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COMPUTATIONAL AND THEORETICAL ASPECTS OF A GRAIN-BOUNDARY MODEL THAT ACCOUNTS FOR GRAIN MISORIENTATION AND GRAIN-BOUNDARY ORIENTATION

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ABSTRACT

A detailed theoretical and numerical investigation of the infinitesimal single-crystal gradient-plasticity and grain-boundary theory of Gurtin (2008) “A theory of grain boundaries that accounts automatically for grain misorientation and grain-boundary orientation". *Journal of the Mechanics and Physics of Solids* **56** (2), 640–662, is performed. The governing equations and flow laws are recast in variational form. The associated incremental problem is formulated in minimization form and provides the basis for the subsequent finite element formulation. Various choices of the kinematic measure used to characterize the ability of the grain boundary to impede the flow of dislocations are compared. A three-dimensional numerical example serves to elucidate the theory.

Key Words: *grain boundaries; crystal plasticity; finite elements; gradient plasticity*

1. Introduction

The miniaturisation of mechanical components composed of crystalline material requires a continuum theory that accounts for the role of the grain boundary and for size-dependent effects. The grain-boundary model should incorporate both the *misorientation in the crystal lattice* between adjacent grains, and the *orientation of the grain boundary* relative to the crystal lattice of the adjacent grains. Classical theories of plasticity are unable to describe the well-known size-dependent response exhibited by crystalline material at the micro- and nanometre scale. Numerous extended (gradient and non-local) continuum theories of single-crystal plasticity have been presented in the last two decades to circumvent these limitations. The thermodynamically consistent gradient theory of Gurtin and co-workers a [see e.g. 2] have received particular attention.

The gradient theory of [2] provides a basis to account for the role of the grain boundary [see 3]. Neumann and Dirichlet-type boundary conditions on the slip and the flux of the vectorial microforce respectively, can be prescribed and are often assumed homogeneous. The homogeneous Dirichlet condition, known as the micro-hard boundary condition, has been widely used to account for the grain boundary. Clearly this boundary condition ignores the complex geometric structures in the vicinity of the grain boundary.

Central to the theory of Gurtin [3] is the introduction of the *grain-boundary Burgers tensor* to parametrize the grain-boundary free energy. The grain-boundary Burgers tensor can be expressed in terms of the *intra-* and *inter-grain interaction moduli*. The inter-grain interaction moduli account for mismatch in the slip systems adjacent to the grain boundary and the orientation of the grain boundary.

The objective here is to investigate computational and theoretical aspects of the grain-boundary theory proposed by Gurtin [3]. For further details see [1], the finite-strain extension of this work is considered in [4].

Gurtin [3] proposes two thermodynamically admissible plastic flow relations for the grain boundary (denoted Gurtin I and II). The flow relations define the structure of the dissipative microscopic stress in the grain boundary microscopic force balance. The flux of dislocations from the grains drives the microscopic force balance. In the first proposal, the grain boundary Burgers tensor is used to parametrize the flow relations, while in the second it is the slip. The first approach accounts for the interaction of slip systems adjacent to the grain boundary. This approach also allows for a recombination of the plastic distortion contributions from adjacent sides via the definition of the grain boundary Burgers tensor. The second approach does not directly account for the structure of the adjacent grains or the orientation of the grain boundary in the plastic flow relation. Both approaches account for the geometric structure of the adjacent grains and the grain boundary via the flux terms from the grains.

A series of three-dimensional numerical examples, performed using the finite element method, elucidate the grain-boundary theory.

2. Governing Relations

The governing relations in the grain and on the grain boundary are now summarised.

2.1. Grain

The relations governing the response of a grain $\mathcal{V}$ are obtained from a macroscopic and a microscopic force balance and are given given by

$$\mathrm{div}\boldsymbol{T} = \boldsymbol{0} \quad \text{in } \mathcal{V} \tag{1}$$

$$\mathrm{div}\boldsymbol{\xi}^{\alpha} + \tau^{\alpha} - \pi^{\alpha} = 0 \quad \text{in } \mathcal{V} \,. \tag{2}$$

