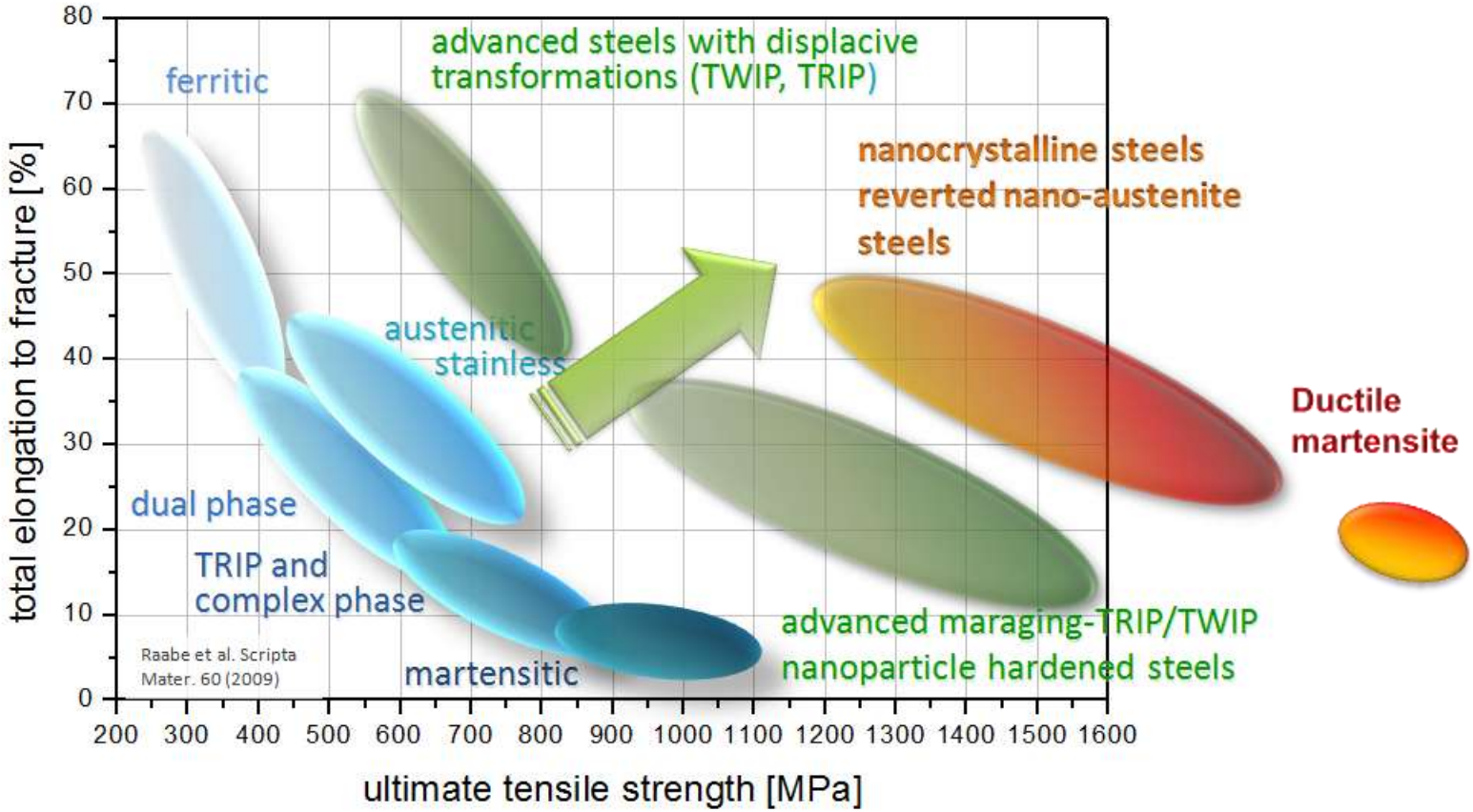
- Why designing new structural alloys?
- Go horizontal: RAP (Rapid Alloy Prototyping)
- Go vertical: Strain hardening in complex alloys: multi-mechanisms
- Conclusions

Alloy production, processing and manufacturing accounts for 46% of all EU manufacturing value and 11% of the EU's total gross domestic product.

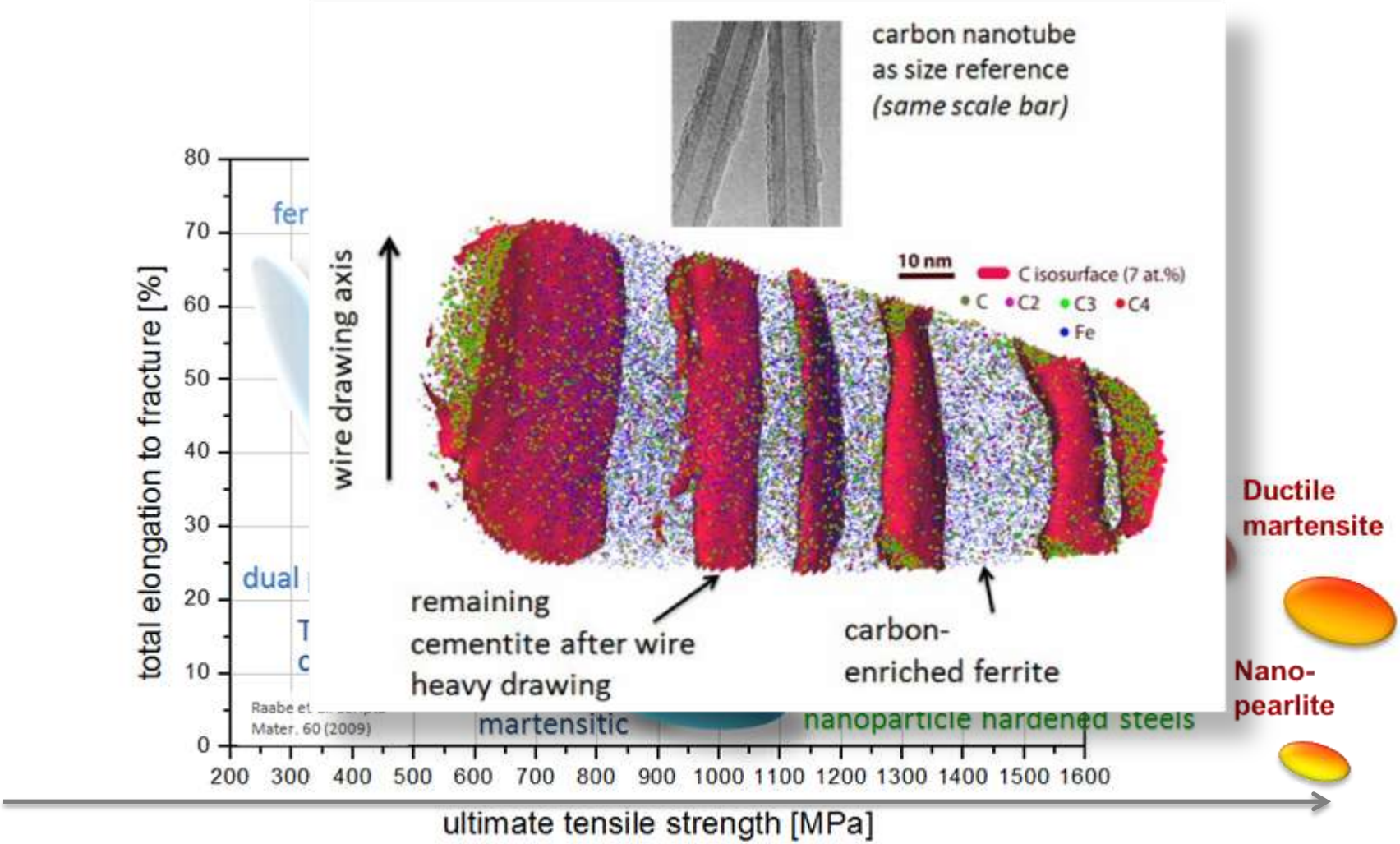
1.3 trillion € per year or 3.5 billion € per day in the EU

[World Trade Organisation; International Metalworkers' Federation]

New mechanisms and their combinations



New bulk steels: understanding the nanoscopic length scales



> 6 GPa

Overview

- Why designing new structural alloys?
- Go horizontal: RAP (Rapid Alloy Prototyping)
- Go vertical: Strain hardening in complex alloys: multi-mechanisms
- Conclusions

