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Application of non-convex rate dependent gradient plasticity to the modeling and simulation of inelastic microstructure development and inhomogeneous material behavior

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ABSTRACT

In this study, a two-dimensional rate-dependent gradient crystal plasticity model for non-convex energetic hardening is formulated and applied to the simulation of inelastic microstructure formation. In particular, non-convex hardening is modeled via a Landau–Devonshire potential for self-hardening and two interaction-matrix-based forms for latent hardening. The algorithmic formulation and the numerical implementation treats the displacement and the glide-system slips as the primary field variables. The numerical simulations are carried out for the case of tensile loading with periodic displacement and slip boundary conditions. The results for the formation of inelastic microstructures and their evolution under mechanical loading are illustrated together with the macroscopic stress–strain responses.

1. Introduction

Although now a basic tenet of modern material modeling and material science, the idea that material properties and mechanical behavior are determined by the presence and evolution of an underlying inhomogeneous inelastic microstructure is still an issue of detailed research. Typical examples of such inelastic microstructure include Lüders band (e.g., [35]) or Portevin–Le Chatelier bands [34,49], or dislocation cell structures (e.g., labyrinth, mosaic, fence or carpet structures) (e.g., [37,43,44,18,42,19]).

The fact that materials with microstructure are widely spread in nature leads to a thorough research in the field of computational modeling. Crystal plasticity is of particular interest in the class of materials with plastic behavior since the deformation is mainly determined by the deformation of the underlying microstructure (e.g., [15,21]). To include micro-effects in a macroscopic model, a complete scale separation is usually required. However, standard crystal plasticity models do not contain intrinsic material length-scales. This implies that these models are not capable of capturing macroscopic size-dependent effects. With regards to model development, the focus in recent years has been on the formulation of models encompassing multiple length- and/or timescales. Therefore extensions of the non-local crystal plasticity theory have been developed. For example, in Ortiz and Repettto [33] and Ortiz et al. [32] a non-local extension based on an idealization of dislocation microstructures as sequential laminates is presented, which is algorithmically performed with the procedure of incremental energy minimization. In further works (e.g., [11,29,23]), it has been proven that with the help of their incremental form, inelastic initial boundary-value problems (IBVPs) can be formulated in a variational setting to obtain evolving deformation microstructures. Alternative, two recent developments in the context of inelastic behavior of single- and polycrystal metals are (i) the development of gradient crystal plasticity (e.g., [17,39,14,2,7,16,24,27,28,41,6,4]) at the glide-system level and (ii) the application of microscopic phase field methods (e.g., [45]) at the single dislocation level. A prominent aspect of phase field models is the modeling of energetic microstructure interaction via non-convex contributions to the free energy of the sys-

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tem. It is known in materials science that almost all microstructure evolution processes are accompanied by non-convex free energies serving as driving force for microstructure evolution (for an overview see Ortiz and Repettto [33]). From these observations it is clear that non-convexity has to be incorporated in crystal plasticity, enabling plasticity-driven evolving microstructures. Recently, gradient plasticity has been extended in this direction in Yalcinkaya et al. [47], Klusemann et al. [20], Yalçinkaya et al. [46], Klusemann and Yalcinkaya [22], resulting in a type of coarse-grained phase field form for gradient plasticity (e.g., [45]). In particular, a polynomial-based Landau–Devonshire form for non-convex energy storage due to inelastic local deformation was examined in one dimension (1D) by Yalcinkaya et al. [47]. They demonstrated that such a form models the transition from elastic to inelastic deformation as well as the accompanying stress relaxation. From the point of view of the formulation of the corresponding initial-boundary-value problem (IBVP), the work of Yalcinkaya et al. [47] treats inelastic deformation as global and the dislocation density as local. Examples of analogous deformation-based formulations can be found in the literature (e.g., [8,1,2,9]). Alternatively (e.g., [14,7,13,5,25]), the formulation of the IBVP can be based on the dislocation density, in which case the inelastic local deformation (i.e., in the form of the flow rule) is modeled as a internal variable. These two formulations of the 1D IBVP were examined in detail with the help of continuum thermodynamic rate-variational methods [40] by Klusemann et al. [20]. As shown there, both formulations generally predict the same microstructure development and material behavior in the bulk. Near the boundaries, however, differences arise which may be due to the formulation-dependent representation of the boundary conditions.

