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Hardening and strengthening behavior in rate-independent strain gradient crystal plasticity

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Two rate-independent strain gradient crystal plasticity models, one new and one previously published, are compared and a numerical framework that encompasses both is developed. The model previously published is briefly outlined, while an in-depth description is given for the new, yet somewhat related, model. The difference between the two models is found in the definitions of the plastic work expended in the material and their relation to spatial gradients of plastic strains. The model predictions are highly relevant to the ongoing discussion in the literature, concerning 1) what governs the increase in the apparent yield stress due to strain gradients (also referred to as strengthening)? And 2), what is the implication of such strengthening in relation to crystalline material behavior at the micron scale? The present work characterizes material behavior, and the corresponding plastic slip evolution, by use of the finite element method. The pure shear problem of an infinite material slab is investigated, with the previously published model displaying strengthening, while the new model does not. In addition to the numerical approach an exact closed form solution, to the pure shear problem, is obtained for the new model, and it is demonstrated that the model predicts proportional straining in the entire plastic regime. Somewhat surprising it is found that the predictions for strain gradient hardening coincide for the two models.

1. Introduction

Formulating strain gradient plasticity theories, without compromising thermodynamics or allowing temporal discontinuities in key stress measures, has been and continues to be, a great challenge to the scientific community. The general experimental trend that *smaller is stronger* is well-established (Greer and Hosson, 2011), but conclusive experiments are yet to unveil if the effect of strain gradients gives rise to additional hardening, strengthening, or a combination of the two. This work defines strengthening as an apparent delay in plastic flow, while hardening is defined by the combined effect of conventional strain hardening and the additional hardening related to gradients of plastic strain. Recent experiments display evidence of a strengthening behavior in polycrystalline wires under cyclic loading (Liu et al., 2015), and in the average compressive load for thin confined copper films (Mu et al., 2014). However, in the majority of micron-scale experiments (e.g. nano-indentation and torsion Ma and Clarke, 1995; Guo et al., 2017, respectively), the complexity of the deformation obscures whether the size dependent observations link to hardening, strengthening, or both. With off-set in isotropic theories, Fleck et al. (2015) recently brought new insight into how the mathematical structure of theories influences the predicted material behavior, in their work entitled “Guidelines for Constructing Strain Gradient Plasticity Theories”. Fleck et al. (2015) focus on the apparent elastic gap at initial yield (referred to as strengthening in the present work) that results from a number of existing theories. Their intention is not to remedy theories, but rather to understand the underlying mathematical structure governing this effect. Distinct changes to the predicted material behavior are found for slight modifications to the definition of plastic work expended in the material. By leaving out the enrichment of strain gradients in the lowest order contribution to the plastic work, the model prediction is shown to preclude strengthening behavior. The present work intends to extend these guidelines to crystal plasticity. Following the findings of Fleck et al. (2015), the present work takes as off-set the three key objectives, for “proper model development”, put forward by Hutchinson (2012). That is, the proposed theoretical framework has to;

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1) reduce to that of conventional J_2 plasticity theory in the limit of sufficiently small strain gradients.
2) take as input the elastic material properties, the uni-axial tensile relation between stress and plastic strain, and a length parameter to characterize the gradient effects.
3) coincide with J_2 deformation theory, with same inputs, throughout a proportional straining history.

In Nellemann et al. (2017), the development of an "easy-to-treat" rate-independent model of strain gradient plasticity, which followed the theory of Hutchinson (2012), proved somewhat complicated to handle in a numerical framework (referred to as Model B in the present work). In contrast to this the new model proposed in the present work (referred to as Model B) is shown to obey all three objectives, demonstrating the following features; 1. no strengthening is predicted, such that initial yield occurs at the conventional yield stress, whereby strain gradients only contribute to hardening. As a consequence, 2. the proposed model predicts proportional straining in the entire plastic regime and, hence, allows for an exact closed form solution to be developed for the pure shear problem investigated. Moreover, both models take as input; elastic parameters, a relation between the resolved shear stress and the slip and a material length parameter, following objective 2). It is emphasized that the three objectives above are highlighted since they are desirable features of rate-independent plasticity theories, which allow for an analytical treatment of a proposed framework. Objective 3) only speaks to model predictions which display proportional straining. The theories developed will involve directional derivatives of higher order stresses that may be interpreted as back-stresses which influence model predictions under general loading conditions. The constitutive nature of these higher order stresses determine whether gradient effects arise as strengthening, hardening or a combination of the two. In the present work, Model B is compared to Model A, and the differences between the two models are emphasized. The present research extends the findings of Fleck et al. (2015) regarding strengthening behavior of an isotropic solid to crystal plasticity. The paper is structured as follows. The proposed strain gradient crystal plasticity framework is outlined in Section 2, where two different approaches to defining the plastic work expended in the material are presented. Section 3 lays out the numerical model, and Section 4 presents the pure shear problem considered along with a closed form solution. Numerical results are given in Section 5 and a direct comparison to the exact solution is demonstrated. Finally, concluding remarks are given in Section 6.

