Grain boundary mechanics in Crystal Plasticity
Finite Element Modeling

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Breitnau conference - Freiburg III, lecture by Dierk Raabe, June 2005
Dierk Raabe

References

• D. Raabe, Y. Wang and F. Roters, Computational Materials Science 34 (2005) 221-234. "Crystal plasticity simulation study on the influence of texture on earing in steel"
• A. Ma F. Roters D. Raabe, Acta Materialia Vol. 54 (2006) pages 2169–2179. „A dislocation density based constitutive model for crystal plasticity FEM including geometrically necessary dislocations”
• Crystal mechanics-FEM
• 3D EBSD
• Materials science of arthropods: lobster
crystal plasticity FEM
crystal kinematics and dynamics

multiplicative decomposition of the deformation gradient

flow law

DOF:

\[ \mathbf{\tilde{L}}_p = \sum_{\alpha=1}^{24} \dot{\gamma}_\alpha \mathbf{d}_\alpha \otimes \mathbf{n}_\alpha \]

Definitions:

\[ F^* : \text{"elastic" deformation gradient} \]
\[ F : \text{total deformation gradient} \]
\[ F_p : \text{plastic deformation gradient} \]
\[ L_p : \text{plastic velocity gradient} \]
\[ L_e : \text{elastic velocity gradient} \]

\[ \dot{\gamma} = \frac{d\gamma}{dt} = n \frac{dx}{X} \frac{b}{Z} \frac{1}{dt} = \rho_m b v \]
physics-based constitutive laws

1. set internal variables
   - dyadic flow law based on dislocation mechanics

2. set internal variables
   - plastic gradients, size scale and orientation gradients (implicit)

3. set internal variables
   - interfaces
   - activation concept
uniaxial compression of Al single crystals

uniaxial compression along [110]

force rate = 0.2 N/s, average strain rate: 0.0001 1/s
crystal plasticity FEM at small scales
small scales – single crystals
small scales – single crystals

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<111> Al (Calculated)
100 mN Indent Force
70 µm Indent Radius
Slice at Center of Indent

<111> Cu (Measured)
100 mN Indent Force
69 µm Indent Radius
Slice at Center of Indent

<111> 110 Pole
40 µm

<111> 5°

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small scales – bicrystals - conventional theory

Experiment

Simulation

7.4°

33.2°
small scales – bicrystals

Experiment

Simulation I (phenomen.)

Simulation II

7.4°
small scales – bicrystals

Experiment

Simulation I (phenomen.)

Simulation II

33°
small scales – bicrystals

experiment

phenomen. model

dislocation model

7,4°  16°  33°
3D electron microscopy
schematics of serial sectioning set-up

- FIB column
- Ga⁺
- sample in cutting position (36° tilt)
- sample in EBSD position (70° tilt)
- SEM objective lens
- EDX detector
- x-rays
- EBSD camera

⇒ easy and precise change between cutting and analysing positions
3D EBSD by serial FIB sectioning

Each 300 nm spacing

SE-image
3D rendering of EBSD sections

guided preparation

colour code: RD

1.2 µm milling
guided preparation
guided preparation
extracting and mounting TEM samples

extraction of thin foil with nano-manipulator

TEM sample fixed to a 3-mm TEM grid
Hellfeld

Orientierung
Extract components and background from experiments

Exp. input

Backcalculation

Difference
Fließfelddivergenz und intrinsische Orientierungsgradienten

89 % plane strain
Orientation and band contrast

EBSD pattern quality:
low
high

Experiment

Simulation

5.00 μm = 100 steps
IQ -14.348...76.6936, Orientation

(011)[100]: 0° - 15° Misorientierung
(111)[1-2]: 0° - 20° Misorientierung
(111)[-1-12]: 0° - 20° Misorientierung

NR
WR

TD
RD
Kleine Skalen: Oligokristalle, Al, ebene Dehnung

von-Mises strain
Vielkristallmechanik, große Skalen
crystal plasticity FEM at large scales

TCCP-FEM: the texture component crystal plasticity FEM
a car contains more than 50 billion grains!
components for mapping the start texture
\[ f(g) = F + \sum_{c=1}^{C} w^c f^c(g) = \sum_{c=0}^{C} w^c f^c(g) \]

\[ w^0 = F, \quad f^0(g) = 1 \]

- \(g\): orientation
- \(f(g)\): ODF
- \(F\): random-texture component
- \(w^c\): volume fraction of all crystals belonging to texture component \(c\)

Textur-Komponenten für Abbildung der Starttextur

Dierk Raabe
Use texture components for mapping

\[ \tilde{\omega}^c = \tilde{\omega}(g^c, g) \]

\[ f^c(g) = N^c \exp(S^c \cos \tilde{\omega}) \]

\[ S^c = \frac{\ln 2}{1 - \cos(b^c/2)} \]

and \[ N^c = \frac{1}{I_0(S^c) - I_1(S^c)} \]

\[ I_1(x) \]

generalized Bessel functions

\[ b^c \]

value is the halfwidth
(mean diameter of a spherical component in orientation space)

Extract components and background from experiments

Sample reference

Main texture components

Symmetry
components for mapping the start texture
local stress homogenization of more than one component possible
Beispiel, Al, Vielkristall, Würfeltextur+"random"

Simulation vs. Experiment

relative ear hight [1]

angle to rolling direction [°]
Large scale anisotropy: TCCP-FEM

3 Pole figures
(Textur goniometer)

Texture components
(Multex Software - freeware)

texture component crystal plasticity FEM
(ABQ or MARC in conjunction with MPI - Subroutines)
### The team

<table>
<thead>
<tr>
<th>Name</th>
<th>Position</th>
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</thead>
<tbody>
<tr>
<td>F. Roters (MPI)</td>
<td>CP-FEM</td>
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<td>A. Ma (MPI)</td>
<td>CP-FEM</td>
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<td>S. Zaefferer (MPI)</td>
<td>experimental</td>
</tr>
</tbody>
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DFG, MPG