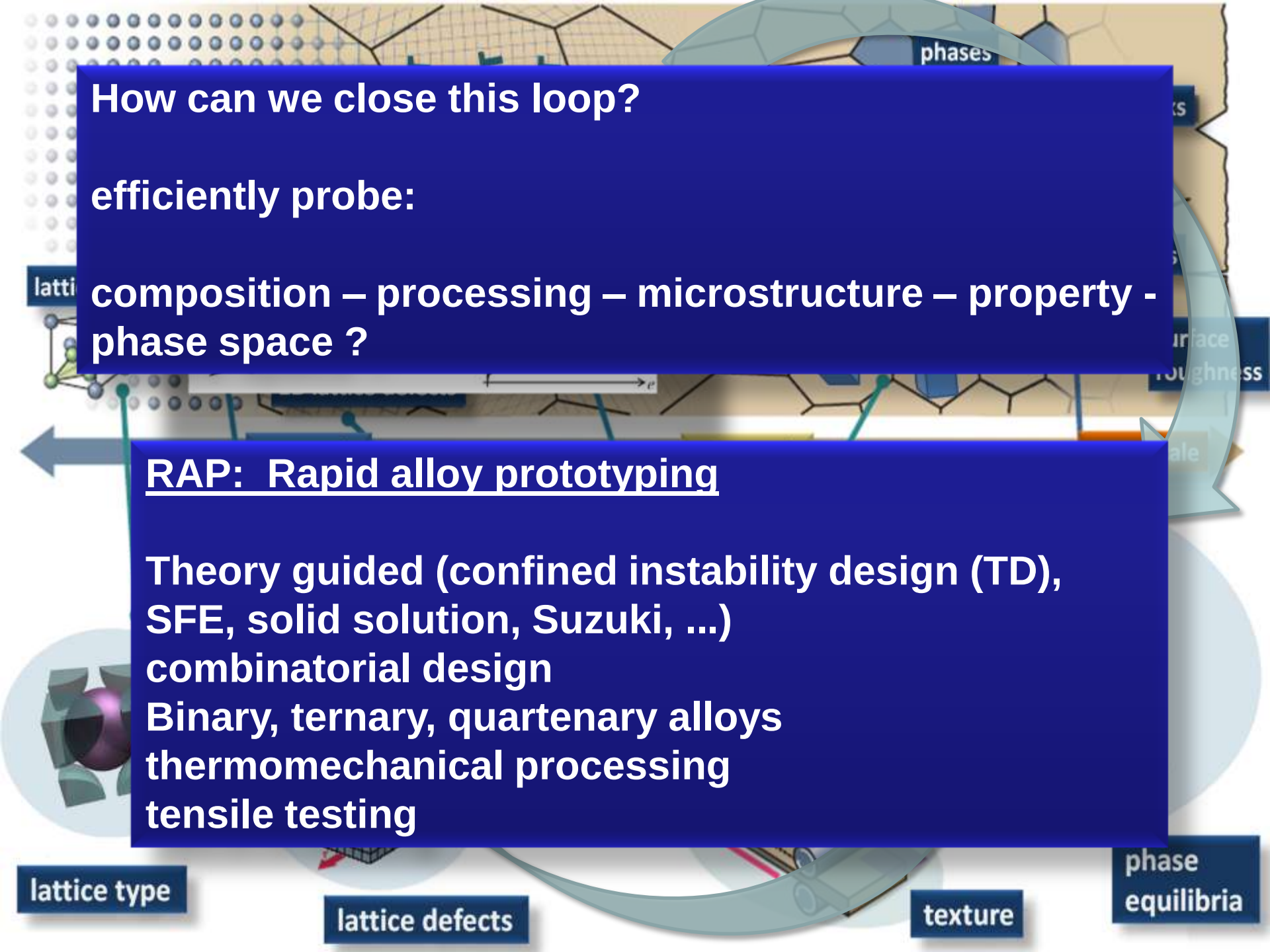
How can we close this loop?

efficiently probe:

composition – processing – microstructure – property - phase space ?

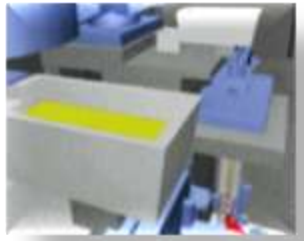
<u>RAP: Rapid alloy prototyping</u>

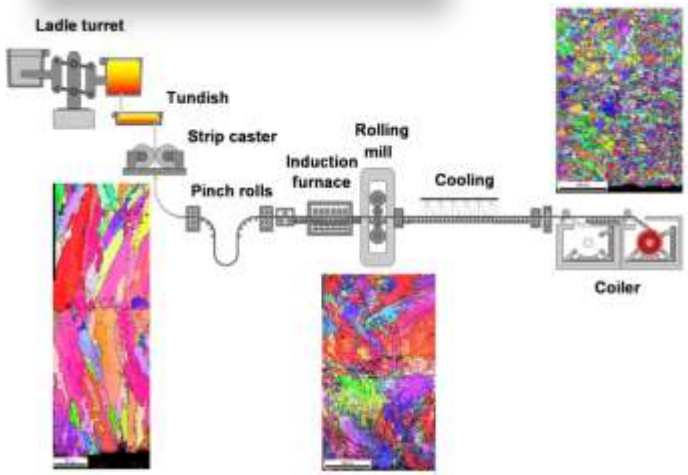
Theory guided (confined instability design (TD), SFE, solid solution, Suzuki, ...)
combinatorial design
Binary, ternary, quartenary alloys
thermomechanical processing
tensile testing



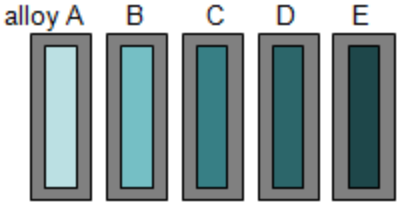
RAP: rapid alloy prototyping

Combinatorial strip casting

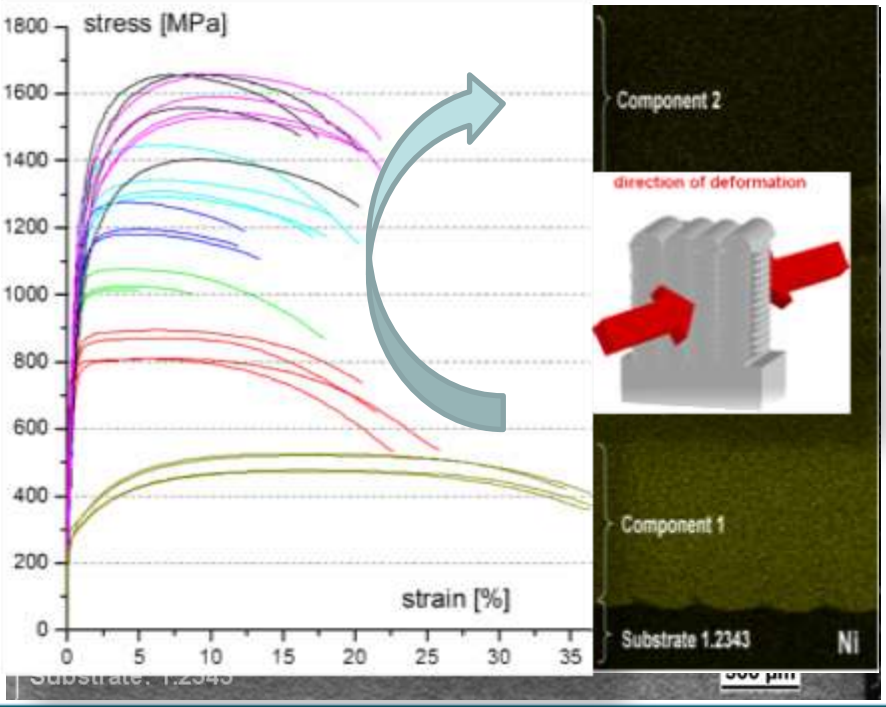




RAP: Steel-plant-in-a-box



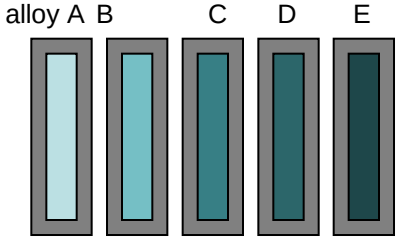
Plasma-powder synthesis



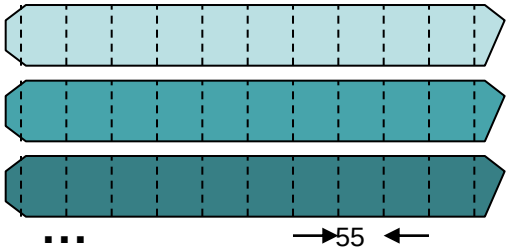
Springer and Raabe, Acta Mater. 60 (2012) 5791

Rapid alloy prototyping: ‘Steel plant in a box’

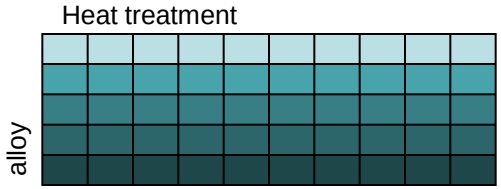
1. **Multi-ingot vacuum or inert gas inductive melting and casting**



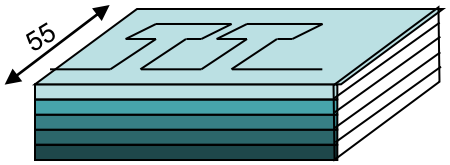
2. **Homogenization and hot rolling**



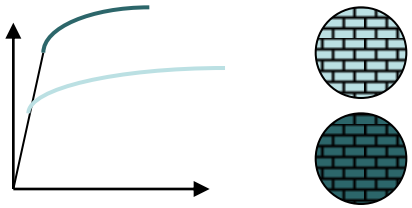
3. **Heat treatment and / or thermomechanical processing**



