Chair for Continuum Mechanics
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Single Crystal Gradient Plasticity – Part III

Chair for Continuum Mechanics – Institute of Engineering Mechanics

Outline

Motivation

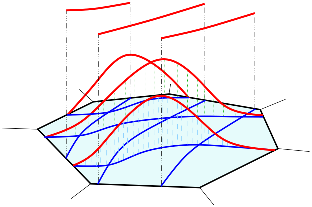
Dislocation continuum theories – overview

The concept of lifted curves

Modelling of pile-ups

Numerical results

Conclusion and Outlook



Literature

- Fundamental dislocation theory

  e.g. Taylor (1934); Orowan (1935); Schmid and Boas (1935); Hall (1951); Petch (1953)
- Kinematics and crystallographic aspects of GNDs

  Nye (1953); Bilby, Bullough and Smith (1955); Kröner (1958); Mura (1963); Arsenlis and Parks (1999)
- Thermodynamic gradient theories

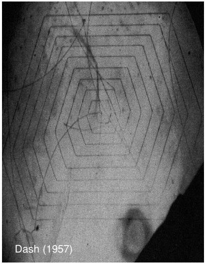
  e.g. Fleck et al. (1994); Steinmann (1996); Menzel and Steinmann (2001); Liebe and Steinmann (2001); Reese and Svendsen (2003); Berdichevski (2006); Ekh et al. (2007); Gurtin, Anand and Lele (2007); Fleck and Willis (2009); Bargmann et al. (2010); Miehe (2011)
- Slip resistance dependent on GNDs and SSDs

  e.g. Becker and Miehe (2004); Evers, Brekelmans and Geers (2004); Cheong, Busso and Arsenlis (2005)
- Micromorphic approach

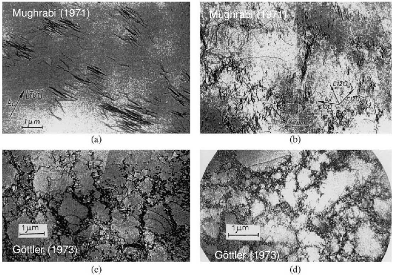
  e.g. Forest (2009); Cordero et al. (2010); Aslan et al. (2011)
- Continuum Dislocation Dynamics

  e.g. Hochrainer (2006); Hochrainer, Zaiser and Gumbsch (2007); Hochrainer, Zaiser and Gumbsch (2010); Sandfeld, Hochrainer and Zaiser (2010); Sandfeld (2010)

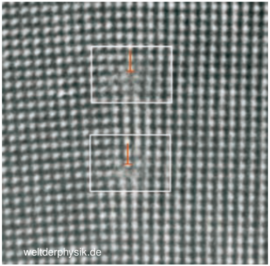
Dislocation Microstructure



Spiral source



Cell structures at different deformation stages



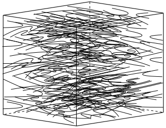
Single dislocations

Important features of the microstructure

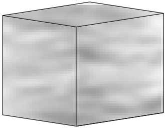
- Total line length/density
- Dislocation sources
- Dislocation motion/transport
- Lattice distortion

Classical Continuum Dislocation Measures

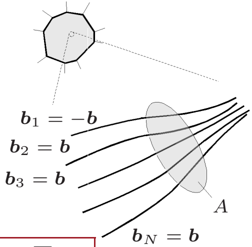
Total line length per unit volume



$$\rho = \frac{\Delta l_{\text{tot}}}{\Delta V}$$



Typical (local) evolution law: $\partial_t \rho = f(\dot{\gamma}, \rho)$ **Transport neglected!**

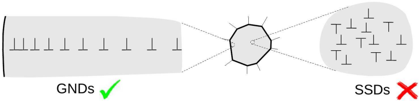


$\boldsymbol{b}_{\text{eff}} = \sum_i \boldsymbol{b}_i$

Nye's dislocation density tensor

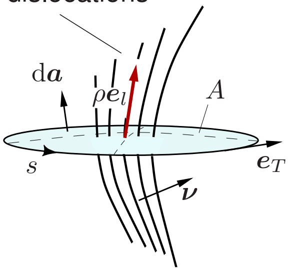
$\boldsymbol{\alpha} = \text{curl}\,(\boldsymbol{H}^p)$ **SSDs neglected!**

$\boldsymbol{H}^p$: plastic displ. gradient



Smooth Dislocation Bundles

Mura (1963)



