Karlsruhe Institute of Technology

Chair for Continuum Mechanics
Institute of Engineering Mechanics (Prof. Böhlke)
Department of Mechanical Engineering

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Single Crystal Gradient Plasticity – Part I

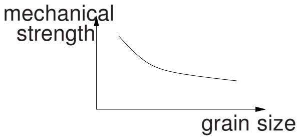
Chair for Continuum Mechanics – Institute of Engineering Mechanics

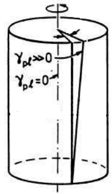
Motivation

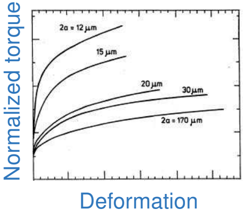
Materials exhibit strong size effects, when the length scale associated with non-uniform plastic deformation is in the order of microns.

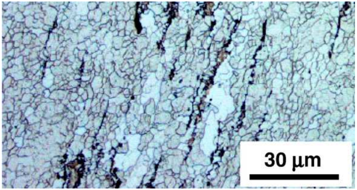
Examples:

- Fine-grained steels
- Precipitation hardening
- Torsion of thin wires Fleck et al. (1994)









B. Eghbali (2007)

Motivation

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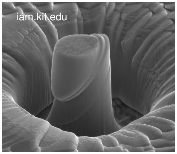
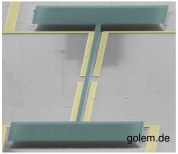
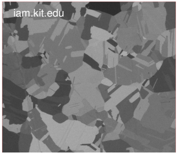
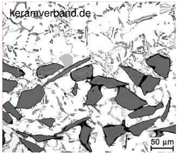


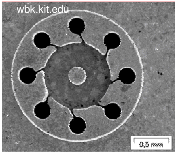


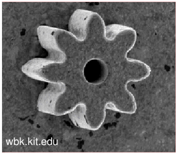
Understanding micro-plasticity

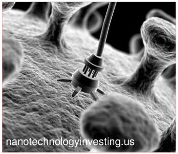




Design of materials



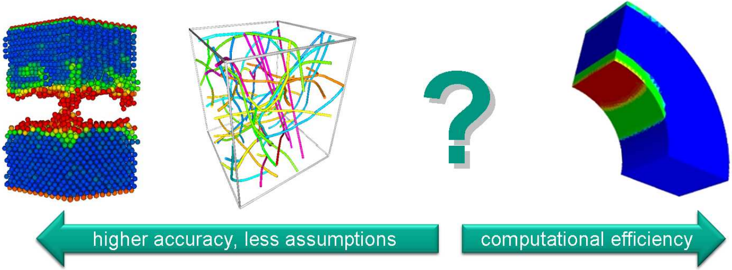




Dimensioning of micro-components and micro-systems

How to identify physically based continuum mechanical micro-plasticity models?

Motivation

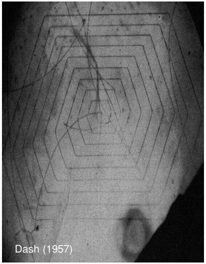


- Atomistic and DDD-simulations are limited to very small systems
- Classical continuum mechanical plasticity fails at the micro-scale

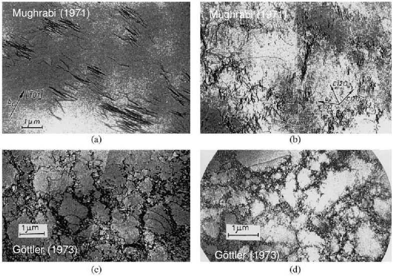
Need for a **Continuum Dislocation Theory** to bridge the scales

DFG Research Group 1650 "Dislocation based Plasticity"

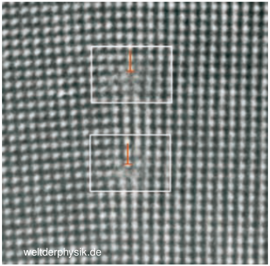
Dislocation Microstructure



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

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)