2. **Discharge sample preparation**



3. **Tensile testing (3 test per state)**



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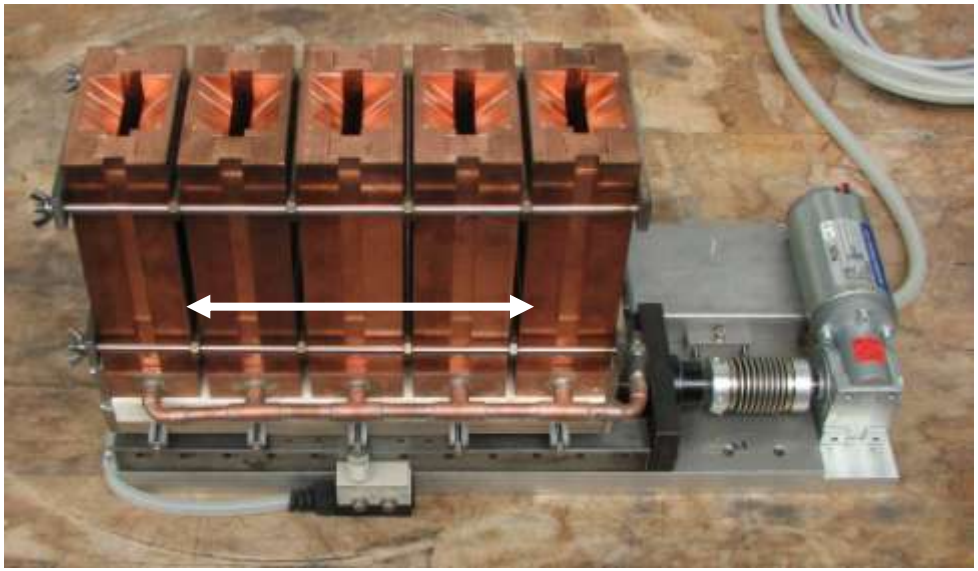
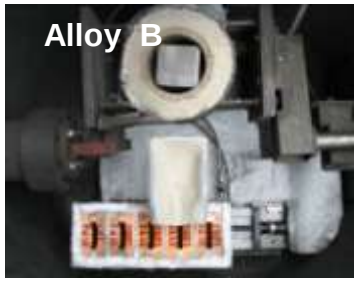
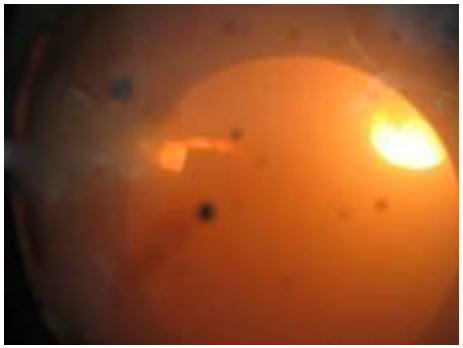
Rapid alloy prototyping: multiple ingot casting



5 Cu-moulds, 60 kW vacuum induction furnace (vacuum, Ar, air)

10 x 50 x 150 mm^3





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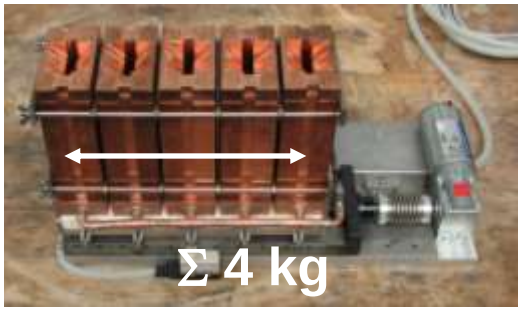
Rapid alloy prototyping: multiple ingot casting

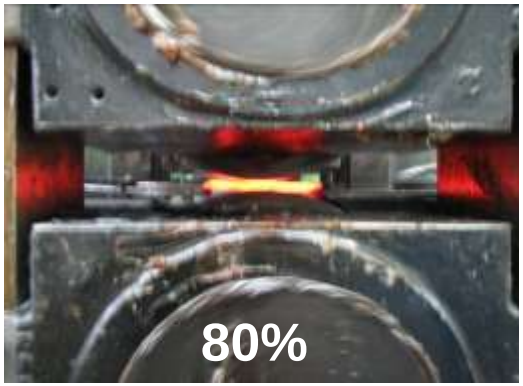
1. Multiple casting VIM

5 alloys in one step



2. Hot rolling, cutting

10 segmente per alloy



3. Heat treatments

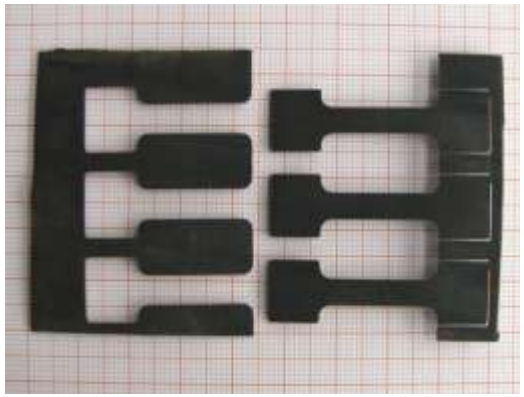
50 combinations (matrix)

4. Sample prep., tensile tests

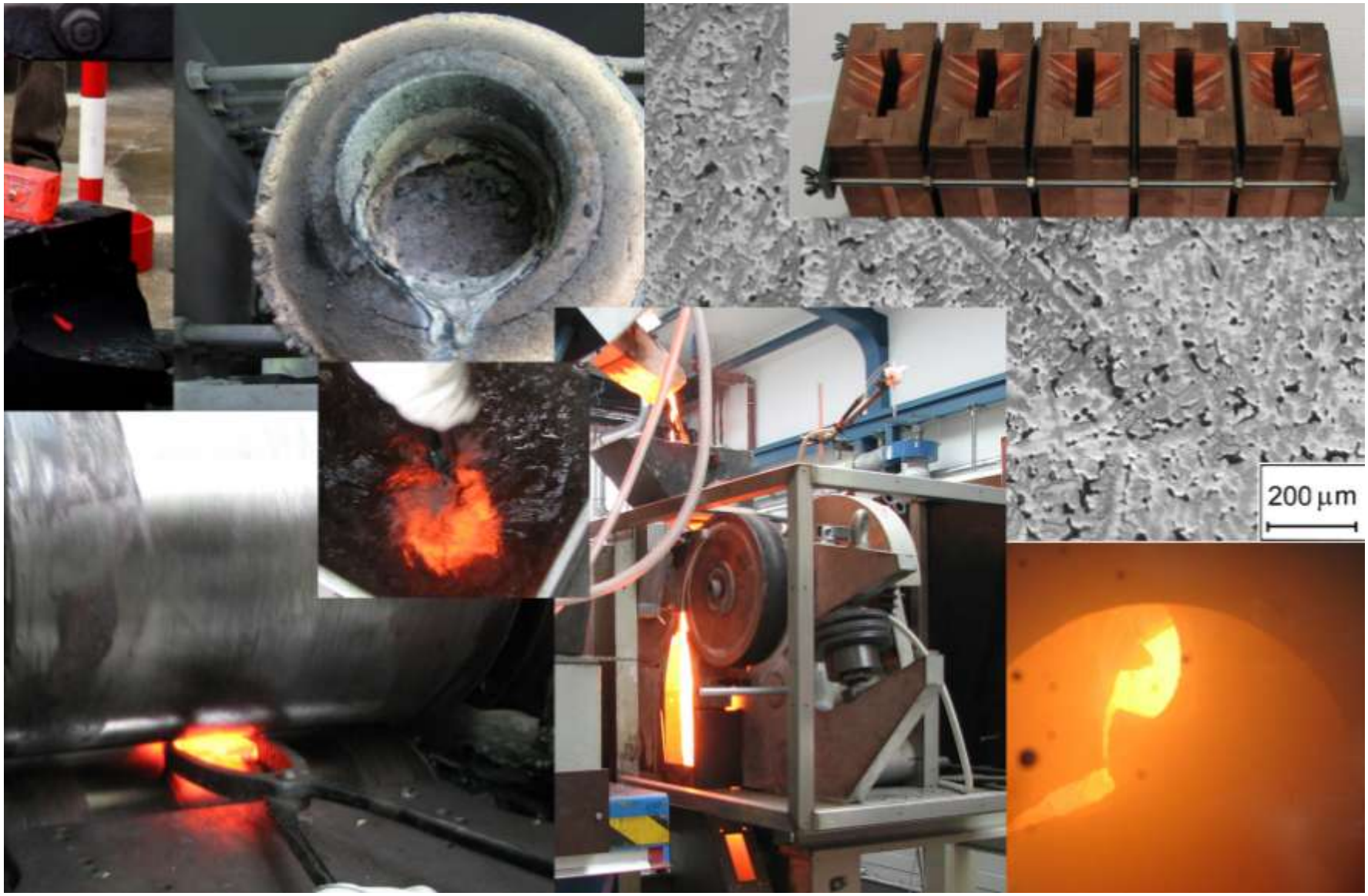
150 samples (statistics)

