Microstructure Mechanics
Crystal Mechanics
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RWTH Class on Microstructure Mechanics 2016
<table>
<thead>
<tr>
<th>Date / Location</th>
<th>Topics</th>
<th>Lecturer</th>
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<tr>
<td>15. April 2016 IMM / RWTH</td>
<td>Introduction to materials micromechanics, multiscale problems in micromechanics, case studies, crystal structures and defects, relation to products and manufacturing</td>
<td>Raabe</td>
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<tr>
<td>22. April 2016 IMM / RWTH</td>
<td>Crystal structures, dislocation statics, crystal dislocations, dislocation dynamics</td>
<td>Raabe</td>
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<td>29. April 2016 IMM / RWTH</td>
<td>Dislocations, crystalline anisotropy and crystal mechanics in hexagonal metals</td>
<td>Sandlöbes</td>
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<td>6. May 2016 IMM / RWTH</td>
<td>No classes</td>
<td>-</td>
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<tr>
<td>13. May 2016 IMM / RWTH</td>
<td>Fracture mechanics, Introduction to FEM</td>
<td>Shanthraj</td>
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<td>20. May 2016 IMM / RWTH</td>
<td>Athermal phase transformations in micromechanics</td>
<td>Wong</td>
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<td>27. May 2016 IMM / RWTH</td>
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<td>3. June 2016 IMM / RWTH</td>
<td>Crystal micromechanics, single crystal mechanics, yield surface mechanics, polycrystal models, Taylor model, Integrated micromechanical experimentation and simulation for complex alloys, hydrogen embrittlement</td>
<td>Raabe</td>
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<tr>
<td>17. June 2016 IMM / RWTH, 12:15</td>
<td>Applied micromechanics: multiphase and composite material design</td>
<td>Springer</td>
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- Single crystal yield surface
- Empirical yield surface
- Taylor model for the mechanics of polycrystals
- Examples
Single crystal plasticity: constructing the yield surface

- Yield criterion for single slip:
  \[ \sigma_{ij} b_i n_j = \tau_{\text{crss}} \]
- In 2D this becomes (\(\sigma_1 = \sigma_{11}\)):
  \[ \sigma_{11} b_1 n_1 + \sigma_{22} b_2 n_2 = \tau_{\text{crss}} \]
What is the straining direction?
The strain increment is given by:
\[ d\varepsilon = \sum_s d\gamma^{(s)} b^{(s)} n^{(s)} \]

2D case:
\[ d\varepsilon_1 = d\gamma b_1 n_1; \quad d\varepsilon_2 = d\gamma b_2 n_2 \]
vector perpendicular to the line for yield
straining direction in stress space

*normality rule* for crystallographic slip

Any given stress state can in a crystal in large-strain elasto-plasticity act only in the form of shear (except hydrostatic effects)
Single crystal plasticity: constructing the yield surface

slip system $s$

$n_i^s, b_i^s$

orientation factor for $s$

$m_{ij}^s = n_i^s b_j^s$

symmetric part

$m_{ij}^{sym,s} = \frac{1}{2} \left( n_i^s b_j^s + n_j^s b_i^s \right)$

rotate crystal into sample

$m_{kl}^s = a_{ki}^c n_i^s a_{lj}^c b_j^s$

symmetric part

$m_{kl}^{sym,s} = \frac{1}{2} \left( a_{ki}^c n_i^s a_{lj}^c b_j^s + a_{lj}^c n_j^s a_{ki}^c b_i^s \right)$

yield surface (active systems)

$m_{kl}^{sym,s=aktiv} \sigma_{kl} = \sigma_{aufg}^s = \tau_{krit,(+)}^s$

yield surface (non-active systems)

$m_{kl}^{sym,s=inaktiv} \sigma_{kl} = \sigma_{aufg}^s < \tau_{krit,(\pm)}^s$
Cube texture component:
(001)[100]
Active slip system:

\[ \tau^\alpha = \tau_{\text{crit}} \]

\[ \tau^\alpha \approx T_e \cdot S_0^\alpha \]

with \[ S_0^\alpha = m_0^\alpha \otimes n_0^\alpha \]

bcc 48 slip systems
orientation \{001\}<100>

12 x \{110\}<111>

12 x \{112\}<111>

24 x \{123\}<111>
Single crystal plasticity: constructing the yield surface

FCC, BCC
12 systems section

BCC
24 systems section

BCC
48 systems section

yield surface, bcc

single crystal, bcc, (001)[100]
Macroscopic – empirical yield criteria

Yield criterion: determine the critical stress required to cause permanent deformation

