MODELING OF INELASTIC MICROSTRUCTURE DEVELOPMENT AND INHOMOGENEOUS MATERIAL BEHAVIOUR VIA NON-CONVEX RATE-DEPENDENT GRADIENT PLASTICITY

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Summary The formulation of gradient inelasticity models has generally been focused on the effects of additional size-dependent hardening on the material behavior. Recently, the formulation of such models has taken a step in the direction of phase-field-like models in the sense that energetic microstructure interaction and development is accounted for via non-convex contributions to the free energy of the system. In the current work, the formulation of such free energy models and the corresponding IBVP using rate variational methods are briefly discussed. With the help of two simple models for such interaction non-convexity, it is shown that phenomena like stress relaxation after yielding as well as PLC-like serrated flow result from the corresponding inelastic deformation microstructure development and non-convexity.

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 underlying microstructure is still an issue of research in detail. In particular, with regards to model development, the focus in recent years has been on the formulation of models encompassing multiple length- and/or timescales. For the case of the inelastic behavior of single- and polycrystalline metals, for example, two recent developments in this direction are (i) the development of gradient crystal plasticity (e.g., [1, 2, 3, 4, 5, 6]) at the glide-system level, and (ii) the application of microscopic phase field methods (e.g., [7]) at the single dislocation level, in such systems. A prominent aspect of phase field models is the modeling of energetic microstructure interaction via non-convex contributions to the free energy of the system. Recently, gradient plasticity has been extended in this direction in [8, 9, 10], resulting in a type of coarse-grained phase field form for gradient plasticity (e.g., [11, 7]).

MODEL FORMULATION & EXAMPLE RESULTS

The model formulation is carried out in the framework of continuum thermodynamics and rate variational methods (e.g., [11, 6]). For simplicity, attention is restricted to isothermal, supply-free, quasi-static, infinitesimal deformation processes. In this context, besides the displacement field $\boldsymbol{u}$, the principle global unknown is the set $\boldsymbol{\gamma} = (\gamma_1, \ldots)$ of shears associated with glide systems having unit normals $(\boldsymbol{n}_1, \ldots)$. In some cases, one can also work with the corresponding dislocation densities $(\boldsymbol{\rho}_1, \ldots)$ as unknowns (e.g., [9]), where $\boldsymbol{\rho}_a = \mathrm{curl}(\gamma_a\, \boldsymbol{n}_a)$. For brevity, attention is restricted here to kinematic boundary conditions; many other types of boundary conditions (e.g., flux-type) may be considered as well (e.g., [11]). On this basis, the IBVP can be formulated with respect to a configuration B of the material in terms of the rate functional

$$R(\ldots, \dot{\boldsymbol{u}}, \dot{\boldsymbol{\gamma}}) = \int_B r(\ldots, \nabla\dot{\boldsymbol{u}}, \dot{\boldsymbol{\gamma}}, \nabla\dot{\boldsymbol{\gamma}})\, dv \tag{1}$$

and corresponding rate density $r = \zeta + \chi$, where ζ represents the stored energy rate density, and χ is the dissipation-rate density. Stationarity of R with respect to admissible variations $\delta\dot{\boldsymbol{u}}$ and $\delta\dot{\gamma}_a,\ a = 1, \ldots$, then yields the weak field relations

$$0 = \int_B \partial_{\nabla\dot{\boldsymbol{u}}} r \cdot \nabla\delta\dot{\boldsymbol{u}}\, dv\ , \quad 0 = \int_B (\partial_{\dot{\gamma}_a} r\ \delta\dot{\gamma}_a + \partial_{\nabla\dot{\gamma}_a} r \cdot \nabla\delta\dot{\gamma}_a)\, dv\ ,\ a = 1, \ldots, \tag{2}$$

of the formulation. The first of these represent the weak form of quasi-static momentum balance, while the second is the non-local flow rule.