Dislocation density vector

$$\boldsymbol{\kappa} := \rho \boldsymbol{e}_l$$

Effective 'Number' of penetration points

$$N_{\mathrm{eff}} = \int_A \boldsymbol{\kappa} \cdot \mathrm{d}\boldsymbol{a},$$

Dislocation flux into A

$$\dot{N}_{\mathrm{eff}} = -\int_{\partial A} (\boldsymbol{\kappa} \times \boldsymbol{\nu}) \cdot \boldsymbol{e}_T \, \mathrm{d}s,$$

$$\Rightarrow \quad \partial_t \boldsymbol{\kappa} = -\mathrm{curl}\,(\boldsymbol{\kappa} \times \boldsymbol{\nu})$$

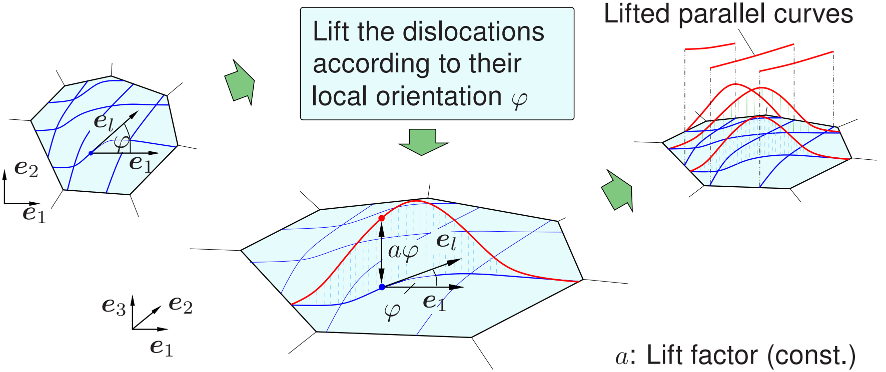
Closed evolution equation

Holds if nearby dislocations are parallel!

How to treat **non-parallel** dislocations?

Concept of lifted dislocations

Hochrainer (2006); Hochrainer, Zaiser and Gumbsch (2007)

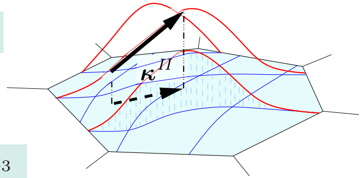


If curvature depends on position and orientation $k = k(x_1, x_2, \varphi, t)$:

Adjacent lifted dislocations are **parallel**!

Concept of lifted dislocations

Hochrainer (2006); Hochrainer, Zaiser and Gumbsch (2007)



Density vector of lifted dislocations $\boldsymbol{\kappa}^{II} = \rho^{II}\boldsymbol{e}_l^{II}$

ρ^{II} : Density of lifted dislocations

$\boldsymbol{e}_l^{II}$: line direction

Velocity of the lifted dislocations $\boldsymbol{V} = \boldsymbol{\nu} + a\vartheta\boldsymbol{e}_3$

$\boldsymbol{\nu}$: real dislocation velocity

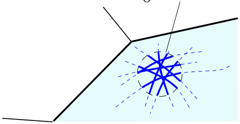
ϑ: angular velocity

Evolution equation (by analogy) $\partial_t\boldsymbol{\kappa}^{II} = -\mathrm{curl}\left(\boldsymbol{\kappa}^{II}\times\boldsymbol{V}\right)$

Planar projection of $\boldsymbol{\kappa}^{II}$

Derivation of orientation dependent density $\rho^{\varphi}(x_1, x_2, \varphi, t) = a\boldsymbol{\kappa}^{II}\cdot\boldsymbol{e}_l$

$$\int_0^{2\pi}\rho^{\varphi}\,\mathrm{d}\varphi$$



Total dislocation density $\rho(x_1, x_2, t) = \int_0^{2\pi}\rho^{\varphi}\,\mathrm{d}\varphi$

Averaged Theory

Hochrainer, Zaiser and Gumbsch (2010)

Continuum Dislocation Dynamics (CDD)

Evolution equation of lifted dislocation density vector

$$\partial_t \boldsymbol{\kappa}^{II} = -\mathrm{curl}\left(\boldsymbol{\kappa}^{II} \times \boldsymbol{V}\right)$$

$$\boldsymbol{\kappa}^{II} = \frac{\rho^{\varphi}}{a}\boldsymbol{e}_l + \rho^{\varphi} k \boldsymbol{e}_3$$