Outline

- Single crystal kinematics at small strains
- Free-energy ansatz
- Field and boundary equations
- Constitutive modeling
- Numerical examples

Kinematics of Single Crystals at Small Strains

- Displacement gradient

$$\boldsymbol{H} = \boldsymbol{H}_e + \boldsymbol{H}_p$$

- Plastic part of the displacement gradient

$$\boldsymbol{H}_p = \sum_\alpha \gamma_\alpha \boldsymbol{d}_\alpha \otimes \boldsymbol{n}^\alpha$$

- Additive decomposition of the strain tensor

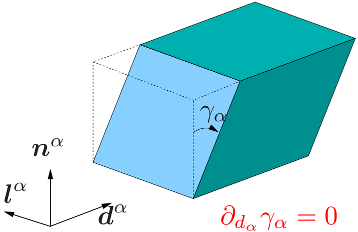
$$\boldsymbol{\varepsilon} = \mathrm{sym}(\boldsymbol{H}) = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p$$

- Flow rule

$$\dot{\boldsymbol{\varepsilon}}_p = \sum_\alpha \dot{\gamma}_\alpha \boldsymbol{M}_\alpha \quad \boldsymbol{M}_\alpha = \frac{1}{2}(\boldsymbol{d}_\alpha \otimes \boldsymbol{n}^\alpha + \boldsymbol{n}^\alpha \otimes \boldsymbol{d}_\alpha)$$

Example:

Homogeneous plastic shear



$$\partial_{d_\alpha} \gamma_\alpha = 0$$

Kinematics of Single Crystals at Small Strains

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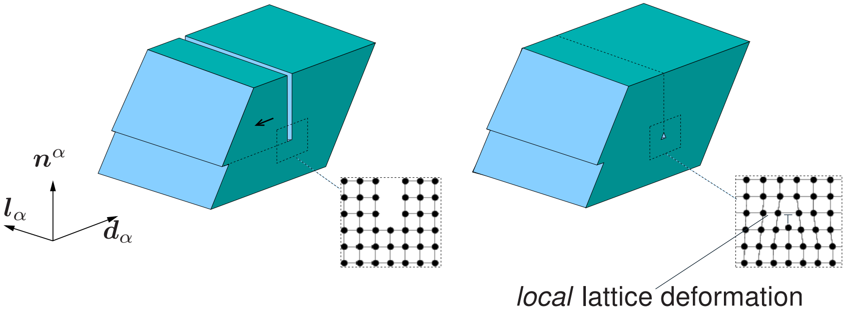
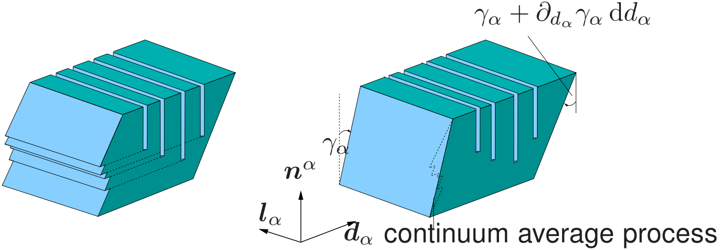
Introduction of a pure edge dislocation (with negative sign)



- Real crystal $\Rightarrow$ *discontinuous* slip
- *Local* lattice deformation **not** captured precisely by classical theory

Kinematics of Single Crystals at Small Strains

Graphical representation of the averaging process of γ_α in continuum mechanics



Kinematics of Single Crystals at Small Strains

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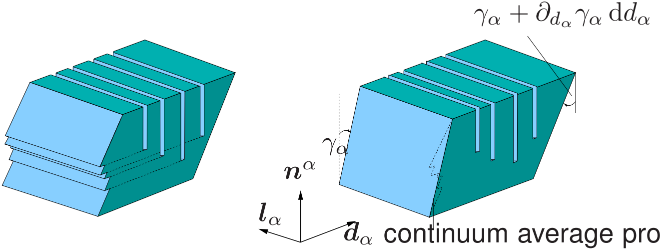


continuum average process

$\Rightarrow$ Dislocations of *equal sign* lead to **non-homogeneous** plastic shear