→ **data-management**

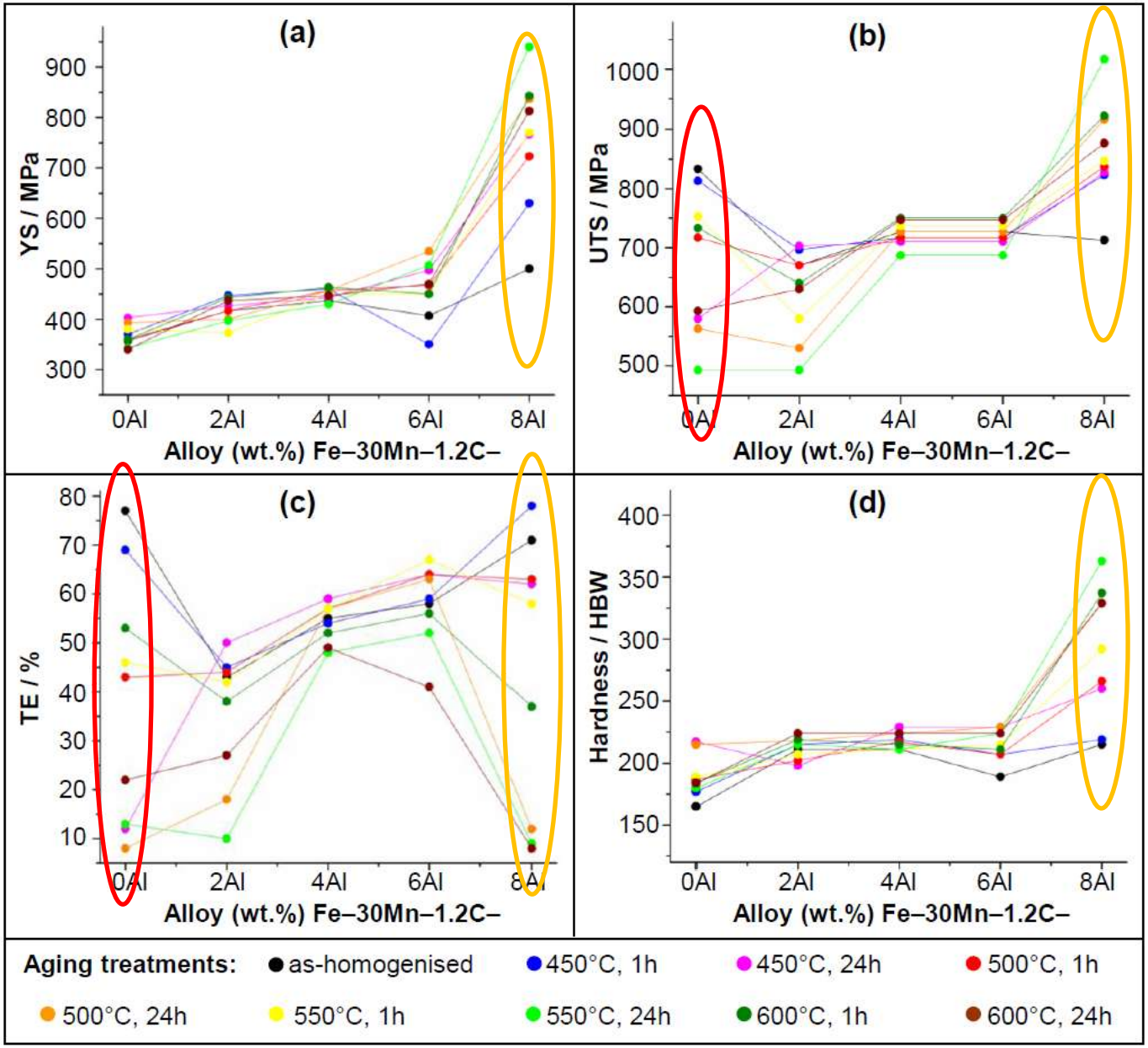
→ **standards**



Rapid alloy prototyping: multiple ingot casting



Rapid alloy prototyping: applied to TRIPLEX Fe-Mn-Al-C steels



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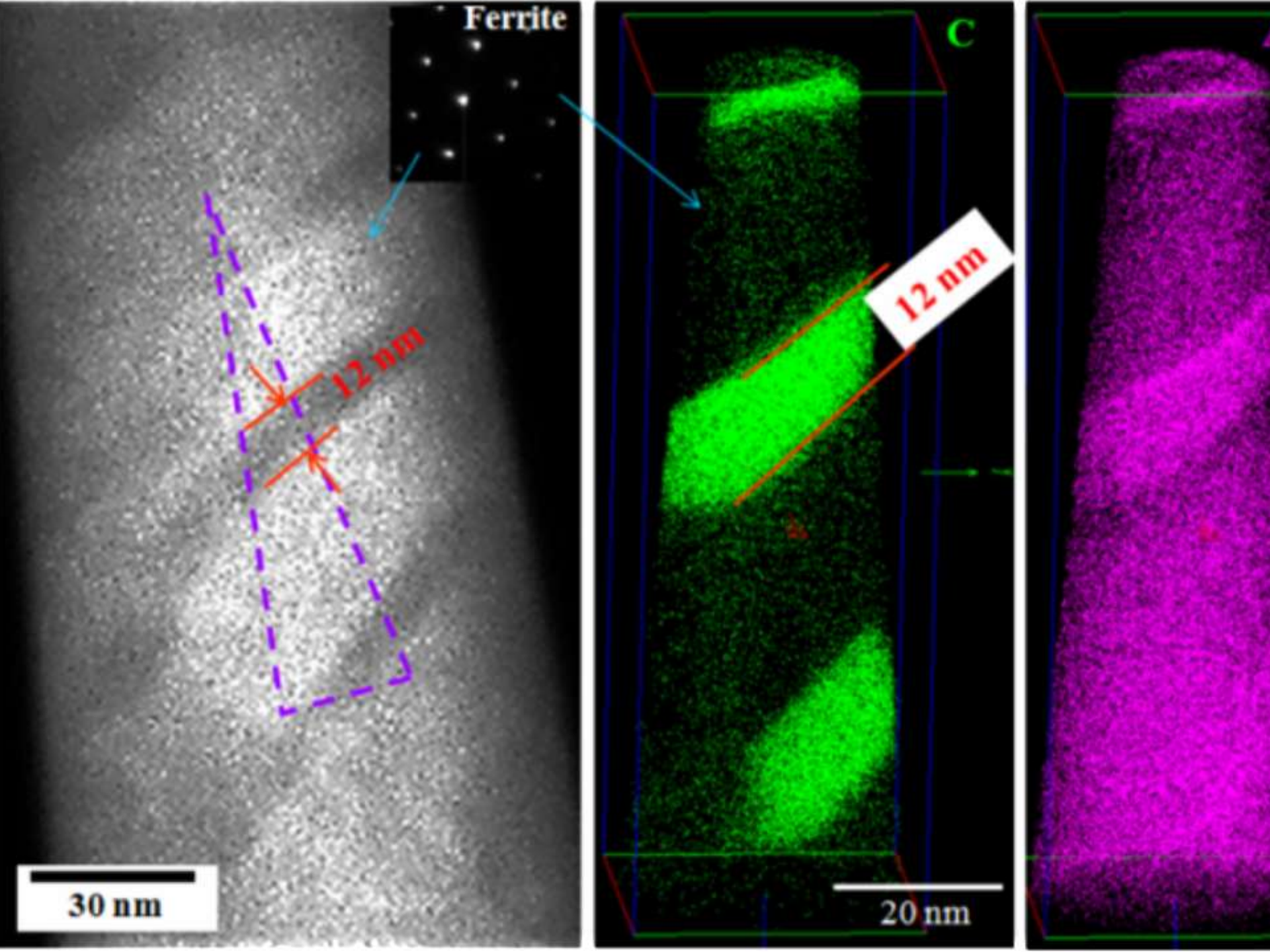
Ferrite
12 nm
30 nm
C
12 nm
20 nm