Equivalent: Evolution equations of density ρ^{φ} and curvature k

$$\partial_t \rho^{\varphi} = -\mathrm{div}\left(\rho^{\varphi}\boldsymbol{\nu}\right) - \partial_{\varphi}(\rho^{\varphi}\vartheta) + \rho^{\varphi} k \nu$$

$$\partial_t(\rho^{\varphi} k) = -\mathrm{div}\left(\rho^{\varphi} k \boldsymbol{\nu} - \rho^{\varphi}\vartheta \boldsymbol{e}_l\right)$$

Averaged/Simplified Theory (sCDD)

Averaged field variables

$$\rho(x_1, x_2, t) = \int_0^{2\pi} \rho^{\varphi} \mathrm{d}\varphi$$

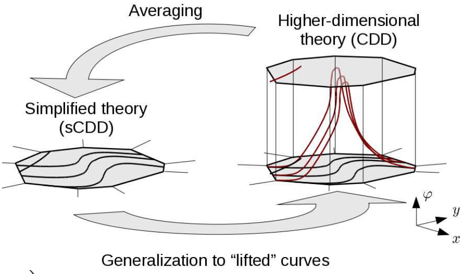
$$\overline{\rho k}(x_1, x_2, t) = \int_0^{2\pi} \rho^{\varphi} k \, \mathrm{d}\varphi$$

$$\boldsymbol{\kappa}^{\perp} = \int_0^{2\pi} \rho^{\varphi} \boldsymbol{e}_{\nu} \mathrm{d}\varphi$$

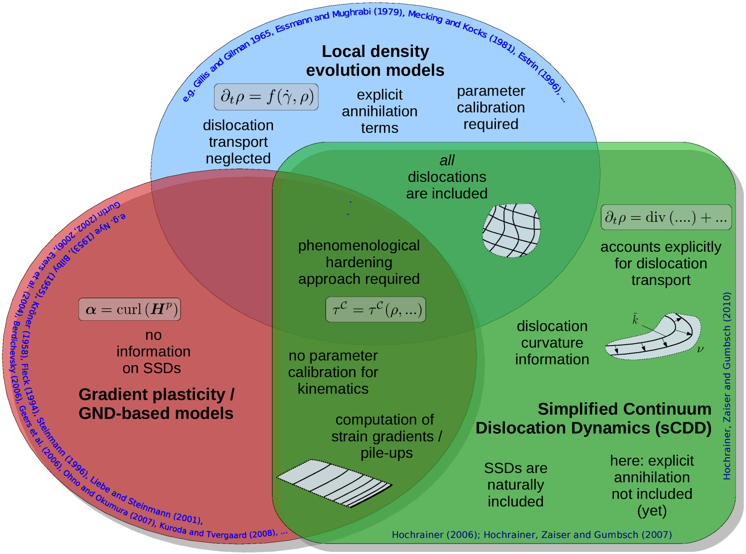
Averaged evolution equations

$$\partial_t \rho = -\mathrm{div}\left(\boldsymbol{\kappa}^{\perp}\nu\right) + \overline{\rho k}\nu$$

$$\partial_t \overline{\rho k} = -\mathrm{div}\left(\overline{\rho k}/\rho \, \nu \boldsymbol{\kappa}^{\perp} + \rho/2 \, \nabla_p \nu\right)$$



Comparison of Dislocation Theories



Coupling to Crystal Plasticity

Single slip framework

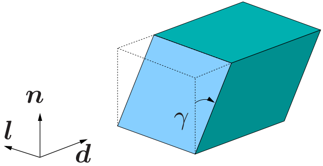
Additive decomposition	$\operatorname{grad}(\boldsymbol{u}) = \boldsymbol{H} = \boldsymbol{H}^e + \boldsymbol{H}^p$
Plastic distorsion	$\boldsymbol{H}^p = \gamma \boldsymbol{d} \otimes \boldsymbol{n} = \gamma \boldsymbol{M}$
Elastic strain	$\boldsymbol{\varepsilon}^e = \operatorname{sym}(\boldsymbol{H}^e)$
Stress	$\boldsymbol{\sigma} = \mathbb{C}[\boldsymbol{\varepsilon}^e]$
Resolved shear stress	$\tau = \boldsymbol{\sigma} \cdot \boldsymbol{M}$

Coupling equations

Orowan equation	$\dot{\gamma} = \rho b \nu$
Overstress modell	$\nu = \nu_0 \operatorname{sgn}(\tau) \left\langle \frac{\lvert\tau + \operatorname{div}(\boldsymbol{\xi})\rvert - \tau^c}{\tau^d} \right\rangle^p$
Taylor hardening	$\tau^c = \tau_0^c + aGb\sqrt{\rho}$