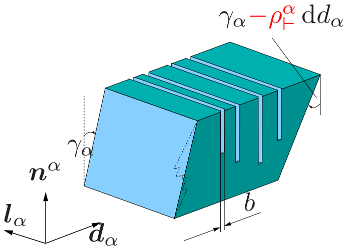
$$\partial_{d_\alpha}\gamma_\alpha \neq 0$$

$\Rightarrow$ *Geometrically neccessary* dislocations

Kinematics of Single Crystals at Small Strains

Edge and screw dislocation densities

$$\rho_{\vdash}^{\alpha} := -\partial_{d_\alpha} \gamma_\alpha = -\nabla \gamma_\alpha \cdot \boldsymbol{d}_\alpha$$



- Dislocation density tensor

$$\boldsymbol{\alpha} = \sum_\alpha [(-\nabla \gamma_\alpha \cdot \boldsymbol{d}_\alpha) \boldsymbol{l}_\alpha \otimes \boldsymbol{d}_\alpha + (\nabla \gamma_\alpha \cdot \boldsymbol{l}_\alpha) \boldsymbol{d}_\alpha \otimes \boldsymbol{d}_\alpha]$$

Kinematics of Single Crystals at Small Strains

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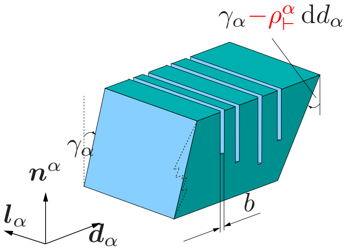

Edge and screw dislocation densities

$$\rho_\vdash^\alpha := -\partial_{d_\alpha}\gamma_\alpha = -\nabla\gamma_\alpha \cdot \boldsymbol{d}_\alpha$$
$$\rho_\odot^\alpha := \partial_{l_\alpha}\gamma_\alpha = \nabla\gamma_\alpha \cdot \boldsymbol{l}_\alpha$$

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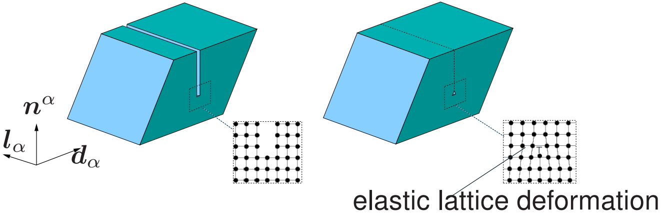
$$\boldsymbol{\alpha} = \sum_\alpha [(-\nabla\gamma_\alpha \cdot \boldsymbol{d}_\alpha)\boldsymbol{l}_\alpha \otimes \boldsymbol{d}_\alpha + (\nabla\gamma_\alpha \cdot \boldsymbol{l}_\alpha)\boldsymbol{d}_\alpha \otimes \boldsymbol{d}_\alpha]$$

Free Energy Ansatz



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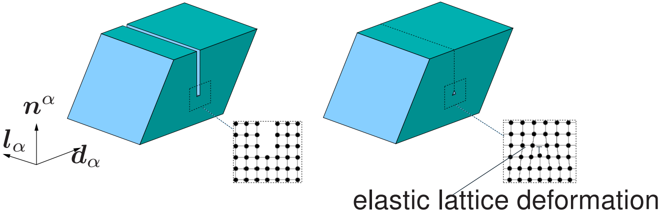
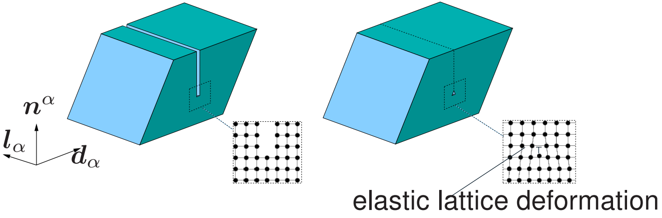


