Microstructure Mechanics of Complex Materials

Introduction

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class times
Friday, 12 am – 2 pm at IMM / RWTH

Course Lecturers:
Prof. B. Svendsen, Prof. D. Raabe, Dr. H. Springer, Dr. S.-L. Wong, Dr. S. Sandlöbes, Dr. M. Diehl
<table>
<thead>
<tr>
<th>Date / Location</th>
<th>Topics</th>
<th>Lecturer</th>
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<tbody>
<tr>
<td>5. April 2019 IMM / RWTH</td>
<td>Introduction to materials micromechanics, multiscale problems in micromechanics, crystal structures and defects, relation to products and manufacturing</td>
<td>Raabe</td>
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<tr>
<td>12. April 2019 IMM / RWTH</td>
<td>Discrete and statistical dislocation dynamics, Crystal micromechanics, single crystal mechanics, yield surface, polycrystal models</td>
<td>Raabe</td>
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<td>19. April 2019 IMM / RWTH</td>
<td>No classes</td>
<td>-</td>
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<tr>
<td>26. April 2019 IMM / RWTH</td>
<td>Micromechanics of polymers and biological materials</td>
<td>Raabe</td>
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<td>3. May 2019 IMM / RWTH</td>
<td>Athermal phase transformations in micromechanics</td>
<td>Wong</td>
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<td>10. May 2019 IMM / RWTH</td>
<td>Fatigue of materials</td>
<td>Sandlöbes</td>
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<tr>
<td>17. May 2019 IMM / RWTH</td>
<td>Dislocations and micromechanics in hexagonal materials</td>
<td>Sandlöbes</td>
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<td>31. May 2019 IMM / RWTH</td>
<td>No classes</td>
<td>-</td>
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<tr>
<td>14. June 2019 IMM / RWTH</td>
<td>No classes</td>
<td>-</td>
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Further reading

- Gottstein: Physical Metallurgy
- Reed-Hill: Physical Metallurgy Principles
- Hull and Bacon: Introduction to Dislocations, Butterworth-Heinemann
- Hirth and Lothe: Theory of Dislocations


Roters, Eisenlohr, Bieler, Raabe: Crystal plasticity finite element methods: in materials science and engineering 2011, John Wiley & Sons
Answering societies' grand challenges with complex alloys

70% of all **industrial innovations** are associated with progress in **materials science and engineering**

**Complex Materials** occupy key roles (energy, transportation, health, safety, infrastructure)

Materials-related industries account for 46% of all EU manufacturing value and 11% of the EU’s total domestic product

3.5 billion € per day in the EU

World Trade Organisation

Mission: Understanding micromechanics of complex materials from first principles and the defect level upwards

Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
- Introduction to the scales
- Introduction to the engineering background
- Quantum mechanics primer
- Examples
Scientific mission: complex materials in real environments

- multiple elements, phases, defects
- interacting mechanisms (non-linearity)
- kinetic transients / local equilibrium
- history dependent (synthesis, processing)
- multiple scales (modeling, experiment)
- real environments (systems science)
- multi-functionality
Martensite: Hierarchical microstructure analysis

Integrated Computational Materials Engineering: DP steel


Understanding mechanics of complex materials down to atomic scale
Martensite: Microstructure scales
In-situ tensile testing: role of coarse lath in martensite fracture

Coarse lath

Fine lath

SEM – in-situ tensile
In-situ tensile testing: role of coarse lath in martensite fracture
Inverse strength-ductility: phenomenological analysis

\[ \frac{d\sigma}{d\varepsilon} \]

\( \sigma \) true strain

\( \sigma \) stress

\( \varepsilon \) true strain

Inverse strength-ductility relation
Inverse strength-ductility: phenomenological analysis
Inverse strength-ductility: phenomenological analysis

- Twinning Shearbands
- Martensite
- Damage tolerance

\[
\frac{d\sigma}{d\varepsilon}
\]

\[\sigma\]

\[\varepsilon\]
Inverse strength-ductility: phenomenological analysis

Design of ductile high strength alloys requires **permanent** strain hardening and **damage tolerance**

\[
\frac{d\sigma}{d\varepsilon}
\]

\[
\sigma
\]

\[
\varepsilon
\]