Overview

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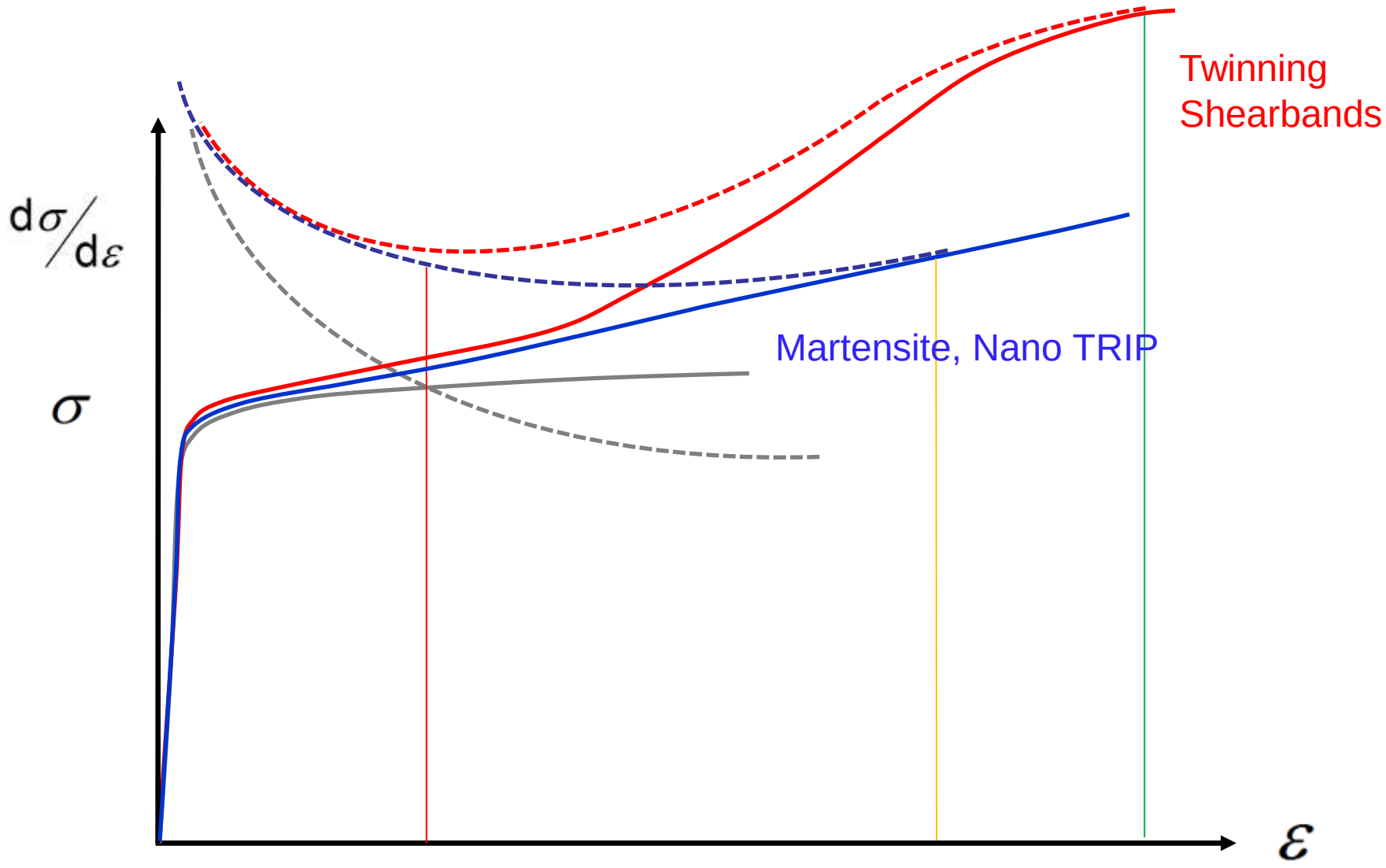
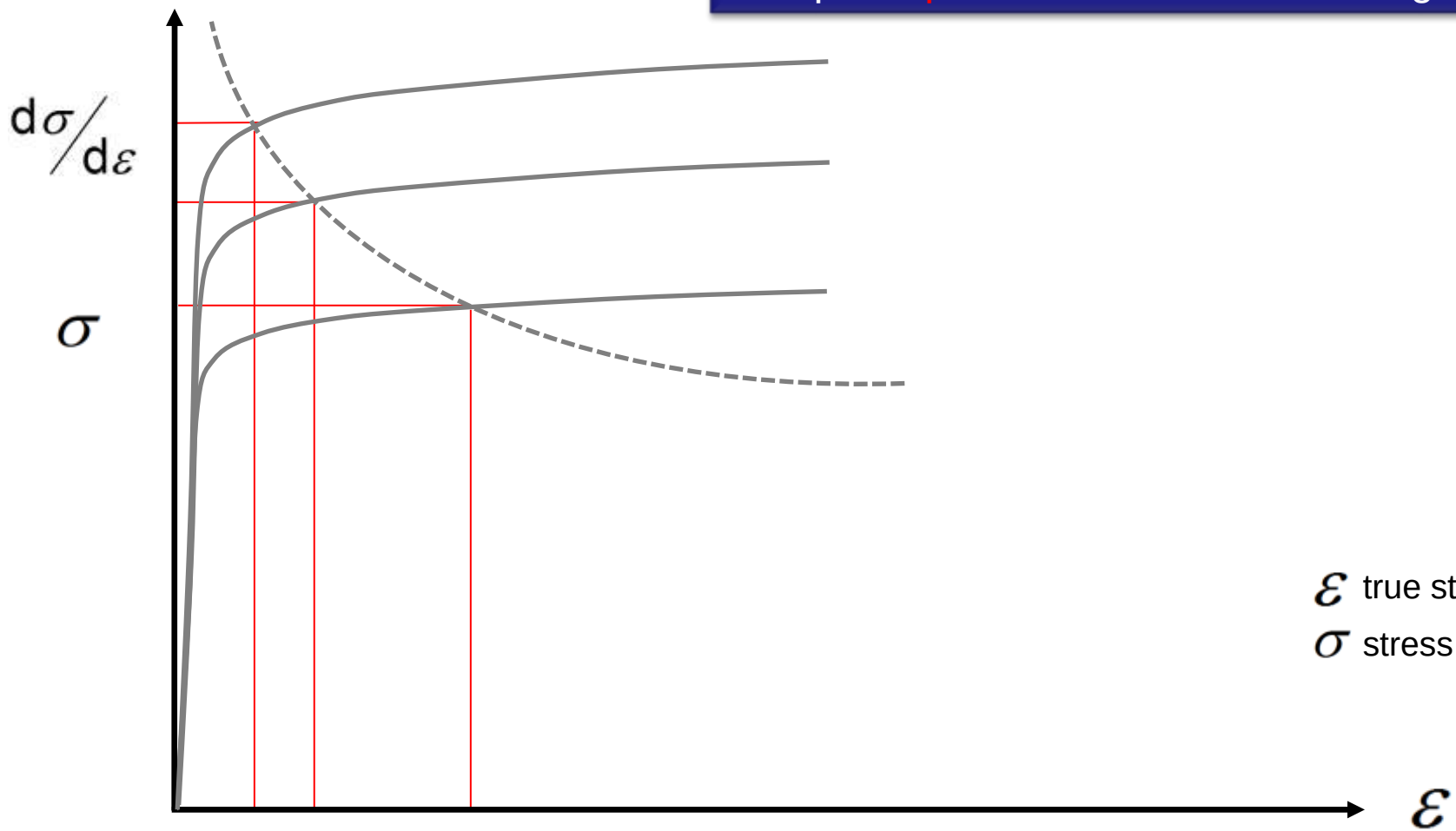
- Go horizontal: RAP (Rapid Alloy Prototyping)
- Go vertical: Strain hardening in complex alloys: multi-mechanisms
- Conclusions

Inverse strength-ductility: phenomenological analysis



Inverse strength-ductility: phenomenological analysis

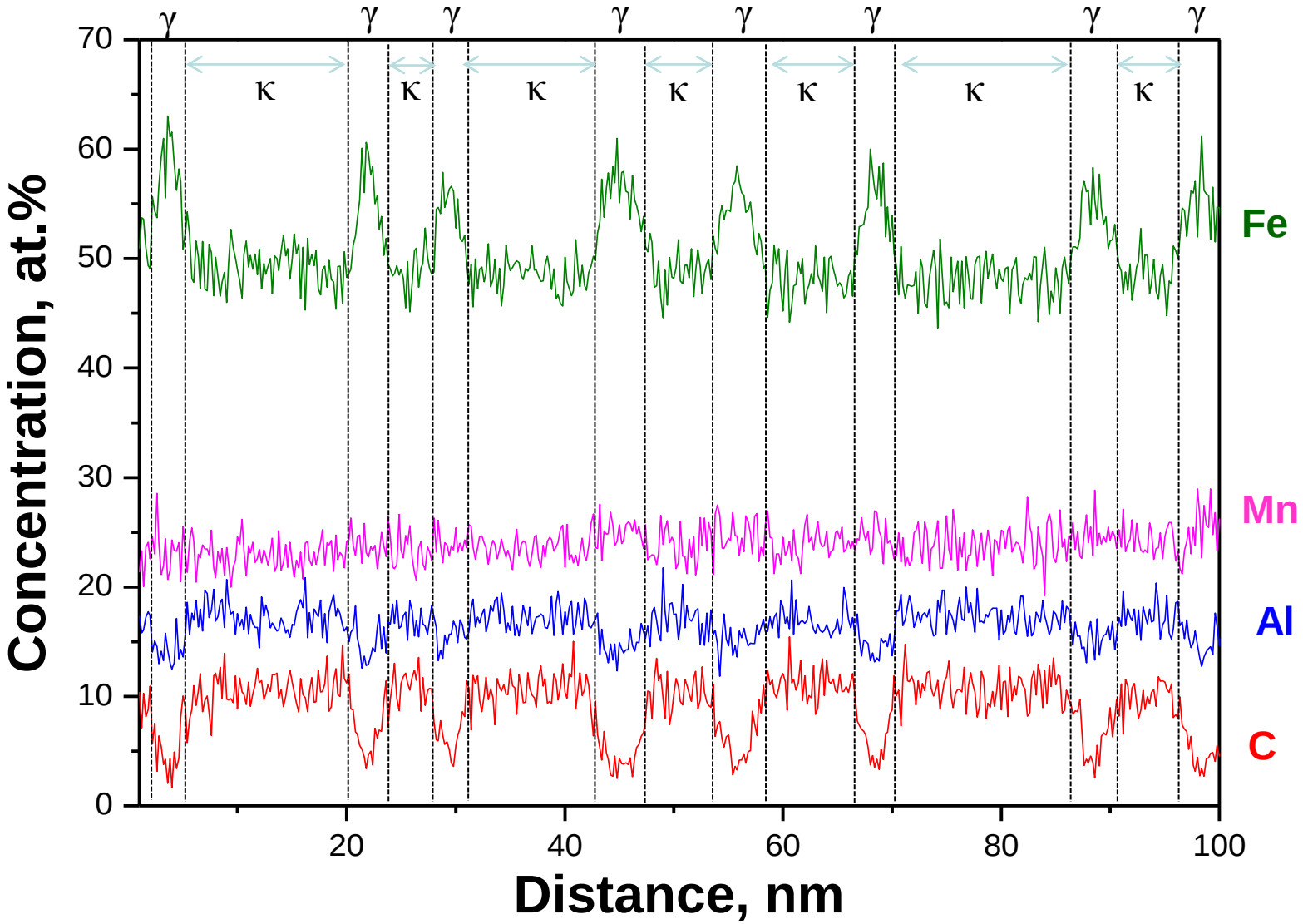
Design of ductile high strength alloys requires permanent strain hardening