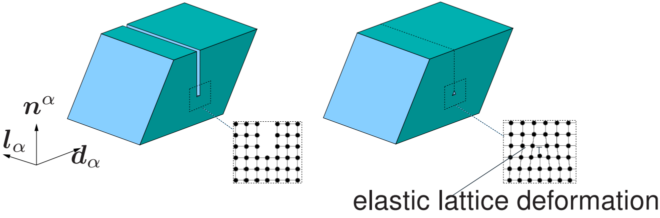
- Illustrated elastic lattice deformation is *averaged* by classical theory and thereby **not** accounted for correctly

Free Energy Ansatz



- Illustrated elastic lattice deformation is *averaged* by classical theory and thereby **not** accounted for correctly
  $\Rightarrow$ Free energy $W \geq W_e := \frac{1}{2}\boldsymbol{\varepsilon}_e \cdot \mathbb{C}[\boldsymbol{\varepsilon}_e]$

Free Energy Ansatz



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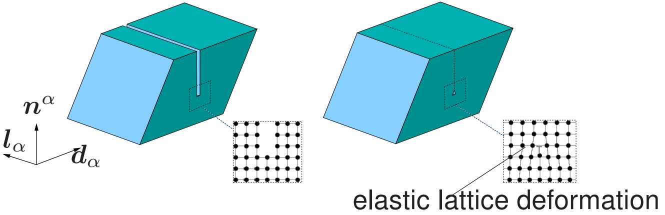
Ansatz

- Free energy $W = W_e(\boldsymbol{\varepsilon}_e) + W_d(\rho^\alpha_\vdash, \rho^\alpha_\odot)$

Free Energy Ansatz



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Ansatz

- Free energy $W = W_e(\boldsymbol{\varepsilon}_e) + W_d(\rho_\vdash^\alpha, \rho_\odot^\alpha)$
- Dissipation $\mathcal{D}_{tot} = \sum_\alpha \mathcal{D}(\dot{\gamma}_\alpha) = \sum_\alpha \tau_\alpha^{\mathcal{D}} \dot{\gamma}_\alpha$

Field and Boundary Equations

Virtual work of external forces δW_{ext} and internal forces δW_{int}

$$\delta W_{ext} \stackrel{!}{=} \delta W_{int} \qquad \forall \delta \boldsymbol{u},\ \delta\gamma_\alpha$$

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$$\delta W_{ext} \overset{!}{=} \delta W_{int} \qquad \forall \delta \boldsymbol{u},\ \delta\gamma_\alpha$$

$$\begin{aligned}
\delta W_{int} &= \delta \int_V W\, dV + \int_V \sum_\alpha \tau_\alpha^{\mathcal{D}} \delta\gamma_\alpha dV \\
&= \int_V \left[\partial_{\boldsymbol{\varepsilon}_e} W_e \cdot \delta\boldsymbol{\varepsilon}_e + \sum_\alpha \left(\partial_{\rho_\vdash^\alpha} W_d \delta\rho_\vdash^\alpha + \partial_{\rho_\odot^\alpha} W_d \delta\rho_\odot^\alpha \right) \right] dV \\
&\quad + \int_V \sum_\alpha \tau_\alpha^{\mathcal{D}} \delta\gamma_\alpha dV.
\end{aligned}$$

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\end{aligned}$$

$\delta W_e = \boldsymbol{\sigma} \cdot \delta\boldsymbol{\varepsilon}_e$ $\qquad$ $\boldsymbol{\sigma} := \partial_{\boldsymbol{\varepsilon}_e} W_e$ $\qquad$ stress

$\delta W_d = \sum_\alpha \boldsymbol{\xi}_\alpha \cdot \nabla\delta\gamma_\alpha$ $\qquad$ $\boldsymbol{\xi}_\alpha := -\partial_{\rho_\vdash^\alpha} W_d \boldsymbol{d}_\alpha + \partial_{\rho_\odot^\alpha} W_d \boldsymbol{l}_\alpha$ defect stress