More recently, these considerations have been extended to two dimensions (2D) in Yalçinkaya et al. [46] and Klusemann and Yalcinkaya [22]. Yalçinkaya et al. [46] investigated the microstructure evolution due to glide-system interaction (latent hardening) neglecting the self-hardening. In Klusemann and Yalcinkaya [22] the effect of an Landau–Devonshire potential, representing a form of self-hardening and neglecting the interaction between different glide systems, was investigated. In the current work the evolution of laminate-like microstructures were obtained in 2D considering both self- and latent-hardening mechanisms via direct extension of corresponding 1D works [47,20]. In addition, all models and IBVPs are formulated now in rate-variational form. The work begins in Section 2 with a synopsis of the basic model formulation together with a brief summary of the algorithmic formulation and numerical implementation. This is followed in Section 3 by a presentation and discussion of the simulation results for the case of plane strain tension. Finally, the work is summarized in Section 4.

2. Model formulation and numerical implementation

The physical model is formulated in the framework of continuum thermodynamics (e.g., [36]) history-dependent behavior. Given the resulting potential-based model form, the corresponding IBVP is amenable to formulation using rate-variational methods (e.g., [40,41]). For simplicity, attention is restricted to isothermal, quasi-static, and infinitesimal deformation processes. All external supplies of momentum, energy, and so on, are negligible in the current context. Let B represent the reference configuration of material of interest with boundary ∂B. Besides the displacement $\boldsymbol{u}$, the glide system slips $\boldsymbol{\gamma} = (\gamma_1, \ldots)$ represent the unknown fields in the model.

In the current thermodynamic setting, the material behavior is either kinetic/dissipative or energetic in nature. The former is accounted for by a simple rate-dependent power-law form

$$\chi = \sum_{\alpha} \frac{1}{m_0+1}\ \sigma_{\mathrm{D}0}\ \dot{\gamma}_0\ \left|\frac{\dot{\gamma}_\alpha}{\dot{\gamma}_0}\right|^{m_0+1} \tag{2.1}$$

for the dissipation potential. Here, $\dot{\gamma}_0$ denotes the material deformation rate, $\sigma_{\mathrm{D}0}$ the drag stress, and m_0 is the rate sensitivity. Since this form of χ is non-negative and convex in $\dot{\gamma}_\alpha$, it satisfies the dissipation principle (e.g., Silhavy [36]) sufficiently. Note that this form tacitly assumes zero activation energy or stress for the initiation of inelastic flow. Since the current work is concerned with purely qualitative effects, $m_0 = 1$ is chosen for simplicity; as will be seen below, this results in a Ginzburg–Landau–/Allen–Cahn phase-field-like relation for each $\gamma_\alpha \in \boldsymbol{\gamma}$, with $\sigma_{\mathrm{D}0}^{-1}\ \dot{\gamma}_0$ the corresponding "mobility" in the context of (2.1).

Turning next to energetic effects on the material behavior, these include contributions from elastic strain, hardening and non-convexity reflected in the form of the free energy density ψ. In the case of non-convex gradient inelasticity [47,20], this is then modeled by the sum

$$\begin{aligned}\psi &= \frac{1}{2}\ \lambda_0\ (\boldsymbol{I}\cdot\boldsymbol{E}_{\mathrm{E}})^2 + \mu_0\ \boldsymbol{E}_{\mathrm{E}}\cdot\boldsymbol{E}_{\mathrm{E}} + \psi_\gamma \\ &\quad + \frac{1}{2}\ a_{\mathrm{E}0}\ \left(\ell_{\mathrm{E}0}^2/b^2\right)\ \sum_\alpha \varrho_\alpha(\nabla\gamma_\alpha)^2 \\ &= \psi_{\mathrm{E}} + \psi_\gamma + \psi_{\nabla\gamma}\end{aligned} \tag{2.2}$$

of elastic ψ_{E}, non-convex ψ_γ and gradient $\psi_{\nabla\gamma}$ parts, respectively. Here, λ_0 and μ_0 denotes the longitudinal and shear elastic moduli, and

