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INELASTIC BEHAVIOR AND GRAIN-BOUNDARY EFFECTS IN POLYCRYSTALLINE MATERIALS

Jibin Shi, Mohammed Zikry, and Tarek Moustafa Hatem
Mechanical and Aerospace Engineering, North Carolina State University, 2601 Stinson Dr, Campus Box 7910, Raleigh, NC, 27695

ABSTRACT

Dislocation-density based multiple-slip constitutive formulations and specialized computational schemes are introduced to account for grain-boundary (GB) effects in polycrystalline aggregates. New kinematically based interfacial grain-boundary regions and formulations are introduced to account for dislocation-density transmission, absorption, and pile-ups that may occur due to CSL grain-boundary misorientations.

INTRODUCTION

Physically based descriptions are needed that can account for dominant physical mechanisms that may occur at different physical scales. Grain-boundary (GB) structure, orientation, and distribution are essential microstructural features that characterize the initiation and evolution of failure modes in crystalline metals, alloys, and intermetallics. The primary purpose of this study is the introduction of an inelastic dislocation density-based multiple-slip crystalline constitutive formulation that can be used to obtain a detailed understanding and accurate prediction of interrelated local material mechanisms that control and affect global deformation in f.c.c. polycrystalline aggregates with CSL GB orientations and distributions. In this formulation, the length scale between multiple-slip crystalline formulations and dislocation densities is bridged by coupling evolutionary equations for the mobile and immobile dislocation densities, through the temperature dependent flow stress and slip-rates on each slip system, to a multiple-slip rate-dependent crystal plasticity formulation. The derivation of these evolutionary equations are based on accepted physical relations, and generally account for thermally activated dislocation activities such as generation, interaction, and annihilation that are generally representative of the dislocation structures in cubic crystalline metals (see for example [1]).

Most polycrystalline formulations generally do not account for GB effects such as dislocation-density and slip transmission, blockage, and absorption. These effects could result due to GB orientation, structure, or interfacial stress mismatches (see, for example, Zikry and Kao [2], Ashmawi and Zikry [3], Randle [4], and Nes [5]). In this study, GB effects are accounted for by the introduction of interfacial regions that are used to track slip and dislocation density transmissions and intersections. These accurate representations of overall polycrystalline aggregate behavior are needed for the prediction of failure initiation and evolution due to GB interactions with void clusters. In the present formulation, dislocation energies are used to obtain pressure dependent formulations that are used to understand how GB ledges act as sources and sinks for the accumulation and decrease of GB dislocations.

MULTIPLE-SLIP CRYSTAL PLASTICITY FORMULATION

The crystal plasticity constitutive framework used in this study is based on the formulation developed in Kameda and Zikry [6]. In that formulation, it has been assumed that the deformation gradient can be decomposed into elastic and inelastic components. Starting from the decomposition of the velocity gradient, $V_{i,j}$, into its symmetric and anti-symmetric parts as

$$V_{i,j} = D_{ij} + W_{ij}, \tag{1}$$

where D_{ij} is the deformation rate tensor, and W_{ij} is the spin tensor. The total deformation-rate tensor, D_{ij}, and the total spin tensor, W_{ij}, are then each additively decomposed into elastic and plastic components, where the inelastic parts are defined in terms of the crystallographic slip-rates as

$$D_{ij}^{P} = P_{ij}^{(\alpha)} \dot{\gamma}^{(\alpha)} \qquad W_{ij}^{P} = \omega_{ij}^{(\alpha)} \dot{\gamma}^{(\alpha)}, \tag{2a-b}$$

where α is summed over all slip-systems, and the tensors $P_{ij}^{(\alpha)}$ and $\omega_{ij}^{(\alpha)}$ are defined in terms of the unit normals and the unit slip vectors. For a rate-dependent inelastic formulation, the slip-rates are functions of the resolved shear and reference stresses, and a power law formulation is used here.

LOCAL DISLOCATION-DENSITY STRUCTURE

To gain a more fundamental understanding of dislocation motion, interaction, and transmission on material failure modes, the crystal plasticity constitutive formulation is coupled to internal variables that account for a local description of the dislocation structure in each crystal. Specifically, we have used the mobile and the immobile dislocation densities as the internal variables in our constitutive formulation. In inelastic deformations of ductile metals, the characteristics of the microstructure are governed by the mechanisms of dislocation production and dynamic recovery. As the material is strained, immobile dislocations are stored in each crystal, and these dislocations act as obstacles for evolving mobile dislocations. Therefore, the immobile and mobile dislocation densities can be coupled, due to the continuous immobilization of mobile dislocations.

