Karlsruhe Institute of Technology

Chair for Continuum Mechanics
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Single Crystal Gradient Plasticity – Part II

Chair for Continuum Mechanics – Institute of Engineering Mechanics

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

Motivation

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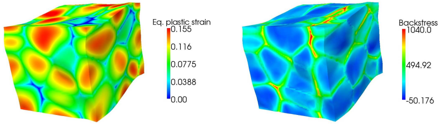
Conclusion and Outlook



Motivation

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- Typical crystal gradient plasticity extension:

$$W(...) \rightarrow W(...) + W_g(\nabla\gamma_1,\ \nabla\gamma_2,\ \dots,\ \nabla\gamma_N)$$

- **Problem**: 15 node variables (FCC)
  →**Gradients massively increase** DOFs

- **Proposition**:

$$W(...) \rightarrow W(...) + W_g(\nabla\gamma_{eq})$$

- Simplification $\boldsymbol{\alpha} \rightarrow \nabla\gamma_{eq}$

- node variables: $15 \rightarrow 4$

Equivalent Plastic Strain Gradient Crystal Plasticity

- Small Strains

$$\boldsymbol{H} = \nabla \boldsymbol{u} = \boldsymbol{H}^e + \boldsymbol{H}^p; \quad \boldsymbol{H}^p = \sum_\alpha \lambda_\alpha \boldsymbol{d}_\alpha \otimes \boldsymbol{n}_\alpha; \quad \boldsymbol{\varepsilon}^p = \sum_\alpha \lambda_\alpha \boldsymbol{M}_\alpha^S$$

  Two slip parameters λ_α per slip system, $\dot{\lambda}_\alpha \geq 0$.

- Equivalent plastic strain $\gamma_{eq} \rightarrow \sum_\alpha \lambda_\alpha = \Sigma_\lambda$

- Equality of γ_{eq} and Σ_λ is weakly enforced

- Stored Energy $W = W_e(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p) + W_h(\Sigma_\lambda) + W_g(\nabla\gamma_{eq}) + \check{p}(\Sigma_\lambda - \gamma_{eq})$
  $\check{p}$: Lagrange multiplier

- Independent variables: $\boldsymbol{u}, \lambda_\alpha, \gamma_{eq}$

Equivalent Plastic Strain Gradient Crystal Plasticity

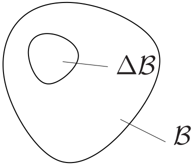
Variation of displacements ($\delta\lambda_\alpha = \delta\gamma_{eq} = 0$)

$$\delta \int_{\Delta\mathcal{B}} W \,\mathrm{d}v = \int_{\Delta\mathcal{B}} \partial_{\boldsymbol{\varepsilon}} W \cdot \delta\boldsymbol{\varepsilon} \,\mathrm{d}v = \int_{\partial\Delta\mathcal{B}} \boldsymbol{t} \cdot \delta\boldsymbol{u} \,\mathrm{d}a \qquad (1)$$

$$\Leftrightarrow \quad \int_{\partial\Delta\mathcal{B}} (\partial_{\boldsymbol{\varepsilon}} W \boldsymbol{n} - \boldsymbol{t}) \cdot \delta\boldsymbol{u} \,\mathrm{d}a - \int_{\Delta\mathcal{B}} \mathrm{div}\,(\partial_{\boldsymbol{\varepsilon}} W) \cdot \delta\boldsymbol{u} \,\mathrm{d}v = 0 \qquad (2)$$

Result:

- Cauchy stress $\boldsymbol{\sigma} = \partial_{\boldsymbol{\varepsilon}} W$
- Linear momentum balance $\mathrm{div}\,(\boldsymbol{\sigma}) = 0$



Equivalent Plastic Strain Gradient Crystal Plasticity

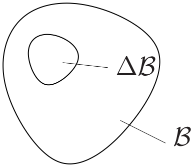
Variation of γ_{eq} $(\delta\lambda_\alpha = 0,\ \delta\boldsymbol{u} = \boldsymbol{0})$

$$\delta \int_{\Delta\mathcal{B}} W \,\mathrm{d}v \quad = \quad \int_{\Delta\mathcal{B}} (\underbrace{\partial_{\gamma_{eq}} W}_{-\check{p}} \,\delta\gamma_{eq} + \underbrace{\partial_{\nabla\gamma_{eq}} W}_{\boldsymbol{\xi}} \cdot \nabla(\delta\gamma_{eq}))\,\mathrm{d}v = \int_{\partial\Delta\mathcal{B}} \Xi\,\delta\gamma_{eq}\,\mathrm{d}a$$

$$\Leftrightarrow \quad \int_{\partial\Delta\mathcal{B}} (\boldsymbol{\xi}\cdot\boldsymbol{n} - \Xi)\cdot\delta\boldsymbol{u}\,\mathrm{d}a - \int_{\Delta\mathcal{B}} (\mathrm{div}\,(\boldsymbol{\xi}) + \check{p})\delta\gamma_{eq}\,\mathrm{d}v = 0$$