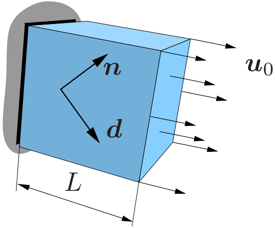
PDEs

$$
\begin{aligned}
\operatorname{div}(\boldsymbol{\sigma}) &= \boldsymbol{0} \\
\partial_t \rho &= -\operatorname{div}\left(\boldsymbol{\kappa}^{\perp} \nu\right) + \overline{\rho k} \nu \\
\partial_t \overline{\rho k} &= -\operatorname{div}\left(\overline{\rho k}/\rho\, \nu \boldsymbol{\kappa}^{\perp} + \rho/2\, \nabla_p \nu\right)
\end{aligned}
$$



Dislocation Starvation Simulation 1

Initial conditions

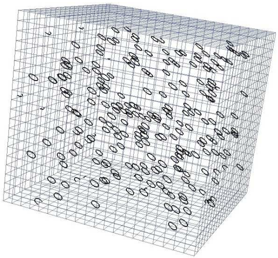


$$
\begin{aligned}
\rho(\boldsymbol{x}, t=0) &= \rho_0 = \text{const.} \\
k(\boldsymbol{x}, t=0) &= k_0 \gg 1/L \\
\Rightarrow \overline{\rho k}(\boldsymbol{x}, t=0) &= \rho_0 k_0
\end{aligned}
$$

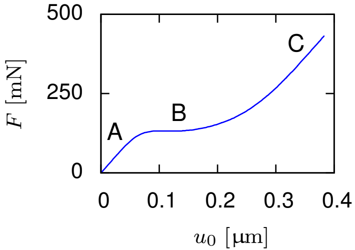
High viscosity required for stabilization

Videos 1, 2, 3

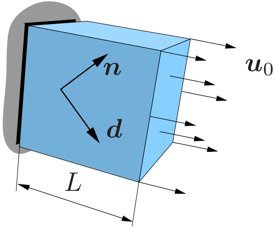
$\Rightarrow$ Homogeneous distribution of small loops



Force displacement curve



Dislocation Starvation Simulation 2



Initial conditions

$\rho(\boldsymbol{x}, t = 0)$: concentrated at center

$k(\boldsymbol{x}, t = 0) = k_0 \gg 1/L$

Videos 4, 5

$\Rightarrow$ Inhomogeneous distribution of small loops

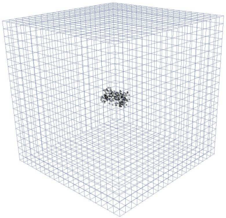


Figure: Initial configuration

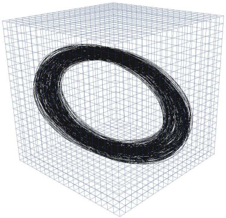
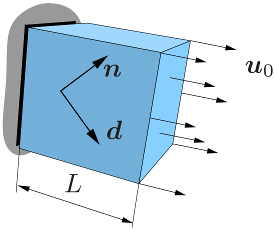


Figure: After loading

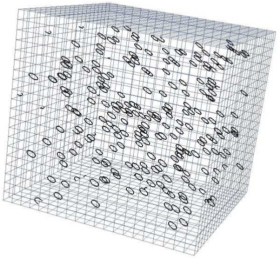
Numerical results



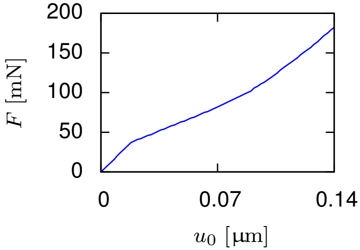
Initial conditions

$$
\begin{aligned}
\rho(\boldsymbol{x}, t=0) &= \rho_0 = \text{const.} \\
k(\boldsymbol{x}, t=0) &= k_0 \gg 1/L \\
\Rightarrow \overline{\rho k}(\boldsymbol{x}, t=0) &= \rho_0 k_0
\end{aligned}
$$

$\Rightarrow$ Homogeneous distribution of small loops

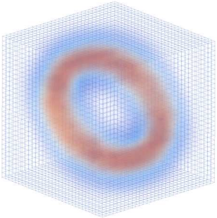


Force displacement curve



Conclusion

- There is a need for a continuum theory of dislocations to bridge the scales
- Concept of lifted curves → physically based continuum theory
- Takes into account
  - SSDs & GNDs
  - transport
  - curvature
- Fits into crystal plasticity framework
- Facilitates the simulation of effects like dislocation starvation



Thank you for your attention

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