Many different macroscopic yield criteria

\( \sigma_{ij} \) stress acting on a solid
\( \sigma_1, \sigma_2, \sigma_3 \) principal values of stress tensor
\( Y \) yield stress of the material in uniaxial tension

\[
(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 = \text{constant}
\]

\[
(\sigma_1 - \sigma_3) = Y \\
(\sigma_1 > \sigma_2 > \sigma_3)
\]
Macroscopic yield criteria

Yield criterion: determine the critical stress required to cause permanent deformation

Many different macroscopic yield criteria

\( \sigma_{ij} \) stress acting on a solid
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\[
(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 = \text{constant}
\]

\[
(\sigma_1 - \sigma_3) = Y \\
(\sigma_1 > \sigma_2 > \sigma_3)
\]
Macroscopic yield criteria

\[ \sigma_1 = \sigma_2 = \sigma_3 \]

Hydrostatic Axis

\[ \pi\text{-plane (Deviatoric Plane)} \]

\[ \sigma_1 + \sigma_2 + \sigma_3 = 0 \]
- How does that work for bimaterials?

- Two extreme cases:
  - iso-strain (Taylor)
  - iso-stress (Schmid)
Iso-stress and iso-strain: general approach

Isostrain
\[ \varepsilon = \varepsilon_s = \varepsilon_d \]
\[ \sigma = \sigma_s + \sigma_d \]
Displacement continuity across layers

Isostress
\[ \varepsilon = \varepsilon_s + \varepsilon_d \]
\[ \sigma = \sigma_s = \sigma_d \]
Stress continuity across layers
Iso-stress and iso-strain: Elastic approach: composite stiffness

Bounding Case - Isostrain

\[ \varepsilon_1 = \varepsilon_2 = \varepsilon_{\text{tot}} \]
\[ \sigma_1 = E_1 \varepsilon_1 = E_1 \varepsilon_{\text{tot}} \quad ; \quad \sigma_2 = E_2 \varepsilon_2 = E_2 \varepsilon_{\text{tot}} \]
\[ P_1 = A_1 \sigma_1 = A_1 E_1 \varepsilon_{\text{tot}} \quad ; \quad P_2 = A_2 \sigma_2 = A_2 E_2 \varepsilon_{\text{tot}} \]
\[ P_{\text{tot}} = P_1 + P_2 = \varepsilon_{\text{tot}} (A_1 E_1 + A_2 E_2) \]
\[ \sigma_{\text{tot}} = \frac{P_{\text{tot}}}{A_1 + A_2} = \varepsilon_{\text{tot}} \left( \frac{A_1}{A_1 + A_2} E_1 + \frac{A_2}{A_1 + A_2} E_2 \right) \]
\[ \sigma_{\text{tot}} = (f_1 E_1 + f_2 E_2) \varepsilon_{\text{tot}} \]

\[ E_{\text{tot}} = f_1 E_1 + f_2 E_2 \]

P_1, P_2 are the loads on 1 and 2.
f_1, f_2 are the volume fractions of 1 and 2.

Bounding Case - Isostress

\[ \sigma_1 = \sigma_2 = \sigma_{\text{tot}} \]
\[ \sigma_1 = E_1 \varepsilon_1 \quad ; \quad \sigma_2 = E_2 \varepsilon_2 \]
\[ \varepsilon_{\text{tot}} = f_1 \varepsilon_1 + f_2 \varepsilon_2 = f_1 \frac{\sigma_{\text{tot}}}{E_1} + f_2 \frac{\sigma_{\text{tot}}}{E_2} \]
\[ E = \frac{\sigma_{\text{tot}}}{\varepsilon_{\text{tot}}} = \frac{1}{f_1 \frac{\sigma_{\text{tot}}}{E_1} + f_2 \frac{\sigma_{\text{tot}}}{E_2}} = \frac{E_1 E_2}{f_1 E_1 + f_2 E_2} \]
Iso-stress and iso-strain

- iso-strain (Taylor-model)

- iso-stress (Sachs-model)
Sachs Model (previous lecture on single crystal):

- All grains with aggregate or polycrystal experience the same state of stress;
- Equilibrium condition across the grain boundaries satisfied;
- Compatibility conditions between the grains violated, thus, finite strains will lead to gaps and overlaps between grains;
- Generally most successful for single crystal deformation with stress boundary conditions on each grain.