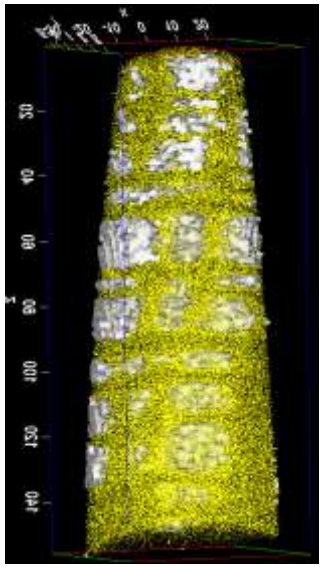
ε true strain

σ stress

Rapid alloy prototyping: applied to TRIPLEX Fe-Mn-Al-C steels



10 at% C



Mn slightly depleted inside particles and enriched in the γ matrix; κ-carbide: not exactly $(Fe,Mn)_3AlC_x$, Mn partitioned to γ matrix is more stable, and Mn-absent k-carbide is most stable

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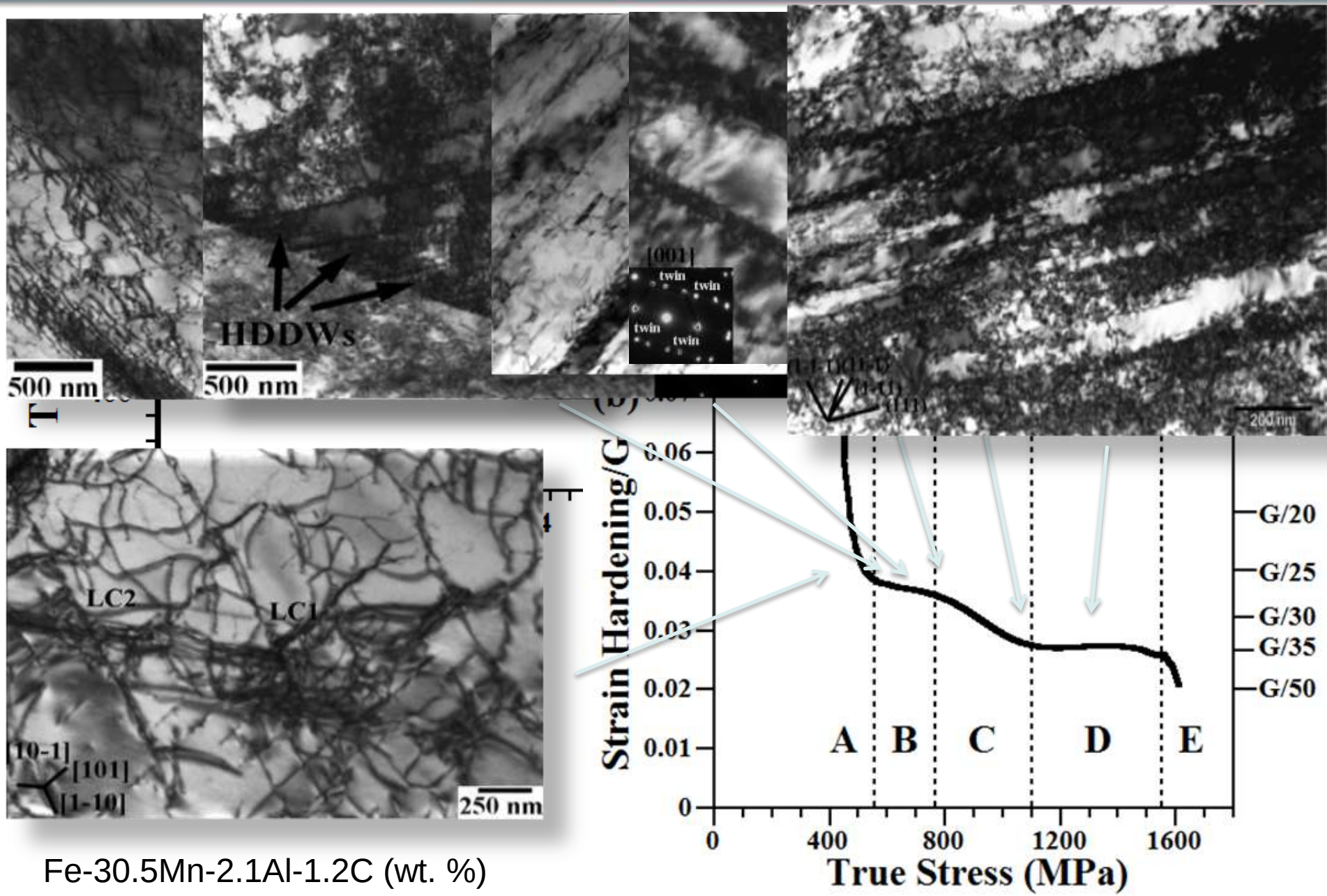
Rapid alloy prototyping: Fe-Mn-Al-C steels: not heat treated



Fe-30.5Mn-2.1Al-1.2C (wt. %)

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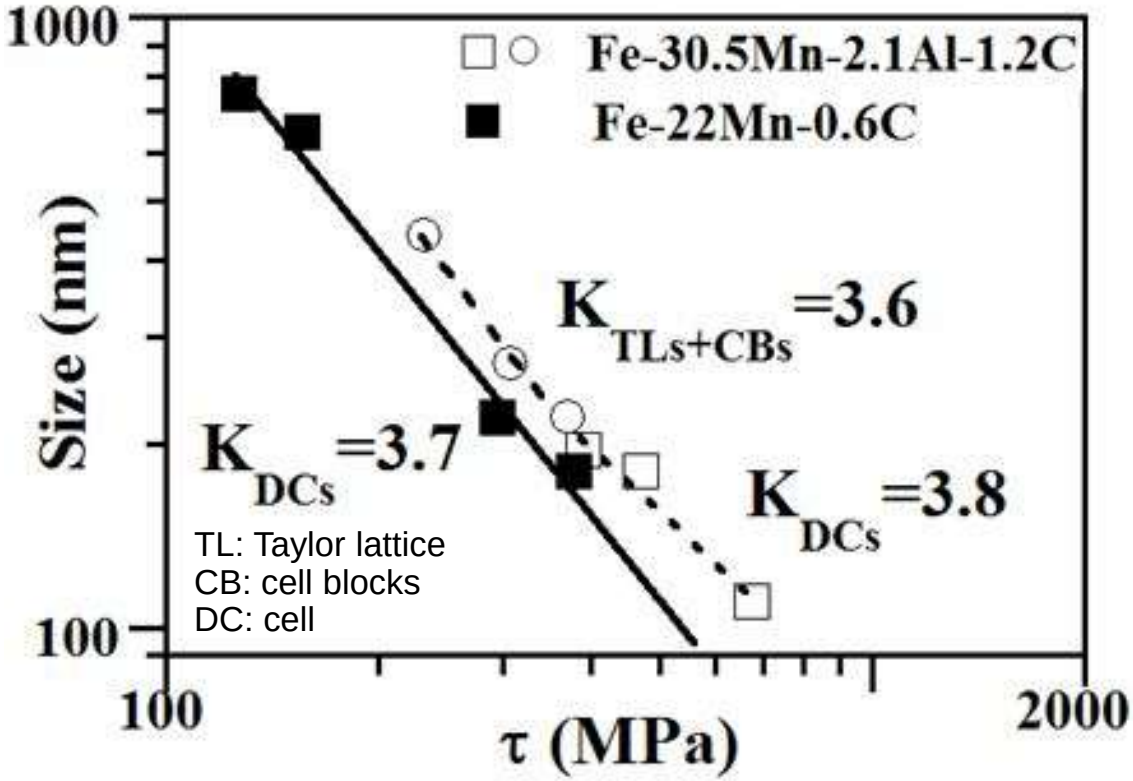
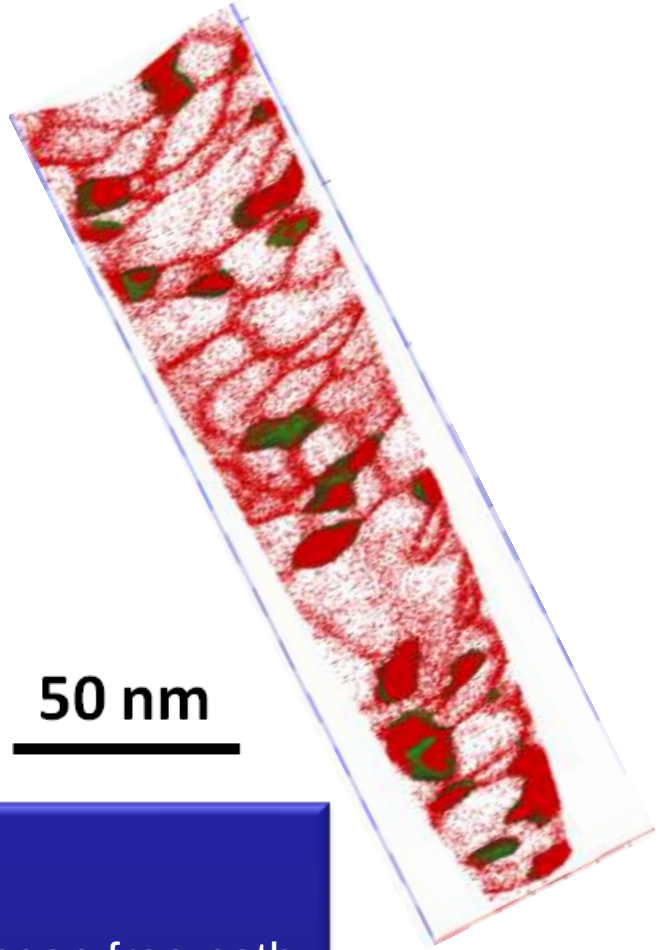
Structure-property relations