Result:

- Micro traction $\Xi = \boldsymbol{\xi}\cdot\boldsymbol{n}$
- Backstress $\check{p} = -\mathrm{div}\,(\boldsymbol{\xi})$



Equivalent Plastic Strain Gradient Crystal Plasticity

Dissipation and flow rule

$$D_{tot}(\Delta\mathcal{B}) = \int_{\partial\Delta\mathcal{B}} (\boldsymbol{t}\cdot\dot{\boldsymbol{u}} + \Xi\,\dot{\gamma}_{eq})\,\mathrm{d}a - \int_{\Delta\mathcal{B}} \dot{W}\,\mathrm{d}v \overset{!}{\geq} 0 \tag{3}$$

with $\mathrm{div}\,(\boldsymbol{\sigma}) = \boldsymbol{0}$, $\quad\boldsymbol{\sigma n} = \boldsymbol{t}$, $\quad\Xi = \boldsymbol{\xi}\cdot\boldsymbol{n}$ and $\check{p} = -\mathrm{div}\,(\boldsymbol{\xi})$:

$$D_{tot}(\Delta\mathcal{B}) = \int_{\Delta\mathcal{B}} \underbrace{\sum_\alpha (\boldsymbol{\sigma}\cdot\boldsymbol{M}_\alpha^S - \partial_{\Sigma_\lambda}W_h - \check{p})\,\dot{\lambda}_\alpha}_{\mathcal{D}}\,\mathrm{d}v \overset{!}{\geq} 0 \tag{4}$$

Local dissipation $\mathcal{D} \overset{!}{\geq} 0 \Rightarrow$ Flow rule, e. g. :

$$\dot{\lambda}_\alpha = \dot{\gamma}_0 \left\langle \frac{\tau_\alpha - (\tau_0^C + \partial_{\Sigma_\lambda}W_h + \check{p})}{\tau^D} \right\rangle^p \tag{5}$$

Equivalent Plastic Strain Gradient Crystal Plasticity

Global residuals for FE-Implementation

$$G^u = \int_{\mathcal{B}} \boldsymbol{\sigma} \cdot \delta \boldsymbol{\varepsilon} \, \mathrm{d}v - \int_{\partial \mathcal{B}_t} \bar{\boldsymbol{t}} \cdot \delta \boldsymbol{u} \, \mathrm{d}a \overset{!}{=} 0$$

$$G^{\gamma_{eq}} = \int_{\mathcal{B}} (\boldsymbol{\xi} \cdot \nabla(\delta \gamma_{eq}) - \check{p} \, \delta \gamma_{eq}) \, \mathrm{d}v - \int_{\partial \mathcal{B}_\Xi} \bar{\Xi} \, \delta \gamma_{eq} \, \mathrm{d}a \overset{!}{=} 0$$

Local (integration point) residuals based on implicit Euler:

$$\boldsymbol{r}^\sigma = \underbrace{\mathbb{C}^{-1}[\boldsymbol{\sigma}]}_{\boldsymbol{\varepsilon}^e} - \left(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p_n - \sum_\alpha \Delta \lambda_\alpha (\boldsymbol{\sigma}, \check{p}) \boldsymbol{M}^S_\alpha \right) \overset{!}{=} \boldsymbol{0}$$

$$r^p = \gamma_{eq} - \left(\gamma_{eq,n} + \sum_\alpha \Delta \lambda_\alpha (\boldsymbol{\sigma}, \check{p}) \right) \overset{!}{=} 0$$

Possible Enhancements/Modifications

- Penalty approximation

$$W = W_e(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p) + W_h(\Sigma_\lambda) + W_g(\nabla\gamma_{eq}) + \check{p}(\Sigma_\lambda - \gamma_{eq})$$

$$\rightarrow \qquad W = W_e(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p) + W_h(\Sigma_\lambda) + W_g(\nabla\gamma_{eq}) + \frac{1}{2}H_\chi(\Sigma_\lambda - \gamma_{eq})^2$$

  - Penalty parameter H_χ: large number
  - Energy $1/2H_\chi(\Sigma_\lambda - \gamma_{eq})^2$ penalizes deviations of Σ_λ from γ_{eq}

