COMPUTATIONAL ISSUES OF GRADIENT-EXTENDED CRYSTAL INELASTICITY

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Summary. In this paper we discuss issues related to the theoretical as well as the computational format of gradient-extended crystal viscoplasticity. The so-called "primal" format uses the internal variables and the displacements as the primary unknown fields. An alternative format is coined the "semi-dual format", which in addition includes microstresses, thereby defining a mixed variational problem. We compare the primal and semi-dual variational formats in terms of pros and cons from a modeling as well as a numerical viewpoint. We perform a set of numerical tests to investigate the rate of convergence for errors in different norms.

1 INTRODUCTION

Crystal plasticity is the accepted model framework for incorporating microstructural information in continuum theory with application to crystalline metals where dislocations constitute the mechanism behind inelastic deformation. Various explicit models based on this conceptual background have been proposed, for example by Gurtin et al[1]. However, several modeling issues still await their resolution. An elegant way of unifying gradient theory for different application models, including inelasticity, damage and phase-field models, was presented by Miehe[2].

The so-called "primal" format uses the internal variables and the displacements as the primary unknown fields. An alternative format is coined the "semi-dual format", which in addition includes the microstresses and thereby define a mixed variational problem.

In this paper we focus on issues related to the theoretical and computational format of material models with gradient variables. We compare the primal and semi-dual variational formats in terms of pros and cons from modeling as well as numerical aspects.

2 PROTOTYPE MODEL OF GRADIENT EXTENDED CRYSTAL VISCO ELASTICITY

In the chosen prototype model for crystal inelasticity, the stress $\boldsymbol{\sigma}$ is given as

$$\boldsymbol{\sigma} = \mathbf{E}^{\mathrm{e}} : [\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^{\mathrm{p}}(\underline{\gamma})], \quad \boldsymbol{\epsilon}^{\mathrm{p}} \stackrel{\mathrm{def}}{=} (\boldsymbol{h}^{\mathrm{p}})^{\mathrm{sym}}, \quad \boldsymbol{h}^{\mathrm{p}} \stackrel{\mathrm{def}}{=} \sum_{\alpha=1}^{M} \gamma_{\alpha} \boldsymbol{s}_{\alpha} \otimes \boldsymbol{m}_{\alpha}, \tag{1}$$

where $\boldsymbol{\epsilon}$ is the strain, $\mathbf{E}^{\mathrm{e}}$ is the elastic modulus and $\boldsymbol{s}_{\alpha}$, $\boldsymbol{m}_{\alpha}$ are the slip direction and the normal to the slip plane, respectively. The "slip" associated with the slip system $(\boldsymbol{s}_{\alpha}, \boldsymbol{m}_{\alpha})$ is denoted γ_{α}. We thus treat $\underline{\gamma}$ as a set of internal variables[*].

Associated with each slip system, we introduce kinematic hardening that is represented by the gradient variables $\boldsymbol{g}_{\alpha} \stackrel{\mathrm{def}}{=} \boldsymbol{\nabla} \gamma_{\alpha}$. The free energy density ψ is then proposed as the additive decomposition

$$\psi\left(\boldsymbol{\epsilon}, \underline{\gamma}, \underline{\boldsymbol{g}}\right) = \psi^{\mathrm{e}}(\boldsymbol{\epsilon}, \underline{\gamma}) + \sum_{\alpha=1}^{M} \psi_{\alpha}^{\mathrm{g}}(\boldsymbol{g}_{\alpha}),$$

where ψ^{e} is the contribution from elastic (stored) energy, whereas $\psi_{\alpha}^{\mathrm{g}}$ are the contributions from gradient hardening in the slip systems. More specifically

$$\psi^{\mathrm{e}}(\boldsymbol{\epsilon}, \underline{\gamma}) = \frac{1}{2}[\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^{\mathrm{p}}(\underline{\gamma})] : \mathbf{E}^{\mathrm{e}} : [\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^{\mathrm{p}}(\underline{\gamma})], \quad \psi_{\alpha}^{\mathrm{g}}(\boldsymbol{g}_{\alpha}) = \frac{1}{2}(l_{\alpha})^{2} \boldsymbol{g}_{\alpha} \cdot \boldsymbol{H}_{\alpha}^{\mathrm{gra}} \cdot \boldsymbol{g}_{\alpha} \tag{2}$$

where we introduced the gradient hardening tensors $\boldsymbol{H}_{\alpha}^{\mathrm{gra}}$.

A dual dissipation function $\phi_{\alpha}^{*}(\tau_{\alpha}^{\mathrm{di}})$, that is associated with each slip system, is chosen as $\phi_{\alpha}^{*} = \frac{1}{t_{*}}\Gamma(|\tau_{\alpha}^{\mathrm{di}}|)$ where $\tau_{\alpha}^{\mathrm{di}}$ are (scalar) "dissipative microstresses" that are energy-conjugated to $\dot{\gamma}_{\alpha}$.