The macroscopic Cauchy stress is defined by $\boldsymbol{T} = \mathbb{C}[\boldsymbol{E} - \boldsymbol{E}^{\mathrm{p}}]$, where $\mathbb{C}$ is the tensor of elastic moduli, $\boldsymbol{E}$ is the strain tensor, and $\boldsymbol{E}^{\mathrm{p}}$ is the plastic strain tensor. The flow of dislocations through the crystal lattice is described kinematically via the assumption that the plastic strain tensor can be expressed in terms of the slip γ^{α} on the individual prescribed slip systems $\alpha = 1, 2, \ldots, N$ as

$$\boldsymbol{E}^{\mathrm{p}} = \sum_{\alpha} \gamma^{\alpha} \frac{1}{2} \left[\boldsymbol{s}^{\alpha} \otimes \boldsymbol{m}^{\alpha} + \boldsymbol{m}^{\alpha} \otimes \boldsymbol{s}^{\alpha} \right] \,. \tag{3}$$

The slip direction and slip plane normal of slip system α are denoted $\boldsymbol{s}^{\alpha}$ and $\boldsymbol{m}^{\alpha}$.

The resolved shear stress on slip system α is denoted by τ^{α}. The energetic contribution arising due to the gradient contribution is described by the vector microscopic force $\boldsymbol{\xi}^{\alpha}$. The flux of dislocations to the grain boundary is described by the term $\boldsymbol{\xi}^{\alpha} \cdot \overline{\boldsymbol{n}}$, where $\overline{\boldsymbol{n}}$ is the grain boundary normal. The (dissipative) scalar microforce is denoted by π^{α}. A viscoplastic flow relation for π^{α} is chosen.

2.2. Grain boundary

A balance of macroscopic and microscopic forces across the grain boundary $\mathcal{G}$ yields

$$[\![\boldsymbol{T}]\!]\overline{\boldsymbol{n}} = \boldsymbol{0} \quad \text{on } \mathcal{G} \tag{4}$$

$$[\![\boldsymbol{\xi}^{\alpha}]\!] \cdot \overline{\boldsymbol{n}} = \overline{\pi}^{\alpha}_{A} + \overline{\pi}^{\alpha}_{B} \quad \text{on } \mathcal{G} \,. \tag{5}$$

Eq. (4) is the standard traction continuity condition for an interface. The microforce balance (5) on the grain boundary states that the internal microforce $\overline{\pi}$ on either side of the grain boundary acts in response to the flux of the vectorial microforce from the grain. The gradient-plasticity formulation adopted in the bulk allows meaningful balance equations for the grain boundary to be constructed in a consistent manner. A micro-hard or micro-free boundary condition could be applied on the grain boundary. However all information about the geometry of neighbouring crystal structures and grain-boundary orientation would be lost.

A plastic flow relation for $\overline{\pi}^{\alpha}$ is required. Two options are considered and referred to as Gurtin I and II.

3. Numerical example

Consider a $100 \times 100 \times 100\ \mu\text{m}^3$ polycrystal subject to tensile loading. The polycrystal is composed of 27 equal sized grains. The crystal lattice in each grain is that of a face-centered-cubic material.

The purpose of the polycrystal example is to explore the various choices of grain boundary models for reasonably complex, three-dimensional problems. A micro-free grain boundary model allows for a high flux of dislocations while the micro-hard model acts as an impenetrable barrier resulting in dislocation pile-up. The ability of the two Gurtin grain boundary models to impede dislocation flow is controlled, in part, by the slip resistance $\overline{S}$ of the grain boundary. The Gurtin I model also accounts for the slip system interaction at the grain boundary. The ability of the two Gurtin models to capture the spectrum of behaviour between the micro-hard and micro-free limits is investigated by examining a range of grain boundary resistances from a low $\overline{S} = 1 \times 10^{-4}$ to an extremely high value of $\overline{S} = 1 \times 10^{10}$.

The discretization of the domain and the boundary conditions are shown in Fig. 1. Each grain is discretized with 6^3 elements. A displacement of $u_y = 5\ \mu\text{m}$ is applied on the boundary with outward normal $\boldsymbol{n} = [0, 1, 0]$. The opposite boundary with outward normal $\boldsymbol{n} = [0, -1, 0]$ is prevented from displacing in the y-direction. The additional constraints to prevent rigid body motion are indicated in Fig. 1.