Consider for example the simplest case of a single glide system and one-dimensional deformation in the glide direction (e.g., [8, 9]). In this case, B reduces to one dimension, e.g., a bar of length l_0. Neglecting any size-dependence of activation or yielding (e.g., [12]) for simplicity, assume (i) linear elasticity, (ii) non-convex local hardening-softening, (iii) linear non-local (i.e., gradient) hardening, and (iv) immediate activation of inelastic deformation. In this case, the simple form

$$r = E_0\,(\nabla u - \gamma) \cdot \nabla\dot{u} + \{\partial_\gamma \psi_\gamma - E_0\,(\nabla u - \gamma)\}\,\dot{\gamma} + a_{\mathrm{E0}}\, l_{\mathrm{E0}}^2\, \nabla\gamma \cdot \nabla\dot{\gamma} + \tfrac{1}{2}\,\sigma_{\mathrm{D0}}\,\dot{\gamma}_0\,|\dot{\gamma}/\dot{\gamma}_0|^2 \tag{3}$$

for r is obtained. Here, E_0 is Young's modulus, a_{E0} is the energetic gradient hardening modulus, and l_{E0} represents the corresponding material lengthscale. In addition, $\dot{\gamma}_0$ denotes the material characteristic inelastic deformation (response) rate, and σ_{D0} is the drag stress. Further, $\psi_\gamma(\gamma)$ represents the interaction hardening contribution to the free energy density. For example, [8] worked with the Landau-Devonshire form $\psi_\gamma(\gamma) = C_1\gamma^4 + C_2\gamma^3 + C_3\gamma^2$ in formal analogy

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with models for phase transitions based on strain as an order paramter (e.g., [13], Chapter 4). A generalization of this is the modified Frenkel form $\psi_\gamma(\gamma) = c_1 \{1 - \cos(c_2\,\gamma)\} + c_3\,\tanh(c_4\,|\gamma|)$ for dislocation-lattice interaction; the first part also appears in the Peierls-Nabarro dislocation model (e.g., [14], Chapter 8) or the overdamped sine Gordon continuum limit of the discrete Frenkel-Kontorova model (e.g., [15]). In particular, for very small γ, this modified Frenkel form for $\psi_\gamma(\gamma)$ reduces to a polynomial form of the Landau-Devonshire type. A comparison of the model response for these two forms is shown in Figure 1. In both cases, a strong rate-dependence of the material response and tendency to form

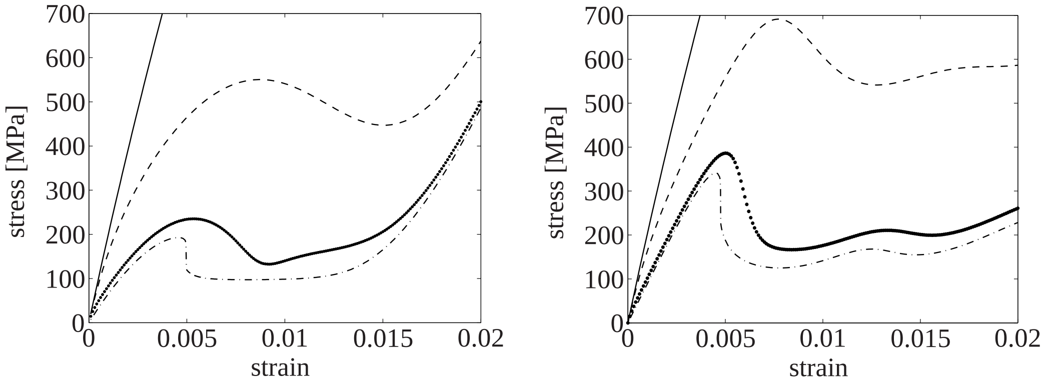

Figure 1: Stress-strain results from the Landau-Devonshire (left) and modified Frenkel (right) forms of $\psi_\gamma(\gamma)$ for hard boundary conditions ($\dot{\gamma} = 0$) and different values of the ratio $\dot{\varepsilon}_0/\dot{\gamma}_0$, with $\dot{\varepsilon}_0$ the external deformation rate: 10^2 (solid line), 10^1 (dashed line), 10^0 (thick-dotted line), 10^{-3} (dash-dotted line). These results are based on the characteristic parameter values $E_0 = 2.1 \times 10^3$ GPa, $a_{\mathrm{E0}}/E_0 = 7.0 \times 10^{-2}$, $l_{\mathrm{E0}}/l_0 = 1.0 \times 10^{-1}$ (Landau-Devonshire), $l_{\mathrm{E0}}/l_0 = 2.5 \times 10^{-1}$ (Frenkel), $\sigma_{\mathrm{D0}}/E_0 = 1.7 \times 10^{-4}$, $C_1 = 1.525 \times 10^8$, $C_2 = -5.2 \times 10^6$, $C_3 = 5.0 \times 10^4$, $c_1 = 1.0 \times 10^{-1}$ MPa, $c_2 = 5.0 \times 10^2$, $c_3 = 1.3 \times 10^0$ MPa, $c_4 = 8.0 \times 10^1$.