Taylor Model (this lecture):

- All single-crystal grains within the aggregate experience the same state of deformation (strain);
- Equilibrium condition across the grain boundaries violated, because the vertex stress states required to activate multiple slip in each grain vary from grain to grain;
- Compatibility conditions between the grains satisfied;
- Generally most successful for polycrystals with strain boundary conditions on each grain.
Polycrystal model

- Taylor model for the mechanics of polycrystals
\[ \varepsilon_{ij} = \frac{1}{2} \sum_{s=1}^{5} \left( n_i^s b_j^s + n_j^s b_i^s \right) \gamma^s \]
The Taylor Model

\[ \varepsilon_{ij} = \frac{1}{2} \sum_{s=1}^{5} \left( n_i^s b_j^s + n_j^s b_i^s \right) \gamma_s \]

plastic spin from polar decomposition

\[ \dot{\omega}_{ij}^K = W_{ij}^K = \frac{1}{2} \left( \dot{u}_{i,j}^K - \dot{u}_{j,i}^K \right) = \sum_{s=1}^{N} m_{ij}^{\text{asym},s} \dot{\gamma}_s \]
The Taylor Model
External Stress

Increasing strain

External Strain

Small arrows indicate variable stress state in each grain

Small arrows indicate identical stress state in each grain

Multiple slip (with 5 or more systems) in each grain satisfies the externally imposed strain, $D$

Each grain deforms according to which single slip system is active
The Taylor Model – comparison to Sachs model

\[
\begin{bmatrix}
  D_2 \\
  D_3 \\
  D_4 \\
  D_5 \\
  D_6
\end{bmatrix} = 
\begin{bmatrix}
  m^{(1)}_{22} & m^{(2)}_{22} & m^{(3)}_{22} & m^{(4)}_{22} & m^{(5)}_{22} \\
  m^{(1)}_{33} & m^{(2)}_{33} & m^{(3)}_{33} & m^{(4)}_{33} & m^{(5)}_{33} \\
  (m^{(1)}_{23} + m^{(1)}_{32}) & (m^{(2)}_{23} + m^{(2)}_{32}) & (m^{(3)}_{23} + m^{(3)}_{32}) & (m^{(4)}_{23} + m^{(4)}_{32}) & (m^{(5)}_{23} + m^{(5)}_{32}) \\
  (m^{(1)}_{13} + m^{(1)}_{31}) & (m^{(2)}_{13} + m^{(2)}_{31}) & (m^{(3)}_{13} + m^{(3)}_{31}) & (m^{(4)}_{13} + m^{(4)}_{31}) & (m^{(5)}_{13} + m^{(5)}_{31}) \\
  (m^{(1)}_{12} + m^{(1)}_{21}) & (m^{(2)}_{12} + m^{(2)}_{21}) & (m^{(3)}_{12} + m^{(3)}_{21}) & (m^{(4)}_{12} + m^{(4)}_{21}) & (m^{(5)}_{12} + m^{(5)}_{21})
\end{bmatrix} 
\begin{bmatrix}
  d\gamma_1 \\
  d\gamma_2 \\
  d\gamma_3 \\
  d\gamma_4 \\
  d\gamma_5
\end{bmatrix}
\]