**true strain**

**\(\sigma\)** stress

inverse strength-ductility relation
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Ab initio-based development of new alloys
Example: 4th generation superalloys for turbine blades (SFB / TR 103)

sources GE; FAU Erlangen Nürnberg und RU Bochum
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Multiscale Modeling and Experimentation
Ab initio Methods for materials science

- Most exact known materials theory
- Combine to atomic scale experiments
- Obtain data not accessible otherwise
- Can be used at continuum scale
- Electronic rules for alloy design: add electrons rather than atoms
time-independent Schrödinger equation

\[ -\frac{\hbar^2}{2m} \nabla^2 \psi(r) + U(r)\psi(r) = E\psi(r) \]

The square of the wave function \( |\psi(r)|^2 \) at position \( r = (x,y,z) \) is a measure of the probability (Aufenthaltswahrscheinlichkeit).

\[ \sum_i \frac{1}{m_i} \nabla_i^2 + U(r_i) \psi(r_i) = E \psi(r_i) \]

many particles
i Electrons: Mass $m_e$; Charge $q_e = -e$; Coordinates $r_{ei}$

j Cores: Mass $m_n$; Charge $q_n = ze$; Coordinates $r_{nj}$

\[
\left(-\frac{\hbar}{2m_e} \sum_i \nabla_i^2 - \frac{\hbar}{2m_n} \sum_j \nabla_j^2 + \sum_{i_1,i_2 \neq i} \frac{e^2}{4\pi\varepsilon_0 |r_{e_{i_1}} - r_{e_{i_2}}|} + \sum_{j_1,j_2 \neq j} \frac{Z_{j_1}Z_{j_2}e^2}{4\pi\varepsilon_0 |r_{n_{j_1}} - r_{n_{j_2}}|} + \sum_{i,j} \frac{Z_je^2}{4\pi\varepsilon_0 |r_{e_i} - r_{n_j}|} \right) \psi(r_{e_i}, r_{n_j}) = E \psi(r_{e_i}, r_{n_j})
\]
Decoupling of cores and electrons

\[ \psi(\mathbf{r}_e, \mathbf{r}_n) = \varphi(\mathbf{r}_e) \phi(\mathbf{r}_n) \]

Electrons

\[
\left( -\frac{\hbar}{2m_e} \sum_i \nabla_i^2 + \sum_{i_1,i_2 \neq i} \frac{e^2}{4\pi \varepsilon_0 |r_{e_{i_1}} - r_{e_{i_2}}|} + \sum_{i,j} \frac{z_j e^2}{4\pi \varepsilon_0 |r_{e_i} - r_{n_j}|} \right) \varphi(r_{e_i}) = E \varphi(r_{e_i})
\]

Atom cores

\[
\left( -\frac{\hbar}{2m_n} \sum_j \nabla_j^2 + \sum_{j_1,j_2 \neq j} \frac{z_{j_1} z_{j_2} e^2}{4\pi \varepsilon_0 |r_{n_{j_1}} - r_{n_{j_2}}|} + \sum_{i,j} \frac{z_j e^2}{4\pi \varepsilon_0 |r_{e_i} - r_{n_j}|} \right) \phi(r_{n_j}) = E \phi(r_{n_j})
\]
Atom Probe: atomic species
Some crystallographic features
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Interdepartmental research: High & Medium Entropy Alloys – from ab initio thermodynamics to properties
Interdepartmental collaboration example

Interdepartmental research: High & Medium Entropy Alloys – from ab initio thermodynamics to properties


Z. Li et al. Nature 2016
Spannungs-Abschattung (Stress shielding)
Elastische Fehlpassung:
Knochenuflösung, Abrasion, Entzündung
ab-initio Simulation of elastic stiffness

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Construct binary alloys in the hexagonal phase

Ti hcp phase

15/1 Ti:X ratio

14/2 Ti:X ratio

Ti atoms

substituent X
Construct binary alloys in the cubic phase

Ti bcc phase

15/1 Ti:X ratio

14/2 Ti:X ratio

Ti atoms

substituent X
Ab initio alloy design: Elastic properties: Ti-Nb system

Young’s modulus surface plots

$A_z = 2 \frac{C_{44}}{(C_{11} - C_{12})}$

- Pure Nb: $A_z = 0.5027$
- Ti - 35 Nb - 7 Zr - 5 Ta: 59.9 GPa (elastic isotropic)
- Ti: 115 GPa

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