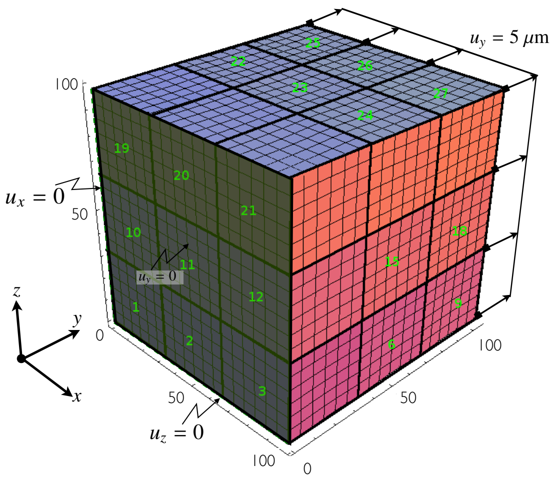

Figure 1: Discretization of the polycrsytal composed of 27 grains.

The y-component of the resultant traction on the right boundary for the Gurtin I, micro-hard and micro-free models is plotted against the prescribed displacement in Fig. 2 (a). As expected the micro-free condition provides a lower bound for the Gurtin models for very low values of $\overline{S}$. From the theory it is reasonable to expect the micro-hard condition to be an upper bound that is approached with increasing $\overline{S}$. It's important to note that the extremely high values of $\overline{S}$ chosen are not physically motivated, rather they penalize the response at the grain boundary. For the high-angle grain boundaries present in the current example it is physically reasonable that the models be capable of producing a response close to micro-hard. It is clear that this is not the case for the Gurtin I model.

The Gurtin II model can capture the range of responses from micro-free to micro-hard, as shown in Fig. 2 (b). A key observation is that the Gurtin II model can be tuned to account for the full range of interactions between micro-free and micro-hard. This observation motivates a possible extension of the current work where the value of the grain boundary slip resistance is chosen as a function of the mismatch at the grain boundary. The Gurtin II has the additional advantage that it is simpler to implement and is computationally more efficient.

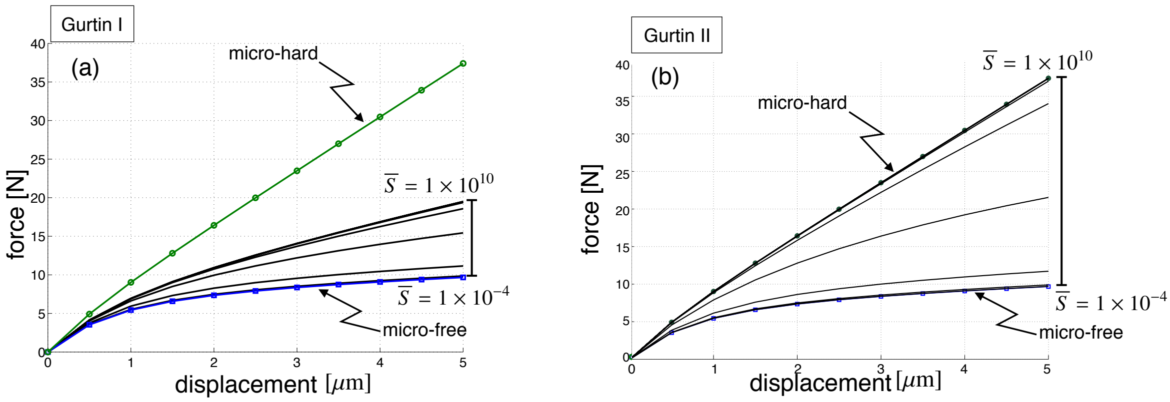

Figure 2: Applied displacement versus the y-component of resultant force on the right boundary for various grain-boundary models. The results of the Gurtin I model are shown in (a), and the Gurtin II model in (b).

4. Discussion and conclusion

Various features of the Gurtin grain-boundary models were illustrated for a polycrystal composed of grains with a face-centered-cubic structure. The Gurtin I model captures the geometric complexity of the grain boundary. A feature of the model is that it does not capture the full range of responses between micro-hard and micro-free. That is, it does not reproduce the widely used micro-hard limit when the grain-boundary slip resistance is used to penalize dislocation flow. The Gurtin II model does not contain the geometrical information concerning the grain boundary but can reproduce the micro-hard limit. The computational efficiency of the formulation is greatly impacted by the choice of the grain boundary flow relation.

The numerical simulations provide valuable insight into the models. They do not, however, allow one to judge the physical correctness of the model. A key challenge is therefore the validation and calibration of this and other grain-boundary models using well-devised experiments and microscopic modelling approaches (e.g. dislocation dynamics).

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