Field and Boundary Equations

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Principle of virtual displacements yields

Field equations

$$\operatorname{div}(\boldsymbol{\sigma}) + \boldsymbol{f} = \boldsymbol{0}, \quad \tau_\alpha^{\mathcal{D}} = \tau_\alpha - (-1)\operatorname{div}(\boldsymbol{\xi}_\alpha) \qquad \forall \boldsymbol{x} \in V$$

- $\tau_\alpha := \boldsymbol{\sigma} \cdot \boldsymbol{M}_\alpha$ resolved shear stress
- $(-1)\operatorname{div}(\boldsymbol{\xi}_\alpha)$ backstress due to GNDs

Field and Boundary Equations

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Boundary equations

$$\begin{aligned} \boldsymbol{\sigma}\boldsymbol{n} &= \boldsymbol{t}, \quad \boldsymbol{\xi}_\alpha \cdot \boldsymbol{n} = \Xi_\alpha \quad \forall \boldsymbol{x} \in \partial V_\sigma \\ \boldsymbol{u} &= \bar{\boldsymbol{u}}, \quad \gamma_\alpha = \bar{\gamma}_\alpha \quad \forall \boldsymbol{x} \in \partial V_u \end{aligned}$$

- $\boldsymbol{t}$ traction
- Ξ_α microtraction, results from evaluation of the PovD

Constitutive Modeling

Strain energy (linearized theory)

$$W_e = \frac{1}{2}\boldsymbol{\varepsilon}_e \cdot \mathbb{C}[\boldsymbol{\varepsilon}_e]$$

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Dissipation

$$\mathcal{D}(\dot{\gamma}_\alpha) = \dot{\gamma}_0 \tau_0 \left|\frac{\dot{\gamma}_\alpha}{\dot{\gamma}_0}\right|^{m+1} \Rightarrow \tau_\alpha^{\mathcal{D}} = \operatorname{sgn}(\dot{\gamma}_\alpha)\tau_0 \left|\frac{\dot{\gamma}_\alpha}{\dot{\gamma}_0}\right|^{m}$$

Constitutive Modeling

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Defect energy (quadratic)

$$W_d = \frac{1}{2}\vec{\rho}\cdot \underline{\underline{E}}\,\vec{\rho}, \qquad \vec{\rho} = (\rho_{\vdash}^{1},\ \rho_{\vdash}^{2},\ ...,\rho_{\vdash}^{N},\ \rho_{\odot}^{1},\ \rho_{\odot}^{2},\ ...,\rho_{\odot}^{N})$$

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- Leads to linear dependence of the defect stress on the dislocation densities

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- Leads to linear dependence of the defect stress on the dislocation densities
- Example – uncoupled quadratic ansatz:

$$W_d = \frac{1}{2}S_0 L^2 \sum_{\alpha} \left[|\rho_{\vdash}^{\alpha}|^2 + |\rho_{\odot}^{\alpha}|^2\right]; \qquad S_0,\ L = \text{const.}$$

Gurtin et al. (2007)

Constitutive Modeling

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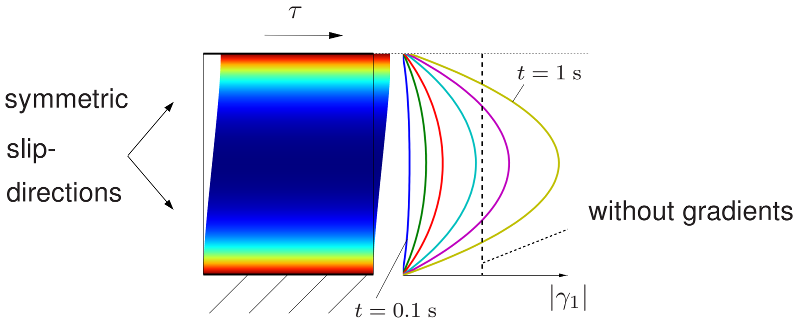
Gurtin et al. (2007)