- Grain Boundary Yield Criterion

$$f_\Gamma = [\![\Xi]\!] - \Xi^C$$

  - Ξ^C: Grain boundary yield stress
  - Grain boundary yield resistance
  - Delays initiation of plastic flow on the grain boundaries

Simulation Results

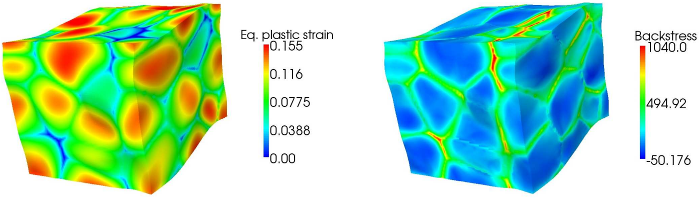


Figure: Periodic Simulation, 2 Mio. Dof

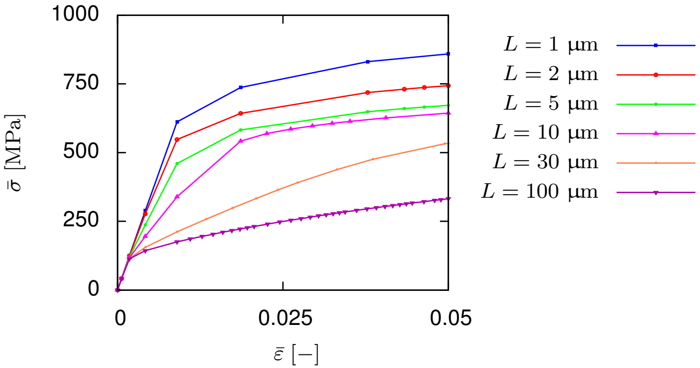
Hardening model

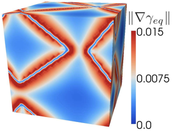
$$W_g = \frac{1}{2} K_G \nabla \gamma_{eq} \cdot \nabla \gamma_{eq}; \quad W_h(\Sigma_\lambda) = \tau_\infty^C \Sigma_\lambda + \frac{1}{\theta_0} (\tau_\infty^C - \tau_0^C)^2 \exp\left(-\frac{\theta_0 \Sigma_\lambda}{\tau_\infty^C - \tau_0^C} \right)$$

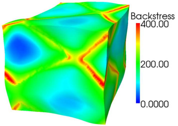
Material Parameters

E	ν	$\dot{\gamma}_0$	p	τ^D	τ_0^C	τ_∞^C	θ_0	K_G
70 GPa	0.34	10^{-3} s^{-1}	50	1 MPa	50 MPa	100 MPa	500 MPa	0.01 N

Macro Response







Comparison With Hall-Petch Relation

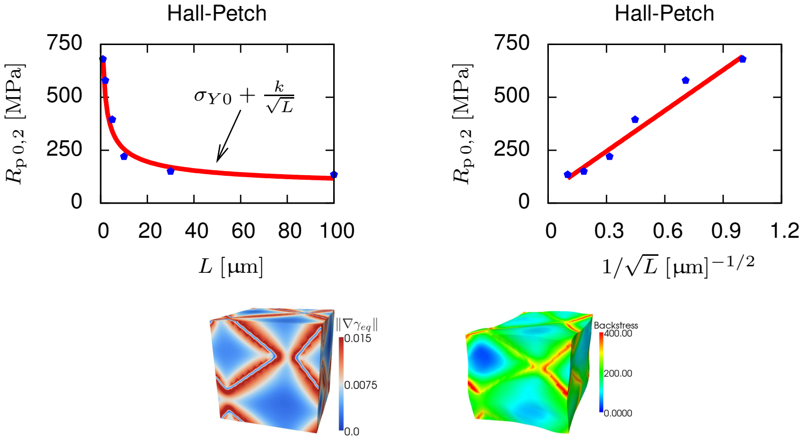
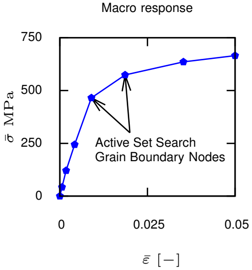


