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Microstructural modeling in f.c.c. crystalline materials in a unified dislocation-density framework

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Abstract

A unified physically based microstructural representation of f.c.c. crystalline materials, has been developed such that evolving microstructural behavior at different physical scales can be accurately predicted. This microstructural framework is based on coupling a multiple-slip crystal plasticity formulation to three distinct dislocation densities, which pertain to statistically stored dislocations, geometrically necessary dislocations, and grain boundary dislocations. This interrelated dislocation-density formulation is then used with specialized finite-element modeling techniques to predict the evolving heterogeneous microstructure and the localized phenomena that can contribute to failure initiation as a function of inelastic deformation.

Keywords: Dislocation-density; Crystal plasticity; Finite-element modeling; Crystallographic microstructure; Non-crystallographic microstructure; Cellular microstructure

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1. Introduction

During inelastic deformations of crystalline aggregates, geometrically necessary boundaries (GNBs) form due to gradients of plastic deformation, which are caused by material texture or loading conditions. Dislocations stored in these boundaries are the geometrically necessary dislocations (GNDs) needed to preserve the lattice continuity through accommodating lattice misorientations across the GNBs (see for example Ref. [1]). Statistically stored dislocations (SSDs) accumulate by the statistical trapping of dislocations during plastic slip. The SSDs are generally heterogeneously distributed, and comprise a cell-type microstructure with low-density cell interiors and high-density cell walls, which are also known as incidental dislocation boundaries (IDBs) [2]. Lattice miorientations across the low-angle grain boundaries (GBs) are accommodated by misfit dislocations. Experimental analyses of the correlation between the slip pattern and the microstructure [3–5] have indicated that some grain orientations develop GNBs that contain Burgers vectors, which belong to one slip plane. These GNBs are commonly denoted as crystallographic boundaries (CBs) [6], and form when two coplanar active slip systems account for a large fraction of the plastic slip. Some other grain orientations result in the formation of GNBs with Burgers vectors belonging to two active slip planes. These GNBs are denoted as non-crystallographic boundaries (NCBs) [6]. It has been further observed [3] that CBs have a mixed tilt and twist characteristic, while the NCBs have predominantly tilt characteristic. Hence, CBs can consist of both types of GNDs, namely edge and screw types, while NCBs are mostly comprised of GNDs of edge type.

This study provides a physically based unified formulation for microstructural evolution through a representation of dislocation densities associated with SSDs, GNDs, and GBDs, coupled to a multiple-slip crystalline plasticity formulation for f.c.c. materials, which is then coupled to specialized finite-element methods to track intergranular and intragranular microstructural evolution. This interrelated microstructural approach together with random grain shapes generated by Voronoi tessellation provides a new framework to examine how GB interfaces, grain interiors, and their interactions can affect evolution of cellular, crystallographic or non-crystallographic microstructural types, collective grain behavior, and grain subdivision.

2. Multiple-slip crystal plasticity formulation

A general crystal plasticity formulation that is based on the additive decomposition of the deformation rate and spin tensors

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into elastic and plastic components is used [7]. The velocity gradient tensor L can be obtained from the deformation gradient tensor F and the rate of change of it $\dot{F}$ as

$$L = \dot{F} \cdot F^{-1}. \tag{1}$$

The velocity gradient can then be decomposed into the deformation-rate tensor D and the spin tensor W. The deformation-rate tensor and the spin tensor can then be additively decomposed into elastic (*) and plastic (p) components as

$$D_{ij} = D^{*}_{ij} + D^{\mathrm{p}}_{ij}, \tag{2a}$$

$$W_{ij} = W^{*}_{ij} + W^{\mathrm{p}}_{ij}. \tag{2b}$$

The plastic components can be defined in terms of the crystallographic slip rates $\dot{\gamma}^{(\alpha)}$. For rate-dependent materials a general power-law relation for crystallographic slip rate, can be stated as

