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A theory for grain boundaries with strain-gradient plasticity

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ABSTRACT

In this work, the effect of the material microstructural interface between two materials (i.e., grain boundary in polycrystalls) is adopted into a thermodynamic-based higher order strain gradient plasticity framework. The developed grain boundary flow rule accounts for the energy storage at the grain boundary due to the dislocation pile up as well as energy dissipation caused by the dislocation transfer through the grain boundary. The theory is developed based on the decomposition of the thermodynamic conjugate forces into energetic and dissipative counterparts which provides the constitutive equations to have both energetic and dissipative gradient length scales for the grain and grain boundary. The numerical solution for the proposed framework is also presented here within the finite element context. The material parameters of the gradient framework are also calibrated using an extensive set of micro-scale experimental measurements of thin metal films over a wide range of size and temperature of the samples.

1. Introduction

It is well known that there is a distinct material behavior when the relevant sizes approach material microstructure length scales such as strong size dependency in the plastic response of the materials (e.g., Fleck et al., 1994; Ma and Clarke, 1995; Chen et al., 2007; Espinosa et al., 2004; Vlassak et al., 2005; Chen et al., 2007; Chen et al., 2011). Moreover, for microstructural optimization of material properties, plastic deformation mechanisms on the grain level play a significant role. A similar strengthening effect is also associated with decreasing the grain size in polycrystalline material due to the increase in yield stress which is referred to as the Hall–Petch effect (Hall, 1951; Petch, 1953).

Such effect in small scale metals can be described by numerous theoretical and numerical models with different resolutions. However, over the aforementioned size scale range the number of dislocations is commonly so large that a continuum formulation is required to describe deformation in an effective and computationally robust manner (Niordson and Hutchinson, 2003). Therefore, it is desirable to advance the theory of continuum plasticity to account for dimensional and microstructural constraints on dislocation activity in the course of plasticity deformation. The collective term for such plasticity models are strain gradient plasticity theories, which have been proposed in a number of studies after the work of Aifantis (1984) (in the spirit of the micromorphic approach following the earlier works of Eringen and Suhubi (1964) and Mindlin (1964)) in order to target the aforementioned size effect. Such continuum theories of plasticity break down at scales when the numbers of dislocations are too small for them to be treated collectively. By increasing the resolution of the theory (e.g., Discrete Dislocation models), individual dislocations can be modeled incorporating other length scales than continuum models.

The experimental observations show the strong effect of free surfaces and interfaces on the plastic deformation in small scale metals (e.g., the effect of surface passivation in free-standing thin films and grain boundary in polycrystalline). Free surfaces can be sources for defects development and its propagation towards the interior while internal interfaces enhance the resistance to plastic flow by blocking the dislocations (e.g., Hirth, 1972; Polcarova et al., 1998) and giving rise to strain gradients to accommodate the GNDs (Geometrical Necessary Dislocations). Moreover grain boundaries may also act as sources of dislocations through the transmission of plastic slip to the adjacent grains (Shen et al., 1988; Clark et al., 1992; Dehosson and Pestman, 1993; Pestman and Dehosson, 1992). Apart from the aforementioned physical observations, in the

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implementation of the higher-order gradient theories, and from mathematical point of view, nonstandard boundary conditions are required at the external boundary of a region and in this way the governing equation is well-posed. In this regard, careful modeling of the interface will supply critical information in the continued development of higher-order strain gradient plasticity theories.

In the present paper a temperature and rate dependent grain boundary flow rule to address the intermediate microscopic boundary conditions is proposed, in the context of higher order gradient plasticity theory allowing for the thermal variation. This model accounts for the energy storage at the grain boundary (i.e., interface) due to the dislocation pile up caused by the presence of surface energy as well as energy dissipation once the dislocation transfer through the grain boundary as a result of both resistance force and change in interfacial area. The paper is structured as follows. Section 2 presents a gradient plasticity theory for grain interior based on a system of microscopic force balances, derived from the principle of virtual power and a thermo-mechanical version of the second law that includes, work performed during plastic flow, and the heat generation due to the plastic work via the energy balance relation. When combined with thermodynamically consistent constitutive relations the microscopic force balances become nonlocal flow rules in the form of partial differential equations requiring boundary conditions. A rate and temperature dependent grain boundary flow rule is also developed which accounts for the energetic state of a plastically strained boundary along with boundary resistance against the plastic strain (i.e., macroscopic measure of slip) transfer. The elaborated details regarding the grain boundary model are presented in Section 3. The free energy and dissipation potentials for the grain and grain boundary are postulated based on micro-mechanical point of views. It is further shown that the backstress and hence kinematic hardening of the grain and grain boundary naturally arise from the free energy potential along with the physical justification by means of dislocation mechanisms. Section 4 provides a physical justification regarding the proposed grain boundary flow rule which can be taken into account in order to make a link between the proposed grain boundary model parameters and the nanoindentation observations conducted near the grain boundary. In Section 5, results of the numerical calculations are presented using finite element implementation of the proposed framework. Particularly, the size effect due to the bulk and interfacial length scale as well as the effect of other parameters on the mechanical and thermal responses of the materials are extensively investigated. The proposed model is then validated over a set of microscale experimental data on thin metal films presenting size effect and initial temperature.