Structure-property relations:

1) Structure evolution: lattice defect population
dislocation production and mean free path
displacive carrier activation

2) Structure property: Obstacle / interaction strength

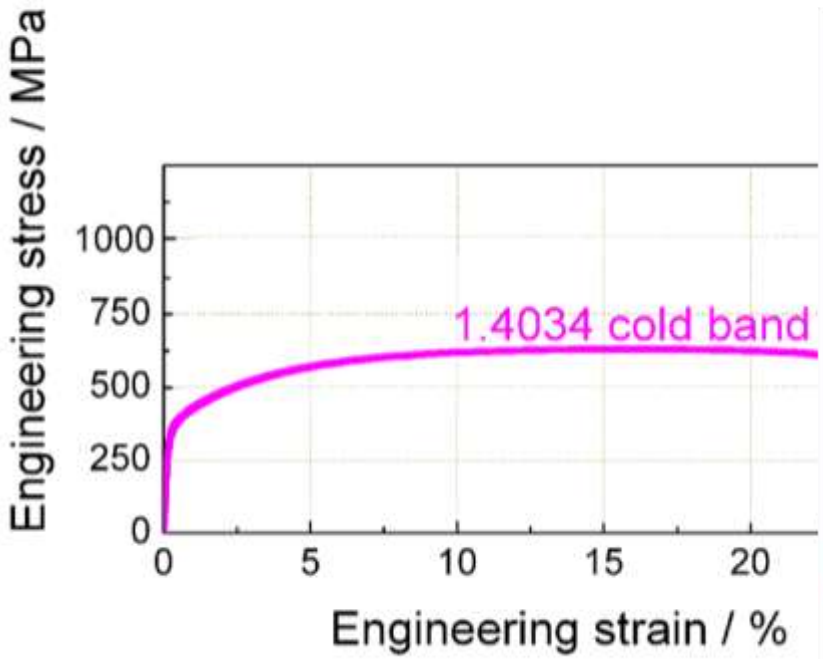
BC treatment: Full-field CPFEM, spectral solvers,homogenization

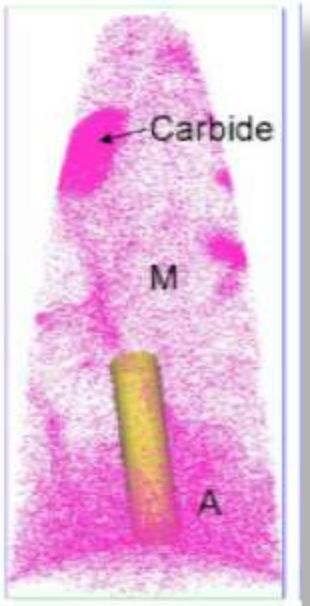
No 'true' models; reasonable models

Martensite relaxation & aging & nanoscale austenite reversion

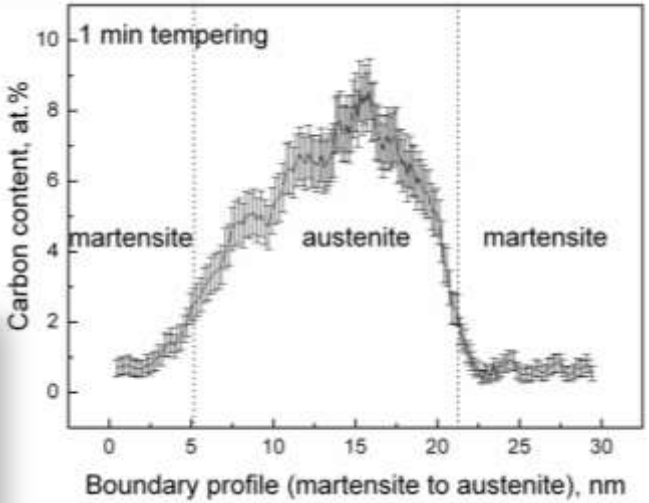
650 MPa to 2 GPa

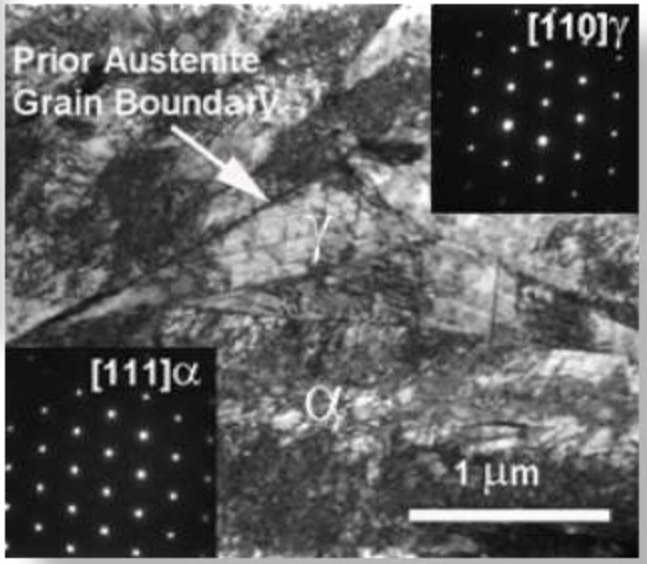
Multiple mechanisms





M: martensite; A: austenite



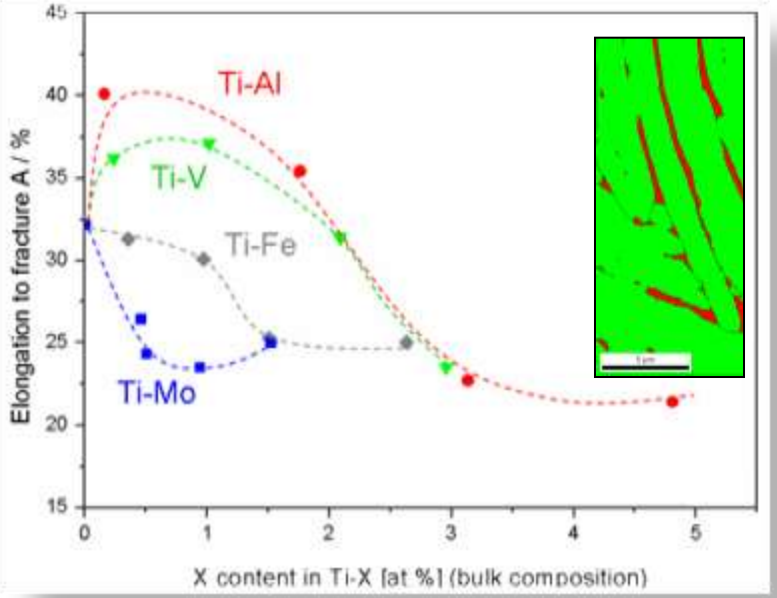


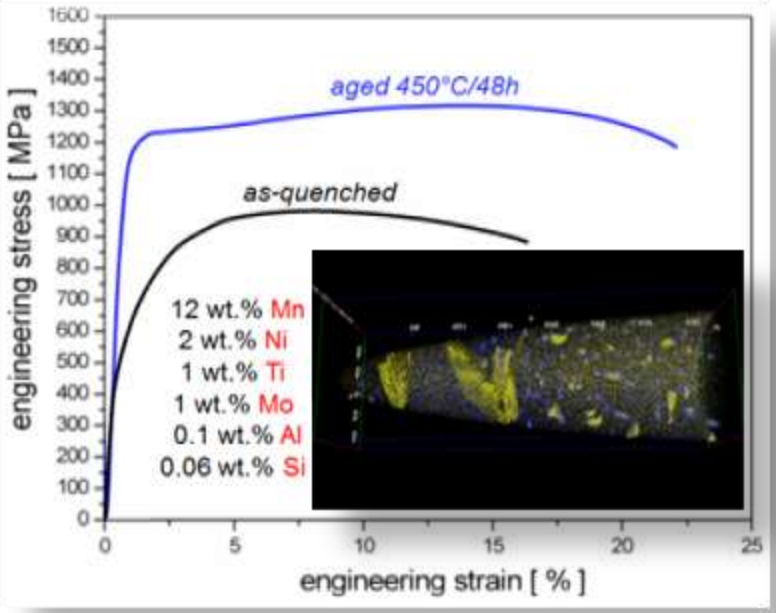
Nanocarbides, transformation GNDs, TRIP, retained austenite stabilization, dislocation decoration, nanoscale austenite reversion, nano-segregation