The reference stress, on each slip-system, can be given as a function of $\rho_{im}^{(\alpha)}$, the immobile dislocation density. The reference stress that is used here is a modification of widely used classical forms (see for example, Mugharbi [8]) that relate the reference stress to a square-root dependence on the immobile dislocation density as

$$\tau_{ref}^{(\alpha)} = \tau_{y}^{(\alpha)} + Gb \sum_{\xi=1}^{12} a_{\xi} \sqrt{\rho_{im}^{(\xi)}}, \tag{3}$$

where G is the shear modulus, b is the magnitude of the Burgers vector, $\tau_y^{(\alpha)}$ is the static yield stress, and the coefficients, a_ξ $(\xi = 1,12)$ are interaction coefficients, and generally have a magnitude of unity.

The total dislocation density $\rho^{(\alpha)}$, is assumed to be additively decomposed, into a mobile dislocation density, $\rho_m^{(\alpha)}$, and an immobile dislocation density $\rho_{im}^{(\alpha)}$. Furthermore, we have assumed that during an increment of strain, an immobile dislocation density rate is generated, which will be denoted by $\dot{\rho}_{im}^{(\alpha)+}$, and an immobile dislocation density rate is annihilated, which will be denoted by $\dot{\rho}_{im}^{(\alpha)-}$. We also assume that $\dot{\rho}_m^{(\alpha)+}$ corresponds to a generation of mobile dislocation densities, and $\dot{\rho}_m^{(\alpha)-}$ corresponds to an annihilation of mobile dislocation densities. Using these balance laws pertaining to the generation and annihilation of mobile and immobile dislocations (see [9] for a detailed presentation), we have derived the following coupled equations that account for the evolution of mobile and immobile dislocation densities that correspond, in an average sense, to dislocation generation, interaction, trapping, and recovery,

$$\frac{d\rho_m^{(\alpha)}}{dt} = \dot{\gamma}^{(\alpha)}\left(\frac{g_{sour}}{b^2}\left(\frac{\rho_{im}^{(\alpha)}}{\rho_m^{(\alpha)}} \right) - \frac{g_{minter}}{b^2}\exp(-\frac{H}{kT}) - \frac{g_{immob}}{b}\sqrt{\rho}_{im}^{(\alpha)} \right), \tag{4}$$

$$\frac{d\rho_{im}^{(\alpha)}}{dt} = \dot{\gamma}^{(\alpha)}\left(\frac{g_{minter}}{b^2}\exp(-\frac{H}{kT}) + \frac{g_{immob}}{b}\sqrt{\rho}_{im}^{(\alpha)} - g_{recov}\exp(-\frac{H}{kT})\rho_{im}^{(\alpha)} \right), \tag{5}$$

where g_{sour} is a coefficient pertaining to an increase in the mobile dislocation density due to dislocation sources, g_{minter} is a coefficient related to the trapping of mobile dislocations due to forest intersections, cross-slip around obstacles, or dislocation interactions, where g_{sour} is a coefficient pertaining to an increase in the mobile dislocation density due to dislocation sources, g_{minter} is a coefficient related to the trapping of mobile dislocations due to forest intersections, cross-slip around obstacles, or dislocation interactions, g_{recov} is a coefficient related to the rearrangement and annihilation of immobile dislocations, g_{immob} is a coefficient related to the immobilization of mobile dislocations, H is the activation enthalpy, k is Boltzmann's constant, and T is the temperature. As these evolutionary equations indicate, the dislocation activities related to recovery and trapping are coupled to thermal activation. These expressions can be modified to account for pressure effects due to dislocation-density evolution based on the following expressions

$$\begin{cases} f_E(p) = \left\{ 1 + \frac{p}{3}\left[\left(\frac{1-v-2v^2}{1-v} \right)\left(\frac{1}{K} \right)\left(\frac{dK}{dp} - 1 \right) + \left(\frac{1-v+v^2}{1-v} \right)\left(\frac{2}{G} \right)\left(\frac{dG}{dp} - \frac{G}{K} \right) + \frac{3}{G}\left(\frac{dG}{dp} \right) \right] \right\}(1-\gamma p), & (6a) \\ f_S(p) = \left[1 + \frac{p}{G}\left(2\frac{dG}{dp} - \frac{G}{K} \right) \right](1-\gamma p), & (6b) \end{cases}$$

where the pressure dependent factor f_e is related to edge dislocations, and f_s is related to screw dislocations. In equations (7a-b), p is the local pressure, K is the bulk modulus, G is the shear

modulus, ν is Poisson's ratio, and γ is the plastic slip. These factors are incorporated within the dislocation-density equations in the GB regions to account for the pressure dependent accumulation and reduction of dislocation-densities.