\[
\begin{bmatrix}
  \tau_1 \\
  \tau_2 \\
  \tau_3 \\
  \tau_4 \\
  \tau_5
\end{bmatrix} = 
\begin{bmatrix}
  m^{(1)}_{11} & m^{(1)}_{22} & m^{(1)}_{33} & (m^{(1)}_{23} + m^{(1)}_{32}) & (m^{(1)}_{13} + m^{(1)}_{31}) & (m^{(1)}_{12} + m^{(1)}_{21}) \\
  m^{(2)}_{11} & m^{(2)}_{22} & m^{(2)}_{33} & (m^{(2)}_{23} + m^{(2)}_{32}) & (m^{(2)}_{13} + m^{(2)}_{31}) & (m^{(2)}_{12} + m^{(2)}_{21}) \\
  m^{(3)}_{11} & m^{(3)}_{22} & m^{(3)}_{33} & (m^{(3)}_{23} + m^{(3)}_{32}) & (m^{(3)}_{13} + m^{(3)}_{31}) & (m^{(3)}_{12} + m^{(3)}_{21}) \\
  m^{(4)}_{11} & m^{(4)}_{22} & m^{(4)}_{33} & (m^{(4)}_{23} + m^{(4)}_{32}) & (m^{(4)}_{13} + m^{(4)}_{31}) & (m^{(4)}_{12} + m^{(4)}_{21}) \\
  m^{(5)}_{11} & m^{(5)}_{22} & m^{(5)}_{33} & (m^{(5)}_{23} + m^{(5)}_{32}) & (m^{(5)}_{13} + m^{(5)}_{31}) & (m^{(5)}_{12} + m^{(5)}_{21})
\end{bmatrix} 
\begin{bmatrix}
  \sigma_{11} \\
  \sigma_{22} \\
  \sigma_{33} \\
  \sigma_{23} \\
  \sigma_{13} \\
  \sigma_{12}
\end{bmatrix}
\]
Grains in polycrystals do NOT experience the same boundary conditions.

Differentiate between GLOBAL boundary conditions (tool, process) and the LOCAL (micromechanical) boundary conditions. The latter are influenced by grain-to-grain interactions and local inhomogeneity.
• Examples
Homogeneity and boundary conditions at grain scale

Crystal Mechanics FEM, grain scale mechanics (2D)

Experiment (DIC, EBSD) v Mises strain

Simulation (CP-FEM) v Mises strain

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Crystal plasticity FEM, grain scale mechanics (3D Al)

exp., grain orientation, side A

exp., grain orientation, side B

FE mesh

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ICME: Integrated Computational Materials Engineering

Experiments and Simulations

- In-situ deformation
- HR-EBSD mapping
- In-lens SE imaging
- Serial sectioning
- Strain mapping

HR-EBSD

Model from EBSD map

Phase properties by nanoindentation & CPFEM

Simulations employing FFT-based spectral solver

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ICME applied to dual phase steel

Experiments

Digital model
Indents
Spectral solver
Strain map & stress map

1µm
SiO₂ pattern
Deformation
Imaging & DIC
Sectioning
Strain map

Integrated Computational Materials Engineering: DP steel
Crystal plasticity FEM for large scale forming predictions

too many grains
Multiscale crystal plasticity FEM for large scale forming

Numerical Laboratory: From CPFEM to yield surface (engineering)
Representative Volume Element

Tension 0° (RD)

Tension 90° (TD)

RVE

Tension 45°

Tension biaxial
Simulation

Experiment

relative ear height [1]

angle to rolling direction [°]

Simulation result: RGC scheme

Color map: Equivalent total strain
Mechanical properties: ... for which structural component?

Component-specific property mix

Front crash ⇒ Energy absorption

Side crash ⇒ Strength
Strain rate 800/s: compare TWIP steel to DP800

\[ W_V = \int_0^{\varepsilon_f} \sigma d \varepsilon \approx \sigma_f \varepsilon_f \]

Awareness of impact situation

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Crystal plasticity & phase field:
Mechanics, damage, phase transformation, diffusion

> 15 years of development
> 50 man years of expertise
> 50,000 lines of code

Pre- and post-processing
Blends with MSC.Marc and Abaqus
Standalone (FFT) spectral solver
Many user groups

http://DAMASK.mpie.de
Average grain size: 5 μm
EBSD step size: 0.2 μm
EBSD scan size: 20 × 70 μm
Target polished thickness: 0.15 μm
Total slices number: 22

Experiment by Dayong An, MPIE
Real 3D Microstructure