Understanding the Elasto-Plasticity of Crystals

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Overview

- Scales in elasto-plasticity, MMM input
- Polycrystal elasto-plasticity homogenization (single phase, focus on kinematics, and b.c.)
- Limits in plasticity continuum models (small scale crystal plasticity)
**Multiscale Models: Scales, Methods**

Far away from thermodynamic equilibrium, only local mechanical equilibrium and compatibility

How does multiscale work?

Understand mechanisms on each scale

- Texture (CPFEM, Taylor)
- Dynamics of defects (MD, DDD)
- Defect topology (kMC, CA, PP)
- Structure of defects (DFT, MD)
- Structure of matter (DFT)

Bottom up

Length \[ [m] \]

- \( 10^{-9} \)
- \( 10^{-3} \)
- \( 100 \)
- \( 10^{-15} \)

Time \[ [s] \]

- \( 10^{-6} \)
- \( 10^{-9} \)
- \( 10^{-3} \)
- \( 10^{3} \)
Multiscale approaches in crystal plasticity

Parameter transfer / Scale hoping:
Elastic constants (Homogenization, feedback, inverse modeling: M. Friak, A. Counts, M. Petrov, J. Neugebauer, L. Limperakis)

Coarse Graining / Statistics:
Statistical dislocation theory (pattern, defect structure formation: F. Roters, P. Dondel, S. Müller)

Polycrystal homogenization theory
Averages mechanical quantities for polycrystals (complex interaction, unknown local b.c., multiple phases, transformations: P. Eisenlohr, M. Friak, J. Neugebauer)
• Brief example (kinetics): dislocation evolution + dislocation-stress relation (talk of F. Roters)
Motivation: Fundamentals of crystal mechanics

- Lattice defects kinematics (dyadics of the shear DOF) plus boundary conditions
- Lattice defect kinetics (Franz Roters)
- Mesoscopic boundary conditions (grain / orientation neighborhood)
- One dislocation
- Parallel loops (Kubin)
- Reactions (Kubin)
- Spin (orientation change)
Motivation: Fundamentals of crystal mechanics

Kinetics: collective dislocation behaviour

- Kinetic equation of state

\[ \frac{d\rho}{d\gamma} = A\rho^+ + B\rho^- \]

- Structure evolution

- Coupling to imposed shape change

\[ \dot{\gamma} = \frac{d\gamma}{dt} = n \frac{dx}{X} \frac{b}{Z} \frac{1}{dt} = \rho_m b v \]

\[ \tau = \alpha G b \sqrt{\rho} \]
Coarse Graining: flow stress only

\[ \tau = G\gamma = \frac{Gb}{2\pi r} \]

\[ \rho = \frac{1}{a^2} \]

\[ \frac{Gb}{2\pi a} = \frac{Gb}{2\pi} \sqrt{\rho} \]
Coarse graining, problems
Coarse graining, problems
Typical issues

Continuum scale coarse graining:

- How much physics is included in a model?
- How transparent are the assumptions?
- What was left out and why?
- Simplify complex systems
- Is there any experimental / theoretical proof?
- Are the experiments trustworthy (better make your own, create new experiments)?
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Crystal mechanics and anisotropy

single crystal level
Origin of plastic anisotropy
single crystal level: stress homogenization

kinematics:
shape change (symmetric part of displacement gradient)

kinematics:
rotation / texture (antisymmetric part of displacement gradient)

Plastically stretched zinc single crystal.
Adapted from Fig. 7.9, *Callister 6e.*
(Fig. 7.9 is from C.F. Elam, *The Distortion of Metal Crystals,* Oxford University Press, London, 1935.)

Adapted from Fig. 7.8, *Callister 6e.*


1 crystal, 1 slip system:

\[ m_{kl} = n_k b_l \]

\[ m_{ij} = a_{ik} n_k a_{jl} b_l \]

**slip systems**

\[ \vec{n} \vec{b} \]

**crystal** (k, l)

**sample** (i, j)

**kinematics**

\[ a_{ik} n_k a_{jl} b_l \sigma_{ij} = \tau_{\text{crit}} \]
single crystal level: stress homogenization

\[ a_{ik} n_k a_{ji} b_l \sigma_{ij} = \tau^{\text{crit}} \]

1 crystal, 1 slip system:
single crystal level: stress homogenization

slip system $s$

$$n^s_i, b^s_i$$

orientation factor for $s$

$$m^s_{ij} = n^s_i b^s_j$$

1 crystal, 2 slip systems

symmetric part

$$m_{ij}^{\text{sym},s} = \frac{1}{2} (n^s_i b^s_j + n^s_j b^s_i)$$

rotate crystal into sample

$$m^s_{kl} = a^c_i n^s_i a^c_j b^s_j$$

symmetric part

$$m_{kl}^{\text{sym},s} = \frac{1}{2} (a^c_k n^s_i a^c_l b^s_j + a^c_l n^s_j a^c_k b^s_i)$$

yield surface (active systems)

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

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

(yield surface (non-active systems))

$$m_{kl}^{\text{sym},s=\text{inaktiv}}$$ $\sigma_{kl} = \sigma_{\text{aufg}} < \tau_{\text{krit},(\pm)}^{s=\text{inaktiv}}$
single crystal level: stress homogenization

krz, kfz, Schnitt

krz, 24 Systeme, Schnitt

krz, 48 Systeme, Schnitt

1 crystal, many slip systems

yield surface, bcc

single crystal, bcc, (001)[100]
single crystal level: stress homogenization
Crystal mechanics and anisotropy

polycrystal level
polycrystal: strain homogenization

\[ \varepsilon_{ij} = \frac{1}{2} \sum_{s=1}^{5} \left( n_i^s b_j^s + n_j^s b_i^s \right) \gamma^s \]
polycrystal: strain homogenization?