inelastic microstructure (as evidenced by stress relaxation after yielding) is evident. Clearly, for external rates $\dot{\varepsilon}_0$ much greater than the material rate $\dot{\gamma}_0$, the material has no time to relax the stress via inelastic microstructure formation and the response is elastic (e.g., solid curves in Figure 1). In other words, kinetic effects (i.e., too low dislocation mobility) prohibits microstructure formation. As $\dot{\varepsilon}_0$ approaches $\dot{\gamma}_0$, however, this clearly changes. In addition, in the modified Frenkel case, dislocation-lattice interaction clearly results in a type of "jerky", "wiggly" or serrated flow reminiscent of the PLC effect.

More recently, these considerations have been extended to two dimensions and latent hardening neglecting self-hardening [10]. In this context, work in progress is concerned with the formulation of such interaction models and the corresponding IBVP for both deformation and dislocation-density based approaches, including (i) ideal dislocation-dislocation (e.g., cross slip, latent hardening), (ii) dislocation-lattice, and (iii) dissociation, interactions. Examples will be given.

References

[1] Gurtin, M. E.: A gradient theory of single-crystal viscoplasticity that accounts for geometrically necessary dislocations. *J. Mech. Phys. Solids* **50** (2002), 5–32.

[2] Evers, L. P., Brekelmans, W., Geers, M.: Scale dependent crystal plasticity framework with dislocation density and grain boundary effects. *Int. J. Solids Struct.* **41** (2004), 5209–5230.

[3] Bayley, C., Brekelmans, W. Geers, M.: A comparison of dislocation induced back stress formulations in strain gradient crystal plasticity. *Int. J. Solids Struct.* **43** (2006), 7268–7286.

[4] Ertürk, I., van Dommelen, J., Geers, M.: Energetic dislocation interactions and thermodynamical aspects of strain gradient crystal plasticity theories. *J. Mech. Phys. Solids* **57** (2009), 1801–1814.

[5] Svendsen, B.: Continuum thermodynamic models for crystal plasticity including the effects of geometrically-necessary dislocations. *J. Mech. Phys. Solids* **50** (2002), 1297–1329.

[6] Svendsen, B., Bargmann, S.: On the continuum thermodynamic rate variational formulation of models for extended crystal plasticity at large deformation. *J. Mech. Phys. Solids* **58** (2010), 1253–1271.

[7] Wang, Y., Li, J.: Phase field modeling of defects and deformation. *Acta Mater.* 58 (2010), 1212–1235.

[8] Yalcinkaya, T., Brekelmans, W., Geers, M.: Deformation patterning driven by rate dependent non-convex strain gradient plasticity. *J. Mech. Phys. Solids* **59** (2011), 1–17.

[9] Klusemann, B., Bargmann, S., Svendsen, B.: Comparison of two formulations for the initial-boundary-value problem of a non-convex gradient inelasticity model, *Comput. Mater. Sci.* submitted for publication, 2012.

[10] Yalcinkaya, T., Brekelmans, W., Geers, M.: Non-convex rate dependent strain gradient crystal plasticity and deformation patterning, *Int. J. Solids Struct.* submitted for publication, 2012.

[11] Svendsen, B.: On thermodynamic- and variational-based formulations of models for inelastic continua with internal lengthscales. *Comput. Meth. Appl. Mech. Eng.* **193** (2004), 5429–5452.

[12] Anand, L., Gurtin, M. E., Lele, S. P., Gething, C.: A one-dimensional theory of strain-gradient plasticity: Formulation, analysis, numerical results. *J. Mech. Phys. Solids* **52** (2005), 1289–1826.

[13] Brokate, M., Sprekels, J.: Hysteresis and Phase Transitions. Applied Mathematical Sciences **121**, Springer, 1996.

[14] Hirth, J. P., Lothe, J.: Theory of Dislocations. John Wiley & Sons, 1982.

[15] Braun, O. M., Kivshar, Y. S.: The Frenkel-Kontorova Model. Springer, 2004.