2. Strain gradient crystal plasticity

One unified framework for rate-independent strain gradient crystal plasticity that encompasses both the model (Model A) from Nellemann et al. (2017) and a new and improved model (Model B), is presented in Section 2.1. The definition of the plastic work expended in the material constitutes the only difference between the two models and both mathematical formulations will be discussed. Following the definitions of the plastic work expressions, their incremental counterparts are presented in Section 2.2. The presentation is limited to the assumption of monotonic loading, which allows for a brief presentation of the models, that preserves the characteristics relevant to the current investigation. The reader is referred to Nellemann et al. (2017) for further details on the derivation presented throughout Section 2.

Throughout, tensor notation is adopted and repeated lower case Latin indices imply summation, whereas comma separation implies spatial derivatives. Quantities denoted by superscript Greek letters refers to a specific slip system, while all active slip systems are indicated by the superscript (:). The $\dot{()}$ notation indicates an incremental quantity and a function is indicated by hard brackets e.g. $f[*]$.

2.1. Modeling framework

The present work is restricted to small stain rate-independent material behavior, where u_i are the displacements, $u_{i,j}$ are the spatial gradient of the displacements, and $\varepsilon_{ij} = (u_{i,j} + u_{j,i})/2$ are the total strains. The Cauchy stress is given by the elastic relation; $\sigma_{ij} = L^e_{ijkl}\varepsilon^e_{kl}$, where L^e_{ijkl} is the isotropic elastic stiffness tensor and ε^e_{ij} denotes the elastic strain determined by the total strain and the plastic strain, ε^p_{ij}, as; $\varepsilon^e_{ij} = \varepsilon_{ij} - \varepsilon^p_{ij}$. In accordance with the strain gradient crystal plasticity framework initially proposed by Gurtin (2000), the equations of equilibrium read

$$\sigma_{ij,j} \quad = \quad 0 \tag{1}$$

$$q^{(\alpha)} - \tau^{(\alpha)} - \xi^{(\alpha)}_{,i} s^{(\alpha)}_i \quad = \quad 0 \tag{2}$$

with the conventional equilibrium given by Eq. (1) and the microforce equilibrium given by Eq. (2). Here, the Cauchy stress, σ_{ij}, is work conjugate to the elastic strain, the micro-stress, $q^{(\alpha)}$ (the sum of a recoverable part, $q^{R(\alpha)}$, and a dissipative part, $q^{D(\alpha)}$), is work conjugate to the slip, $\gamma^{(\alpha)}$, and the higher order stress, $\xi^{(\alpha)}$, is work conjugate to the normalized pure edge dislocation density (neglecting screw dislocations) $\gamma^{(\alpha)}_{,i} s^{(\alpha)}_i$. The normalized dislocation density is also known as the net Burgers vector density. The resolved shear stress on a slip system is; $\tau^{(\alpha)} = \sigma_{ij}\mu^{(\alpha)}_{ij}$, with the Schmid orientation tensor $\mu^{(\alpha)}_{ij}$ given by Eq. (3).

In the adopted crystal plasticity framework, the plastic strain relates to the crystallographic slip, $\gamma^{(\alpha)}$, on individual slip systems through the relation

$$\varepsilon^p_{ij} = \sum_{(\alpha)} \gamma^{(\alpha)} \mu^{(\alpha)}_{ij}, \quad \text{with} \quad \mu^{(\alpha)}_{ij} = \frac{1}{2}\left(s^{(\alpha)}_i m^{(\alpha)}_j + s^{(\alpha)}_j m^{(\alpha)}_i\right) \tag{3}$$

with a specific slip system, α, characterized by the slip direction vector, $s^{(\alpha)}_i$, and the vector normal to the slip plane, $m^{(\alpha)}_i$.

The slip increment, $\dot{\gamma}^{(\alpha)}$, is unrestricted with respect to sign, such that both positive and negative slip increments may occur. This results in the evolution of the slip; $\gamma^{(\alpha)} = \int_0^t \dot{\gamma}^{(\alpha)} \mathrm{d}t$. Dissipation of energy is assumed to be associated with the accumulation of statistically stored dislocations (SSDs), while recoverable energy is associated with the build up of geometrically necessary dislocations (GNDs) (Ashby, 1970). Thus, the accumulated slip; $\gamma^{(\alpha)}_{acc} = \int_0^t \left|\dot{\gamma}^{(\alpha)}\right| \mathrm{d}t$ is related to dissipation, while the net Burgers vector density, $\gamma^{(\alpha)}_{,i} s^{(\alpha)}_i$ is related to recoverable energy. A gradient enhanced effective slip is defined by the quadratic relation

$$\gamma^{(\alpha)}_{eff} = \sqrt{\left(\gamma^{(\alpha)}\right)^2 + l^2 \left(\gamma^{(\alpha)}_{,i} s^{(\alpha)}_i\right)^2} \tag{4}$$

where a single length parameter, l, governs the gradient dependence.

A power law hardening relation is adopted, such that; $\overline{\tau}^{(\alpha)}_0[\gamma] = \tau^{(\alpha)}_y + \widehat{\tau}^{(\alpha)}_0[\gamma]$ is the conventional shear hardening curve defined in terms of the initial slip resistance, $\tau^{(\alpha)}_y$, and $\widehat{\tau}^{(\alpha)}_0[\gamma] = \tau^{(\alpha)}_y\ k^{(\alpha)}\ \gamma^n$, is the slip dependent shear hardening curve