Genereralized nonlinear ansatz

$$W_d = c_n \sum_{\alpha} \left[|\rho_{\vdash}^{\alpha} L|^n + |\rho_{\odot}^{\alpha} L|^n \right]; \qquad c_n,\ n,\ L = \text{const.}$$

Numerical Results

Infinite 2d-layer, two slip systems:



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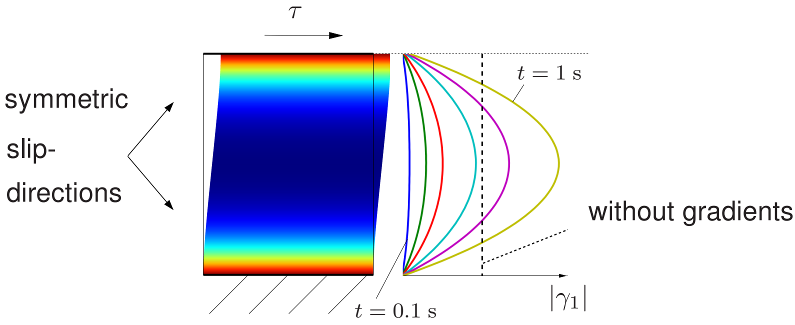

Quadratic defect energy

- leads to smooth strain curves

Numerical Results

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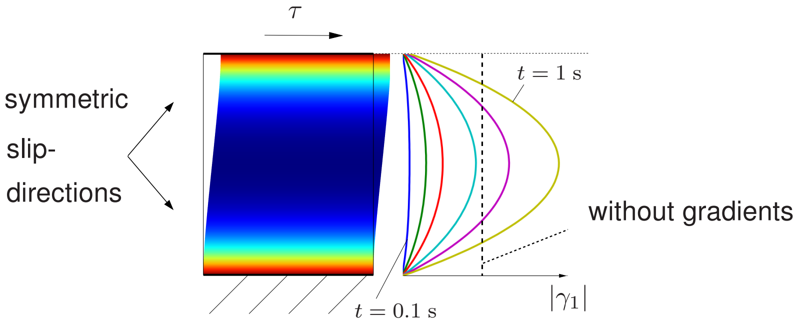
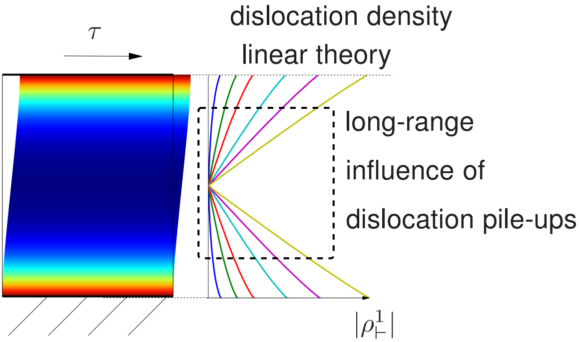


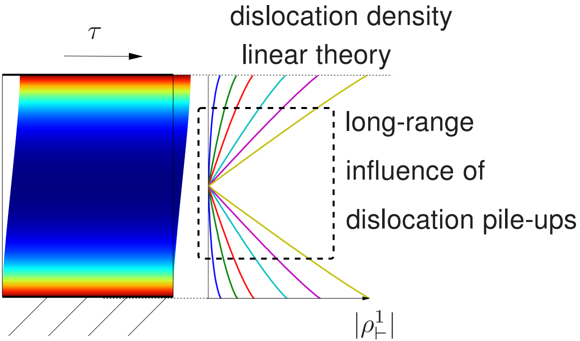
Quadratic defect energy

- leads to smooth strain curves
- long-range dislocation interactions

Numerical Results



Numerical Results



Quadratic energy

- leads to a long-range influence of the dislocation pile-ups at the boundaries on the bulk-dislocations

End of Part I

The support of the German Research Foundation (DFG) in the project "Dislocation based Gradient Plasticity Theory" of the DFG Research Group 1650 "Dislocation based Plasticity" under Grant BO 1466/5-1 is gratefully acknowledged.