$$\frac{\dot{\gamma}^{(\alpha)}}{\dot{\gamma}_0} = \left(\frac{|\tau^{(\alpha)}|}{\hat{\tau}^{(\alpha)}}\right)^{1/m} \cdot \exp\left(-\frac{\Delta F}{kT}\left(1 - \frac{|\tau^{(\alpha)}|}{\hat{\tau}^{(\alpha)}}\right)\right) \cdot \times \operatorname{sign}(\tau^{(\alpha)}), \tag{3}$$

where m is the strain-rate sensitivity parameter, $\dot{\gamma}_0$ is the reference strain-rate, k is Boltzmann's constant, T is the absolute temperature, ΔF is the activation energy, $\tau^{(\alpha)}$ is the resolved shear stress, and $\hat{\tau}^{(\alpha)}$ is the threshold resistance to slip on system α that can be stated as

$$\hat{\tau}^{(\alpha)} = \tau_{\mathrm{y}} + cbG\sqrt{\rho_{\mathrm{o}}^{(\alpha)}}, \tag{4}$$

where τ_{y} is the static yield stress, c is a constant, G is the shear modulus, and b is the magnitude of the Burgers vector. The obstacle density $\rho_{\mathrm{o}}^{(\alpha)}$ depends on how stored dislocations on every slip system interact with mobile dislocations on slip system α, and can be quantified through a set of interaction coefficients $i^{(\alpha s)}$ [8] as

$$\rho_{\mathrm{o}}^{(\alpha)} = \sum_{s=1}^{12} i^{(\alpha s)}(\rho_{\mathrm{SSD}}^{(s)} + \rho_{\mathrm{GND}}^{(s)} + \rho_{\mathrm{GBD}}^{(s)}). \tag{5}$$

3. Dislocation-density evolution

The net rate of change of the SSD density in the cell interiors $\dot{\rho}_{\mathrm{c}}^{(\alpha)}$ for slip system α, can be stated as [9],

$$\dot{\rho}_{\mathrm{c}}^{(\alpha)} = |\dot{\gamma}_{\mathrm{c}}^{(\alpha)}|\frac{1}{bL_{\mathrm{c}}^{(\alpha)}} - A\sqrt{\rho_{\mathrm{c}}^{(\alpha)}}\left(\exp\left(-\frac{w_{\mathrm{f}}^{(\alpha)}}{kT}\right) - \exp\left(-\frac{w_{\mathrm{b}}}{kT}\right)\right), \tag{6}$$

where $\dot{\gamma}_{\mathrm{c}}^{(\alpha)}$ is the crystallographic slip rate of cell interiors, $L_{\mathrm{c}}^{(\alpha)}$ is the mean free path for the mobile dislocations on slip system α, which is equal to $C/\sum_{s=1,12} h^{\alpha s}\rho_{\mathrm{c}}^{(\alpha)}$. C is a material constant and $h^{\alpha s}$ quantifies the mutual immobilization effects of the slip systems [8]. A in Eq. (6) depends on the frequency of the cross-slip attempts and the length of a potential site for such an attempt, w_{f} is the forward activation energy for cross-slip attempts, and w_{b} is the backward activation energy, which is assumed to be equal to the activation energy of cross-slip w_{cs}. The forward activation energy can be assumed to be equal to $w_{\mathrm{cs}}(1 - \tau_{\mathrm{c}}^{(\alpha)}/G)$, where $\tau_{\mathrm{c}}^{(\alpha)}$ is the portion of the resolved shear stress on slip system α that acts over the cell interiors.

Assuming that edge dislocations are stored in the cell walls as mobile screw dislocations glide in the cell interiors, and that the recovery within the cell wall occurs by diffusion controlled climb and the annihilation of oppositely signed edge dislocations, the resultant rate of change in the density of SSDs in the cell walls $\dot{\rho}_{\mathrm{w}}^{(\alpha)}$ becomes [9],

$$\dot{\rho}_{\mathrm{w}}^{(\alpha)} = |\dot{\gamma}_{\mathrm{c}}^{(\alpha)}|\frac{2}{b\delta_{\mathrm{w}}} - \rho_{\mathrm{w}}^{(\alpha)^2} D_{\mathrm{L}}\frac{Gb^3}{kT}, \tag{7}$$

where δ_{w} is the cell wall thickness, and D_{L} is the lattice diffusivity.