2. Strain gradient plasticity framework: bulk (grain interior)

In the following formulation, tensors are represented only by lower case subscripts *i*, *j*, *k* and *l*. All other subscripts and superscripts do not represent tensors but only identify specific functions or variables. However, as an example subscripts such as *en*, *dis*, *int*, *ex*, etc. signify specific quantities respectively such as *energetic*, *dissipative*, *internal*, *external*, etc.

2.1. Principle of virtual power: macroscopic and microscopic force balances

The principle of virtual power is used to determine the associated balance of the forces that contribute to the power expended within the body as well as the appropriate forms of the first two laws of thermodynamics. In this regard, with accounting for the gradient of plastic-strain rate, the structure of the internal virtual power, $\mathcal{P}_{int}$, is expressed in terms of the energy contribution in the arbitrary subregion of the body, V, as shown in the expression below (i.e., Fleck and Hutchinson, 2001; Fleck and Willis, 2009a):

$$\mathcal{P}_{int} = \int_V (\sigma_{ij}\dot{\varepsilon}^e_{ij} + \mathcal{R}\dot{p} + \mathcal{Q}_k\dot{p}_{,k})dV \tag{1}$$

where σ_{ij} is the Cauchy stress tensor, ε^e_{ij} is elastic strain tensor,[4] and $\mathcal{R}$ and $\mathcal{Q}_k$ are the microforces conjugate to the rate of accumulated plastic strain ($\dot{p} = \sqrt{\dot{\varepsilon}^p_{ij}\dot{\varepsilon}^p_{ij}}$)[5] and rate of plastic strain gradient, $\dot{p}_{,k}$.

The internal power is balanced by the power expended by traction ℓ_i on the external surface, S, and an external body force ℓ_i acting within V to account for the inertia. External virtual power is then expressed for any virtual velocity $\dot{u}_i$ as:

$$\mathcal{P}_{ext} = \int_V (\ell_i\dot{u}_i)dV + \int_S (\ell_i\dot{u}_i + m\dot{p})dS \tag{2}$$

In order to account for the microscopic boundary conditions that arise from the strain gradient, it is further assumed here that the external power is affected by the microtraction m that is the conjugate force of the accumulated plastic strain.

By equating the external power to the internal power (i.e., $\mathcal{P}_{ext} = \mathcal{P}_{int}$) and factoring the common terms out, the following relation for local macroforce equilibrium and nonlocal microforce balance can be expressed respectively for volume V:

$$\sigma_{ij,j} + \ell_i = 0 \tag{3}$$

$$\tau_{ij} - (\mathcal{R} - \mathcal{Q}_{k,k})N^p_{ij} = 0 \tag{4}$$

where $\tau_{ij} = \sigma_{ij} - \sigma_{kk}\delta_{ij}/3$ is the deviatoric component of the Cauchy stress tensor (δ_{ij} is the Kronecker delta). The higher-order boundary conditions are required at the external boundary of a region in which plastic flow occurs as well as at the internal boundary of the plastic region. On the external surface, S, the equations for local traction force and nonlocal microtraction condition can be given as follows:

$$\ell_j = \sigma_{ij}n_i \tag{5}$$

$$m = \mathcal{Q}_k n_k \tag{6}$$

where n_k denotes the outward unit normal to S.

The microscopic boundary conditions in Eq. (6) are related to the interfacial energy at the free surfaces (e.g., the surface of a free-standing thin film, the free surface of a void) or interfaces (e.g., the film–substrate interface, grain boundaries, inclusion interface). This interfacial energy introduces an interfacial resistance against dislocation emission/transmission.

The simple class of boundary conditions for these fields on a prescribed subsurface S are: (i) *microfree condition* where dislocations are free in movement across the boundary $m = 0$ and (ii) *microclamped condition* where dislocations are completely blocked at the boundary $p^I = 0$. According to the notion of Gurtin (e.g., Cermelli and Gurtin, 2002), satisfying the insulation condition implies either a micro-free boundary condition imposed at external free surfaces or a micro-clamped boundary condition imposed on the internal boundaries. However, those null boundary conditions of a microscopically rigid interface or a microscopically free surface are very difficult to be satisfied in reality,[6] particularly, for large

[4] The classical theory of isotropic plastic solids undergoing small deformations is based on the additive decomposition of the strain, ε_{ij}, into elastic, ε^e_{ij}, and plastic parts, ε^p_{ij}, such as: $\varepsilon_{ij} = \varepsilon^e_{ij} + \varepsilon^p_{ij}$.

[5] Depending on applied load (tension or compression), the plastic strain can increase or decrease. However, in the current formulation, p is represented as magnitude of the plastic strain (square root of plastic strain) and consequently it will never decrease in case of tension followed by compression.

[6] The examples of such micro-free and micro-clamped boundary conditions can be found in thin films with unpassivated and passivated surfaces (e.g. Xiang et al., 2005).