In order to "close" the problem formulation, we need to establish the Biot equations or *microforce balance*[3] which in this case read

$$\tau_{\alpha}^{\mathrm{en}} + \tau_{\alpha}^{\mathrm{di}} - \boldsymbol{\xi}_{\alpha}^{\mathrm{en}} \cdot \boldsymbol{\nabla} = 0 \tag{3}$$

where the "energetic microstresses" $\tau_{\alpha}^{\mathrm{en}} = \partial\psi/\partial\gamma_{\alpha}$ and $\boldsymbol{\xi}_{\alpha}^{\mathrm{en}} = \partial\psi/\partial\boldsymbol{g}_{\alpha}$ are energy conjugated to γ_{α} and $\boldsymbol{g}_{\alpha}$ respectively.

3 PRIMAL VARIATIONAL FORMAT

In order to establish the proper variational format, we introduce the suitable sets of trial functions for displacements ($\mathbb{U}$), slip variables ($\mathbb{G}$) and dissipative microstresses ($\mathbb{T}$).

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[*]With an underline we denote a tuple with the same number of elements as slip systems, i.e. $\underline{\gamma} = (\gamma_{1}, \gamma_{2}, \dots, \gamma_{M})$.

The primal variational format can be stated as follows: Find $\boldsymbol{u} \in \mathbb{U}$, $\gamma_\alpha \in \mathbb{G}_\alpha$, and $\tau_\alpha^{\mathrm{di}} \in \mathbb{T}$ that solve

$$\int_\Omega \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}], \underline{\gamma}) : \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \, \mathrm{d}\Omega = l^{(u)}(\delta\boldsymbol{u}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0, \qquad (4a)$$

$$\int_\Omega [\tau_\alpha^{\mathrm{en}}(\boldsymbol{\epsilon}[\boldsymbol{u}], \underline{\gamma}) + \tau_\alpha^{\mathrm{di}}]\delta\gamma_\alpha \, \mathrm{d}\Omega + \int_\Omega \boldsymbol{\xi}_\alpha(\boldsymbol{g}[\gamma_\alpha]) \cdot \boldsymbol{g}[\delta\gamma_\alpha] \, \mathrm{d}\Omega = l_\alpha^{(\gamma)}(\delta\gamma_\alpha) \quad \forall \delta\gamma_\alpha \in \mathbb{G}^0, \qquad (4b)$$

$$\int_\Omega \left[\gamma_\alpha - \Delta t \frac{\partial \phi_\alpha^*(\tau_\alpha^{\mathrm{di}})}{\partial \tau_\alpha^{\mathrm{di}}} \right] \delta\tau_\alpha^{\mathrm{di}} \, \mathrm{d}\Omega = \int_\Omega {}^n\gamma_\alpha \delta\tau_\alpha^{\mathrm{di}} \, \mathrm{d}\Omega \quad \forall \delta\tau_\alpha^{\mathrm{di}} \in \mathbb{T}, \qquad (4c)$$

where $\mathbb{U}^0$, $\mathbb{G}^0$ and $\mathbb{T}$ are the pertinent test spaces. Here, we introduced the data in terms of the linear functionals

$$l^{(u)}(\delta\boldsymbol{u}) = \int_\Omega \boldsymbol{b} \cdot \delta\boldsymbol{u} \, \mathrm{d}\Omega + \int_{\Gamma_t} \boldsymbol{t} \cdot \delta\boldsymbol{u} \, \mathrm{d}S \quad \text{and} \quad l_\alpha^{(\gamma)}(\delta\gamma) = \int_{\Gamma_t^{(\gamma)}} \bar{t}_\alpha^{(\gamma)}\delta\gamma_\alpha \, \mathrm{d}S, \qquad (5)$$

while essential boundary conditions are incorporated implicitly in the formulation of the trial sets.

3.1 DUAL VARIATIONAL FORMAT

In the (semi-)dual variational format we exploit a partial Legendre transformation to ψ w.r.t. to the gradient variables $\boldsymbol{g}_\alpha$:

$$\psi_\alpha^{*g}(\boldsymbol{\xi}_\alpha) = \frac{1}{2} \frac{1}{(l_\alpha)^2} \boldsymbol{\xi}_\alpha \cdot \boldsymbol{H}_\alpha^{*\mathrm{gra}} \cdot \boldsymbol{\xi}_\alpha. \qquad (6)$$

The dual variational format thus becomes as follows: Find $\boldsymbol{u} \in \mathbb{U}$, $\boldsymbol{\xi}_\alpha \in \mathbb{X}_\alpha$, $\gamma_\alpha \in \mathbb{T}$, and $\tau_\alpha^{\mathrm{di}} \in \mathbb{T}$ that solve

$$\int_\Omega \boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}], \underline{\gamma}) : \boldsymbol{\epsilon}[\delta\boldsymbol{u}] \, \mathrm{d}\Omega = l^{(u)}(\delta\boldsymbol{u}) \quad \forall \delta\boldsymbol{u} \in \mathbb{U}^0, \qquad (7a)$$