$$\boldsymbol{E}_{\mathrm{E}} = \mathrm{sym}(\nabla\boldsymbol{u}) - \sum_\alpha \gamma_\alpha\ \mathrm{sym}(\boldsymbol{s}_\alpha\otimes\boldsymbol{n}_\alpha) \tag{2.3}$$

is the linear elastic strain tensor, with $\mathrm{sym}(\boldsymbol{A}) := \frac{1}{2}(\boldsymbol{A}+\boldsymbol{A}^{\mathrm{T}})$ representing the symmetric part of any second-order tensor $\boldsymbol{A}$. Further, $\boldsymbol{s}_\alpha$ and $\boldsymbol{n}_\alpha$ are the slip direction and normal of the glide system α, respectively. As well, $\varrho_\alpha := -b\boldsymbol{s}_\alpha\cdot\nabla\gamma_\alpha$ represents the (non-dimensional) density of (edge) geometrically necessary dislocations (GNDs), and b the Burgers vector magnitude as usual. As shown, the gradient energy is assumed a quadratic function of the slip gradient $\nabla\gamma_\alpha$ projected onto the glide system direction $\boldsymbol{s}_\alpha$ depending as well on the material lengthscale $\ell_{\mathrm{E}0}$ and hardening modulus $a_{\mathrm{E}0}$. From Evers et al. [14], for example, $a_{\mathrm{E}0} = E/16(1-\nu^2)$ in terms of the Young's modulus E and Poisson's ratio ν. The specific forms of the non-convex potential ψ_γ are specified explicitly in the following sections (see (3.8) for Landau–Devonshire form, and (3.9) with (3.10) for latent hardening case and (3.9) with (3.11) for the case of both self and latent hardening).

Given the above constitutive relations, application of continuum thermodynamic methods (e.g., Silhavy [36], Svendsen [40]) yields

$$\boldsymbol{0} = -\delta_{\boldsymbol{u}}\zeta = \mathrm{div}(\partial_{\nabla\boldsymbol{u}}\zeta), \quad \partial_{\dot{\gamma}_\alpha}\chi = -\delta_{\dot{\gamma}_\alpha}\zeta = \mathrm{div}(\partial_{\nabla\dot{\gamma}_\alpha}\zeta) - \partial_{\dot{\gamma}_\alpha}\zeta, \tag{2.4}$$

for quasi-static momentum balance and the (now non-local) glide-system flow rule, respectively, in B, with $\delta_x f := \partial_x f - \mathrm{div}\,(\partial_{\nabla x} f)$ the variational derivative. Here,

$$\begin{aligned}\zeta &= \partial_{\nabla\boldsymbol{u}}\psi\cdot\nabla\dot{\boldsymbol{u}} + \sum_\alpha \partial_{\dot{\gamma}_\alpha}\psi\ \dot{\gamma}_\alpha + \partial_{\nabla\dot{\gamma}_\alpha}\psi\ \nabla\dot{\gamma}_\alpha, \\ &= \boldsymbol{T}\cdot\mathrm{sym}(\nabla\dot{\boldsymbol{u}}) + \sum_\alpha (\partial_{\dot{\gamma}_\alpha}\psi - \tau_\alpha)\ \dot{\gamma}_\alpha - a_{\mathrm{E}0}\ (\ell_{\mathrm{E}0}^2/b)\ \varrho_\alpha\ \boldsymbol{s}_\alpha\cdot\nabla\dot{\gamma}_\alpha,\end{aligned} \tag{2.5}$$

is the energy storage rate density,

$\boldsymbol{T} = \partial_{\boldsymbol{E}_{\mathrm{E}}}\psi = \mathcal{C}_{\mathrm{E}}\ \boldsymbol{E}_{\mathrm{E}}$ is the stress tensor, and $\tau_\alpha = \boldsymbol{s}_\alpha\cdot\boldsymbol{T}\boldsymbol{n}_\alpha$ is the resolved Schmid stress as usual. Restricting attention to kinematic-type boundary conditions here for simplicity, $\dot{\boldsymbol{u}}$ and $\dot{\boldsymbol{\gamma}}$ are specified on ∂B. As discussed in detail elsewhere (Svendsen [40], Svendsen and Bargmann [41]), using such relations and assumptions, one can formulate the corresponding IBVP for fields like $\boldsymbol{u}$ and each γ_a -