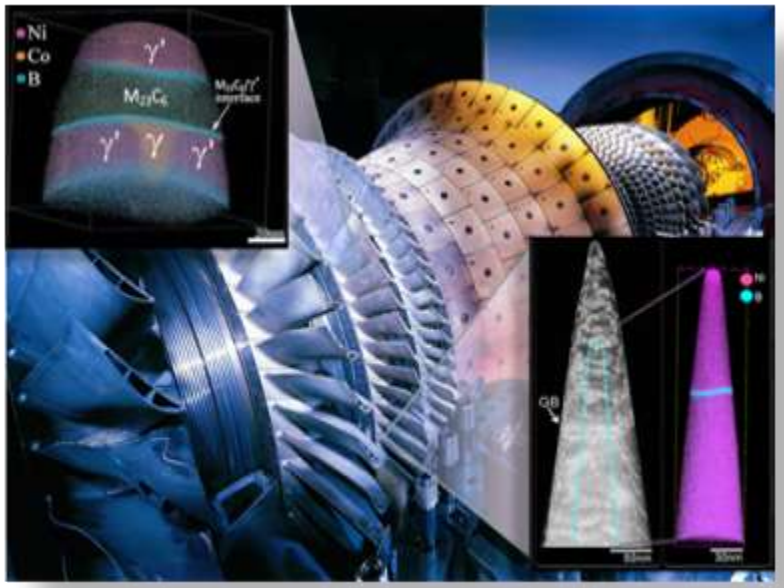
Fe-13.6Cr-0.44C (wt.%)

L. Yuan et al. Acta Mater (2012)

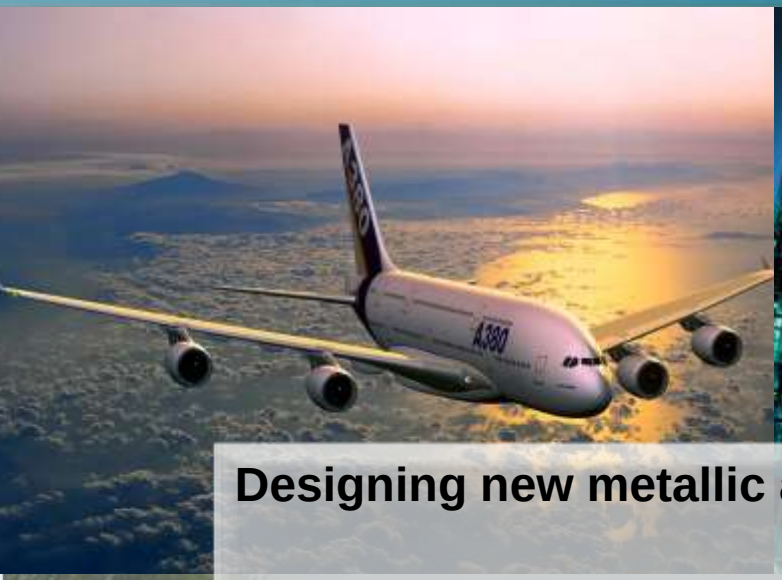
Rapid alloy prototyping: other alloy systems





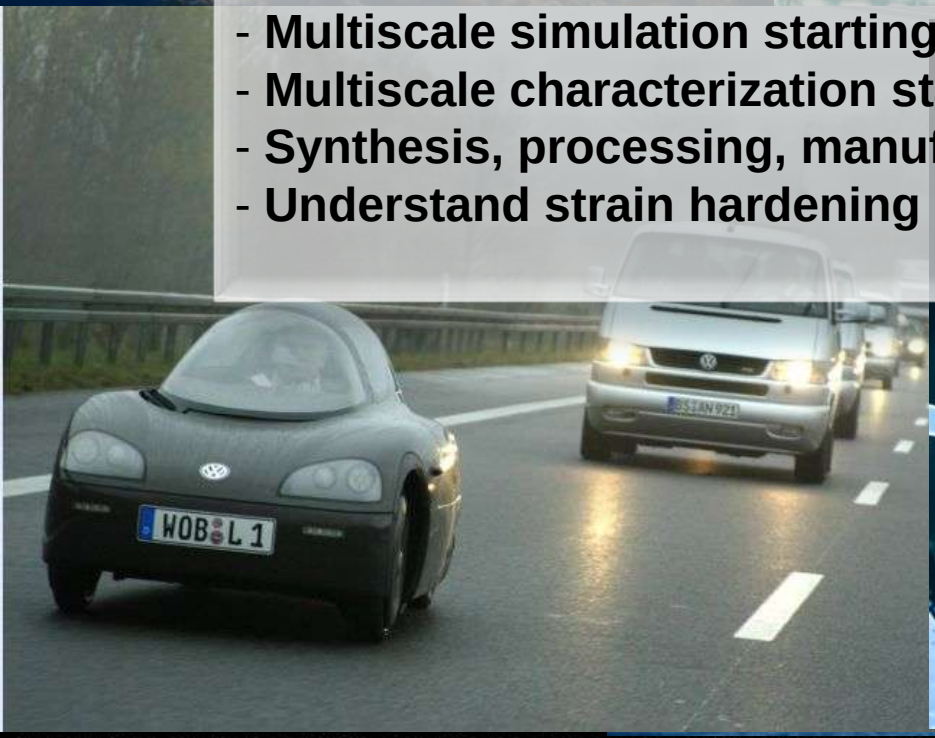


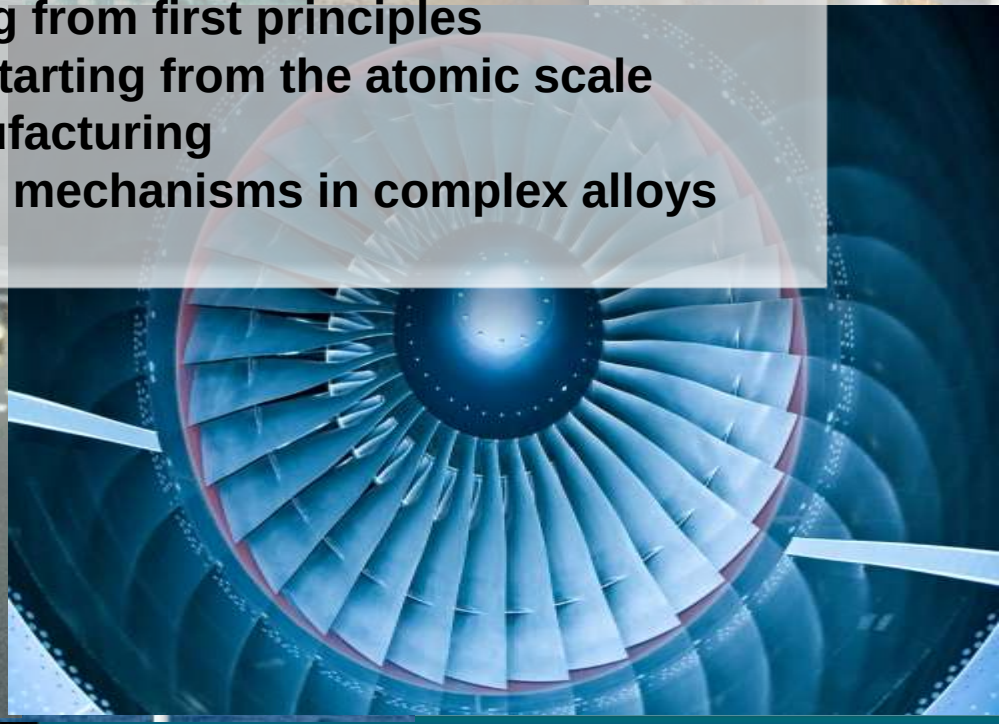
Answering societies' grand challenges with complex alloys



Designing new metallic alloys

- **Multiscale simulation starting from first principles**
- **Multiscale characterization starting from the atomic scale**
- **Synthesis, processing, manufacturing**
- **Understand strain hardening mechanisms in complex alloys**





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Rapid alloy prototyping: Compositional and thermo-mechanical high throughput bulk combinatorial design of structural materials based on the example of 30Mn–1.2C–*x*Al triplex steels

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Received 20 December 2011; received in revised form 7 May 2012; accepted 15 May 2012

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–*x*Al 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.

References

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Acta Materialia 60 (2012) 5791–5802

Acta MATERIALIA

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Multistage strain hardening through dislocation substructure and twinning in a high strength and ductile weight-reduced Fe–Mn–Al–C steel

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Received 20 May 2012; received in revised form 1 July 2012; accepted 3 July 2012
Available online 23 August 2012

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.

References

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Viewpoint Paper

Grain size effect on strain hardening in twinning-induced plasticity steels

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Available online 28 January 2012

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.

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Available online at www.sciencedirect.com

ScienceDirect

Acta Materialia 59 (2011) 6449–6462

Acta MATERIALIA

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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

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Received 11 March 2011; received in revised form 3 July 2011; accepted 4 July 2011
Available online 29 July 2011

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.