The mechanics of a heterogeneous microstructure can then be used to derive relations between the local variables and the average slip system behavior [10,11]. Assuming that the total strain-rate is the same in the cell walls and cell interiors, and that it is equal to the slip system average strain-rate $\dot{\gamma}^{(\alpha)}$ results in

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_{\mathrm{w}}^{(\alpha)} + \frac{\dot{\tau}_{\mathrm{w}}^{(\alpha)}}{G} = \dot{\gamma}_{\mathrm{c}}^{(\alpha)} + \frac{\dot{\tau}_{\mathrm{c}}^{(\alpha)}}{G}, \tag{8}$$

where $\dot{\gamma}_{\mathrm{w}}^{(\alpha)}$ is the slip rate corresponding to the cell walls, and $\dot{\tau}_{\mathrm{w}}^{(\alpha)}/\mathrm{G}$ and $\dot{\tau}_{\mathrm{c}}^{(\alpha)}/\mathrm{G}$ are the local elastic strain-rates of the cell walls and the cell interiors, respectively. It can also be assumed that the local crystallographic slip rates are of the same form as Eq. (3), and that the local slip resistance terms $\hat{\tau}_{\mathrm{c}}^{(\alpha)}$ and $\hat{\tau}_{\mathrm{w}}^{(\alpha)}$ have the general form of Eq. (4). To solve Eq. (8) for the local resolved shear stress rates, $\dot{\gamma}^{(\alpha)}$ needs to be obtained. Therefore, an average SSD density for each slip system has to be known.

The average density of SSDs used in Eq. (5) can be related to $\rho_{\mathrm{c}}^{(\alpha)}$ and $\rho_{\mathrm{w}}^{(\alpha)}$ as

$$\rho_{\mathrm{SSD}}^{(\alpha)} = f_{\mathrm{c}}^{(\alpha)}\rho_{\mathrm{c}}^{(\alpha)} + (1 - f_{\mathrm{c}}^{(\alpha)})\rho_{\mathrm{w}}^{(\alpha)}, \tag{9}$$

where $f_{\mathrm{c}}^{(\alpha)}$ is the average fraction of the cell interiors on slip system α. Since the local fractions must sum to unity, the fraction of the cell walls will be $1 - f_{\mathrm{c}}^{(\alpha)}$. Overall stress equilibrium can then be used to obtain $f_{\mathrm{c}}^{(\alpha)}$, where there must be a balance between the overall slip system resolved shear stress $\tau^{(\alpha)}$ and its local components $\tau_{\mathrm{c}}^{(\alpha)}$ and $\tau_{\mathrm{w}}^{(\alpha)}$,

$$\tau^{(\alpha)} = f_{\mathrm{c}}^{(\alpha)}\tau_{\mathrm{c}}^{(\alpha)} + (1 - f_{\mathrm{c}}^{(\alpha)})\tau_{\mathrm{w}}^{(\alpha)}. \tag{10}$$

Once $f_{\mathrm{c}}^{(\alpha)}$ is known, Eq. (8) can be solved.

The average fraction of cell interiors can also be stated in terms of the average dislocation-cell size $\delta_{\mathrm{c}}^{(\alpha)}$ and cell wall thickness $\delta_{\mathrm{w}}^{(\alpha)}$ as $\delta_{\mathrm{c}}^{(\alpha)}/(\delta_{\mathrm{c}}^{(\alpha)} + \delta_{\mathrm{w}}^{(\alpha)})$. If the cell wall thickness remains constant, $f_{\mathrm{c}}^{(\alpha)}$ can then be used to obtain the average dislocation-cell size for each slip system. When the changes in the temperature are small, cell wall thicknesses can be assumed to be constant. With this assumption, the change in the volume