On the implementation of rate-independent gradient-enhanced crystal plasticity theory

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In the present work, classical local crystal plasticity is reformulated using incremental energy minimization. The resulting constrained optimization problem is efficiently solved by a nonlinear complementary problem, which additionally solves the problem of determination of the set of active slip systems. The model is extended to a nonlocal, gradient-enhanced, formulation by employing and adapting the micromorphic approach. By doing so, the implementation of the gradient-enhanced model is almost identical to that of the original local one, with the exception of additional balance equations.

1 Introduction

Gradient enhancements have been widely discussed and implemented, since they solve many problems known from the classical local formulations. These problems include the pathological mesh-dependencies induced by softening and a missing possibility to introduce plastic size effects like, e.g., the well-known Hall-Petch relationship. In this work, a micromorphic approach (see [1]) is applied, since this approach, additionally to the aforementioned advantages of a general nonlocal model, retains the variational formulation presented (see [2]) and does not affect the underlying local problem.

The local minimization problem, consisting of a set of Karush-Kuhn-Tucker inequalities known from rate-independent plasticity, presents a challenging task, since the set of active slip systems is not known a priori, cf. [3]. This problem is solved by using the nonlinear complementary problem proposed by Fischer and Burmeister, cf. [4].

2 Crystal plasticity theory — Fundamentals and Implementation

2.1 Classical local crystal plasticity theory

The classical, local crystal plasticity theory is based on a multiplicative split of the deformation gradient $F = 1 + \nabla u = F^e \cdot F^p$ into an elastic and a plastic part. The free energy function $\Psi(F^e, \alpha) = \Psi(F^e) + \Psi(\alpha)$ is additively decomposed where $\alpha$ is a set of internal variables related to hardening. After introducing the thermodynamic driving forces $\Sigma(F^p) := -\partial_{F^e} \Psi \cdot [F^p]^T$ and $Q^i(\alpha) := -\partial_{\alpha^i} \Psi$ one can define the well-known Schmid-type yield function

$$\phi^i = \Sigma : \left[ M^i \otimes N^i \right] - \left[ Q^i_0 + Q^i \right] \leq 0,$$

where $M^i$ and $N^i$ are orthogonal vectors describing the $i$-th slip system and $Q^i_0$ denotes the initial yield limit. Exploiting the postulate of maximum dissipation, the associated evolution equations become

$$\dot{F}^p, [F^p]^{-1} = \sum_{i} \dot{\gamma}^i M^i \otimes N^i, \dot{\gamma}^i = \text{sign} \left( \Sigma : \left[ M^i \otimes N^i \right] \right) \lambda^i, \dot{\lambda}^i = -\lambda^i.$$  

For the variational formulation (see e.g. [2]), rate potential $\hat{\mathcal{L}} := \int_{\Omega} \left[ \Psi + D_{\text{int}} \right] dV + \mathcal{P}_{\text{ext}}$ is considered. Here, $D_{\text{int}} = \sum_{i} Q^i \lambda^i$ is the internal dissipation and $\mathcal{P}_{\text{ext}}$ is the power of externally applied forces on a body $\Omega$. The mechanical problem is now expressed by the problem of stationarity

$$\text{stat}_{\delta u, \lambda} \left\{ \hat{\mathcal{L}}(u, \lambda) : (\Sigma, Q) \in \mathbb{E} \right\} \text{ with } \mathbb{E} := \left\{ (\Sigma, Q) \in \mathbb{R}^{3\times3} + n_{\text{sys}} \mid \phi^i(\Sigma, Q^i) \leq 0 \; \forall i \right\}. \tag{3}$$

The stationarity conditions of the aforementioned rate potential w.r.t. the velocity field and the plastic multipliers $\lambda^i$ yield the main governing equations. More precisely,

$$\delta_u \hat{\mathcal{L}} = \int_{\Omega} P : \delta \dot{F} dV + \delta_u \mathcal{P}_{\text{ext}} = 0 \quad \text{and} \quad \delta_{\lambda^i} \hat{\mathcal{L}} = -\phi^i \geq 0. \tag{4}$$

While the first equation is the balance of linear momentum, the second one corresponds to Eq. (1).

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2.2 Numerical implementation

Applying a time discretization using a backward-Euler-scheme, the local problem reduces to the set of inequalities

\[ \partial_{\Delta \lambda^{(i)}} I^{(i)} \geq 0 \land \Delta \lambda^{(i)} \geq 0 \land \partial_{\Delta \lambda^{(i)}} I^{(i)} \Delta \lambda^{(i)} = 0 \quad \forall i, \]

which can be reformulated into the nonlinear complementary problem (NCP) using the approach of Fischer and Burmeister (see [4, 5]),

\[ \tilde{\phi}^{(i)} := \sqrt{[\partial_{\Delta \lambda^{(i)}} I^{(i)}]^2 + [\Delta \lambda^{(i)}]^2 + 2 \delta^2 - \partial_{\Delta \lambda^{(i)}} I^{(i)} - \Delta \lambda^{(i)}} = 0 \quad \forall i. \]

By doing so, no cumbersome search for the set of active slip systems is required. By setting the perturbation parameter \( \delta = 0 \), eqs. (5) are fulfilled strictly. In a numerical implementation however, choosing a numerically small perturbation \( \delta = \epsilon \neq 0 \) has been found to be more stable while approximating the original set of inequalities with sufficient accuracy, see [6].

2.3 Gradient enhanced Crystal Plasticity

In order to extend the local crystal plasticity model, presented in the previous subsection, to a non-local gradient-extended formulation, the micromorphic approach is adopted, see e.g. [1]. Here, additional field variable \( \varphi_p^{(i)} \) for every slip system is introduced and coupled to internal variable \( \alpha^{(i)} \) via penalization energy \( \Psi_{\text{intr}}(\alpha, \varphi_p) \). Then, an additional part of the free energy can be formulated to introduce size effects in dependence of gradients of the new field variable, e.g.

\[ \Psi_{\text{glob}} = \Psi_{\text{glob}}(\varphi, \nabla \varphi). \]

The main advantage of this approach is that the local implementation is almost unaffected — particularly, no inequalities have to be solved at the global, finite element, level. The extended mechanical variational problem reads \( \text{stat}_{(u, \lambda, \varphi)} \{ I(u, \lambda, \varphi) \mid (\Sigma, Q) \in B \} \).

In Fig. 1 one can see the size effect in a tensile-test of a single crystal of length \( L = 84 \mu m \) for varying length scales \( l_c \). Here, a quadratic energy \( \Psi_{\text{glob}} = \frac{1}{2} \mu \| \nabla \varphi_p \|^2 \) and a Neo-Hooke-type elastic energy are assumed, with first Lamé parameter \( \Lambda = 35.9133 \) GPa, shear modulus \( \mu = 21.1 \) GPa and initial yield limit \( Q_{0}^{(i)} = 0.06 \) GPa. The crystal axes are not oriented in specimen direction. It bears emphasis that hardening effects are solely introduced via the gradient enhancement, since the underlying local model does not capture hardening (perfect plasticity).

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