internal boundary conditions

external boundary conditions

?
polycrystal : strain homogenization

1 grain, many systems (stress space)
many grains, 2 systems (strain rate homogenization)
Polycrystal reality

Crystal-scale homogeneity does not exist

Control of boundary conditions essential

3%

8%

15%
polycrystal: homogenization

\[
\langle \sigma_{ij} \rangle = \frac{1}{V} \int \sigma_{ij}(x,g) dV
\]

\[
\langle D_{ij} \rangle = \frac{1}{V} \int D_{ij}(x,g) dV
\]

typical boundary conditions

\[
D_{ij}^{\text{ext}} = \langle D_{ij} \rangle = \frac{1}{V} \int D_{ij}^K(x,g) dV,
\]

\[
D_{ij}^K(x,g) \quad \sigma_{ij}^K(x,g)
\]

\[
D_{ij}^{\text{ext}} = \frac{1}{V} \int D_{ij}^K(x,g) dV \approx \sum_{\text{Komp}} D_{ij}^K(g) \frac{V^{\text{Komp}}}{V} \approx D_{ij}^K(g)
\]

less typical boundary conditions

\[
\sigma_{ij}^{\text{ext}} = \langle \sigma_{ij} \rangle = \frac{1}{V} \int \sigma_{ij}^K(x,g) dV,
\]

\[
\sigma_{ij}^K(x,g)
\]


„Concepts for integrating plastic anisotropy into metal forming simulations“


„On the dependence of in-grain subdivision and deformation texture of aluminium on grain interaction“
complex b.c.: Crystal Plasticity FEM (CPFEM) - Family

- constitutive law on slip system basis
- mesh
- orientation input
- external boundary conditions
- local homogenization geometrical discreteness

70.00 µm = 70 steps
Crystal Mechanics FEM, grain scale mechanics (2D)

Experiment (DIC, EBSD) v Mises strain

Simulation (CP-FEM) v Mises strain

„Micromechanical and macromechanical effects in grain scale polycrystal plasticity experimentation and simulation“
Crystal Mechanics FEM, grain scale mechanics (3D)

- Experimental
- Simulation

Mises strain

- 15.0
- 13.5
- 12.0
- 10.5
- 9.0
- 7.5
- 6.0
- 4.5
- 3.0
- 1.5
- 0.0
Crystal Mechanics FEM + transformation (recrystallization)

"Coupling of a crystal plasticity finite element model with a probabilistic cellular automaton for simulating primary static recrystallization in aluminum"

Nucleation in transformation (recrystallization)

source: Stefan Zaefferer
10 billion grains

too many grains

70.00 μm = 70 steps
map texture functions into FEM

„Using texture components in crystal plasticity finite element simulations“
Crystal Plasticity FEM

- Simulation
- Experiment

Graph showing relative height vs. angle to rolling direction.

Inset images of crystal plasticity FEM models.
Crystal Plasticity FEM
Virtual Material Testing
- Representative Volume Element
- Virtual test program – extrapolation of calibration tests
- Parameter fit of the macro material model
- No performance loss compared to classical deep drawing simulation
- Material behaviour limited to available models in commercial FE codes
- Demonstrated by INPRO for (bcc) HSLA steel

Example: Automobile (Coarse graining, Parametertransfer)

From Crystal Plasticity to Deep Drawing

Vegler-Modell in PamStamp 2G
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Nanoindentierung

[Image of nanoindentation experiment results showing indented (111) plane and cross section.]

(section 1, center line, Ga⁺ beam)
3D electron - microscopy

SEM
FIB
BSED
SED
STED
GIS

EDX
in-lens SED
EBSD

sample in cutting position (36° tilt)

sample in EBSD position (70° tilt)

SEM objective lens

EDX detector

EBSD camera

Ga⁺

FIB column

e⁻

e⁻
N. Zaafarani, D. Raabe, R. N. Singh, F. Roters, S. Zaefferer,
“Three dimensional investigation of the texture and microstructure below a nanoindent in a Cu single crystal using 3D EBSD and crystal plasticity finite element simulations”

Forces: 4, 6, 8, and 10 mN
N. Zaafarani, D. Raabe, F. Roters and S. Zaefferer
Acta Materialia, Volume 56, Issue 1, January 2008, Pages 31-42
On the origin of deformation-induced rotation patterns below nanoindents
Multiscale approaches in crystal plasticity
Multiscale Models: Scales, Methods

MMM: input / handshake in Elasto-Plasticity

- **Structure of matter (DFT):** TD of alloys, impurities, order, T>0K (talk of M. Friak)

- **Structure of defects (DFT, MD):** dislocation cores, dislocation motion, inertia, energy surface during motion, dislocation reactions, impurities, interface properties, T>0K (MD potentials, rates, loads !) (talk of L. Limperakis)

- **Defect topology (DD, kMC, CA, PP):** kinetics, Ostwald, clustering, interface dynamics: physics of interfaces and diffusion

- **Dynamics of defects (MD, DD):** mechanical reactions, interaction with interfaces, role of impurities (talk of L. Limperakis)

- **Texture (CPFEM, Taylor):** any intrinsic anisotropy