$$\int_\Omega [-\boldsymbol{g}_\alpha(\boldsymbol{\xi}_\alpha) \cdot \delta\boldsymbol{\xi}_\alpha - \gamma_\alpha[\delta\boldsymbol{\xi}_\alpha \cdot \boldsymbol{\nabla}]] \, \mathrm{d}\Omega = l_\alpha^{(\xi)}(\delta\boldsymbol{\xi}_\alpha) \quad \forall \delta\boldsymbol{\xi}_\alpha \in \mathbb{X}^0, \qquad (7b)$$

$$\int_\Omega [\tau_\alpha^{\mathrm{en}}(\boldsymbol{\epsilon}[\boldsymbol{u}], \underline{\gamma}) + \tau_\alpha^{\mathrm{di}} - \boldsymbol{\xi}_\alpha \cdot \boldsymbol{\nabla}]\delta\gamma_\alpha \, \mathrm{d}\Omega = 0 \quad \forall \delta\gamma_\alpha \in \mathbb{T}, \qquad (7c)$$

$$\int_\Omega \left[\gamma_\alpha - \Delta t \frac{\partial \phi_\alpha^*(\tau_\alpha^{\mathrm{di}})}{\partial \tau_\alpha^{\mathrm{di}}} \right] \delta\tau_\alpha^{\mathrm{di}} \, \mathrm{d}\Omega = \int_\Omega {}^n\gamma_\alpha \delta\tau_\alpha^{\mathrm{di}} \, \mathrm{d}\Omega \quad \forall \tau_\alpha^{\mathrm{di}} \in \mathbb{T}, \qquad (7d)$$

where we introduced the data in terms of the linear functional

$$l^{(u)}(\delta\boldsymbol{u}) = \int_\Omega \boldsymbol{b} \cdot \delta\boldsymbol{u} \, \mathrm{d}\Omega + \int_{\Gamma_u} \boldsymbol{t} \cdot \delta\boldsymbol{u} \, \mathrm{d}S \quad \text{and} \quad l_\alpha^{(\xi)}(\delta\boldsymbol{\xi}_\alpha) = -\int_{\Gamma_u^{(\gamma)}} \bar{\gamma}_\alpha[\delta\boldsymbol{\xi}_\alpha \cdot \boldsymbol{n}] \, \mathrm{d}S. \qquad (8)$$

In the dual formulation, $\mathbb{X}_\alpha$ and $\mathbb{X}^0$ are the sets of trial and test functions, respectively, for the fields $\boldsymbol{\xi}_\alpha$. A difference in the boundary conditions from the primary format is that the type of the boundary conditions on the different parts of Γ have switched their roles.
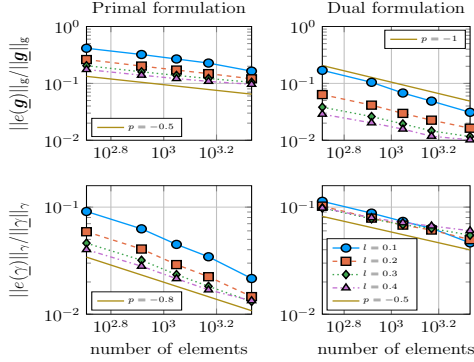
Figure 1: Convergence of errors in the slip $\underline{\gamma}$ and its spatial derivative $\underline{\boldsymbol{g}} = \nabla\underline{\gamma}$ for different values of the internal length scale l.

Parameter	Value
Young's modulus E	$200\,\text{kPa}$
Poisson's ratio ν	0.3
Norton exponent n	2
Edge modulus $H_{\perp,\alpha}$	$0.1\,E$
Norton factor C_α	$1\,\text{kPa}$
Regularization parameter t_*	$1000\,\text{s}$

Table 1: Parameters for the analyses

4 NUMERICAL RESULTS

The two variational formats are solved for approximately using lowest order finite element approximations. We set up a polygon-shaped 2D single crystal with non-homogeneous Dirichlet boundary conditions on the displacement field and microhard boundary conditions for the slip (i.e. $\gamma_\alpha = 0$). The crystal contains two slip systems at with slip direction $20°$ and $40°$. We define the error of a field in a point as the difference in the field between the solution on a coarse mesh and the overkill solution, $e(\bullet) = \bullet - \bullet_h$. Figure 1 shows the convergence with respect to mesh refinement of the error in the gradient of the slip $||e(\boldsymbol{g})||_{\text{g}}/||\boldsymbol{g}||_{\text{g}}$ and the error in the slip $||e(\boldsymbol{\gamma})||_\gamma/||\boldsymbol{\gamma}||_\gamma$. Here $||\underline{\boldsymbol{g}}||$ and $||\underline{\gamma}||_\gamma$ define the pertinent norms for the gradient and plastic slip field, respectively. As expected, we note that the error in slip is smaller for the primal format, whereas the approximation of the gradient is superior in the (semi-)dual formulation.

5 CONCLUSIONS

We have presented two formulations of a crystal viscoelasticity model and examined the convergence rate for different errors and showed that the dual formulation converges faster for the gradient field while the primal formulation converges faster for the slip field.

[1] Gurtin, M. E., Anand, L. & Lele, S. P. Gradient single-crystal plasticity with free energy dependent on dislocation densities. *Journal of the Mechanics and Physics of Solids* **55**, 1853 – 1878 (2007).

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