Figure: Tensile test with periodic 2-grain microstructure

Convergence

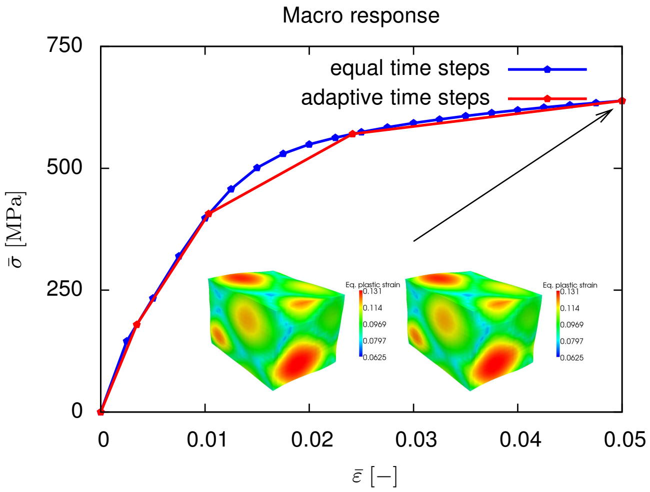
Euclidean Norm of Force Residual

Δt : 0.012 s	0.024 s	0.048 s	0.096 s	0.192 s	0.333 s	0.295 s
1.16e+03	2.33e+03	4.64e+03	9.19e+03	1.83e+04	3.12e+04	2.66e+04
5.20e-01	5.79e+00	1.15e+04	2.55e+04	4.03e+04	3.85e+02	3.45e+02
9.11e-04	2.28e-01	8.26e+01	1.73e+02	2.66e+02	1.64e+02	1.87e+02
1.35e-05	2.20e-04	2.35e+01	3.15e+01	4.13e+01	3.84e+01	9.05e+01
2.01e-07	3.31e-06	3.71e+00	4.30e+00	6.23e+00	9.57e+00	2.09e+01
2.97e-09	5.00e-08	2.10e-01	4.24e-01	5.65e-01	4.12e+00	4.87e+00
		1.63e-02	2.91e-02	1.88e-02	5.67e-01	1.18e+00
		2.48e-04	3.64e-04	5.44e-05	7.97e-03	1.53e-01
		5.35e-07	5.21e-07	4.37e+02	3.94e-05	2.35e-02
		3.16e-09	6.48e+01	9.35e+01	1.24e-06	1.26e-04
			1.22e+00	3.19e+01		1.03e-06
			5.01e-02	3.00e+00		
			3.10e-04	2.80e-01		
			8.44e-07	9.25e-03		
			2.13e+01	5.47e-05		
			2.46e-01	4.67e+01		
			2.56e-03	6.73e-01		
			3.49e-06	8.37e-03		
			4.66e+00	1.71e-05		
			8.48e-03	1.47e-07		
			1.41e-05			
			2.20e-01			
			1.28e-04			
			1.79e-07			
			3.56e-09			



Marked in red: Active set search of grain boundary nodes

Dependence on Time Step Size



Improvement of Cross Hardening Model

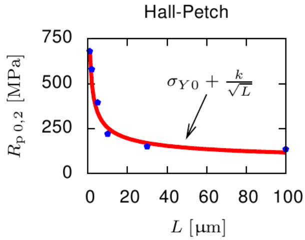
- Cross hardening is modelled by $W_h(\Sigma_\lambda)$
  $\rightarrow$ phenomenological approach
- Replacement by dislocation based approach
  $$\tau^C = \tau^C(\rho) = \tau_0^C + aGb\sqrt{\rho}$$
- Advanced dislocation density model (until now only single slip)

$$\begin{aligned}
\partial_t \rho &= -\operatorname{div}\left(\boldsymbol{\kappa}^\perp \nu\right) + \overline{\rho k}\nu \\
\partial_t \overline{\rho k} &= -\operatorname{div}\left(\overline{\rho k}/\rho\, \nu \boldsymbol{\kappa}^\perp + \rho/2\, \nabla_p \nu\right) \\
\dot{\lambda} &= \rho b \nu \\
\nu &= \nu_0 \operatorname{sgn}(\tau) \left\langle \frac{|\tau| - \tau^C - \check{p}}{\tau^D} \right\rangle^p
\end{aligned}$$

with $\boldsymbol{\kappa}^\perp = 1/b(\boldsymbol{I} - \boldsymbol{n} \otimes \boldsymbol{n})\nabla\lambda$ and $\nabla_p \nu = (\boldsymbol{I} - \boldsymbol{n} \otimes \boldsymbol{n})\nabla\nu$.
Accounts for dislocation transport and curvature-induced line length production.

Summary

- Crystal plasticity model enhanced by gradient of equivalent plastic strain
- DOFs per node massively reduced
- Leads to backstress formally similar to other theories
- Classical FE-implementation + Grain boundary yield condition
- Converging results
- Results close to Hall Petch relation



End of Part II

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.