NUMERICAL SCHEME

The total deformation-rate tensor, D_{ij}, and the plastic deformation-rate tensor, D_{ij}^{p}, are needed to update the stress state of the crystalline material. A brief outline of the numerical method will be presented; for further details see [10]. An implicit finite-element analysis has been used to obtain the total deformation-rate tensor, D_{ij}. The displacements have been obtained by the quasi-Newton methods. Once the displacements are obtained, the deformation tensor can be calculated. To solve for the plastic deformation rate tensor, D_{ij}^{p}, the time derivative of the resolved shear-stress is used together with the objective stress rate, and the assumption that the elastic modulus tensor is isotropic, to obtain a system of coupled nonlinear differential equations for each active slip-system. This computational scheme is also used to update the evolutionary equations (5-6) for the immobile and mobile dislocation densities. Specialized Vornoi algorithms were used to generate the FE meshes.

GRAIN BOUNDARY INTERFACIAL REGIONS

It is clear that GBs play a considerable role in controlling the mechanical and physical properties and response of polycrystalline aggregates, which in combination with other factors influence material flow and fracture. As indicated by Lee et al. [11] and Randle [4] most existing models treat GBs as either one-dimensional rigid walls, or only as interfacial quantities which are not accurately representative of GB morphology, structure and interfacial mismatches that may occur due to stress and strain gradients. In this study, the GB region is modeled as an interfacial region with structure and properties that are different from the bulk grain regions. This layer is assumed to be a crystalline region that has a specific orientation for its crystallographic planes. Special kinematic schemes are introduced that account for slip transmission and impedance at the GB region. These schemes are based on the identification and tracking of rotating slip systems in the interfacial region, as strain evolves, such that slip and dislocation-density compatibilities and incompatibilities are used to delineate regions of transmission and pile-ups; for a detailed presentation, see Ashmawi and Zikry [3, 7].

RESULTS AND DISCUSSION

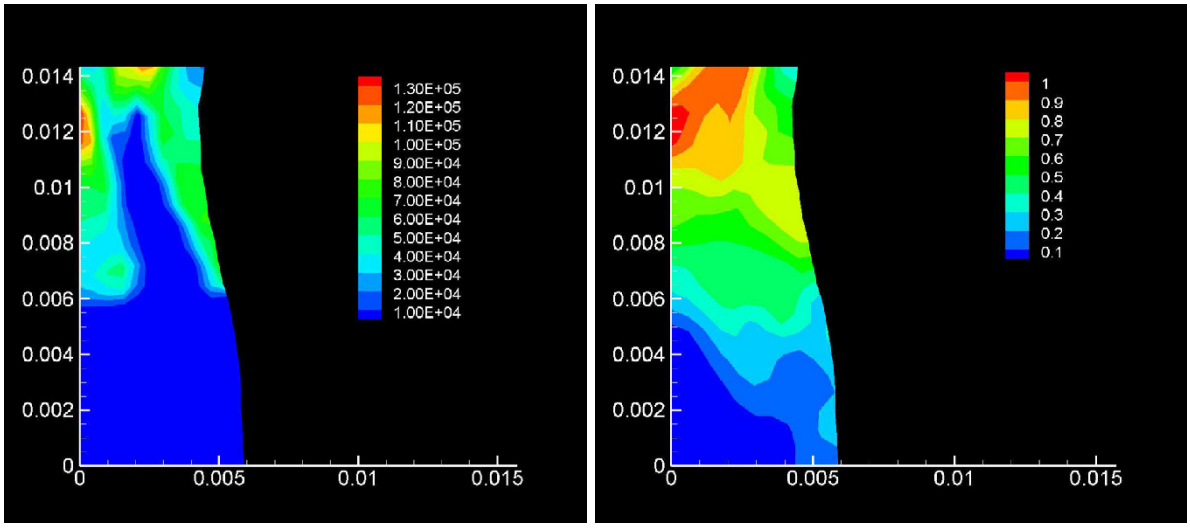
A polycrystalline aggregate was simulated to illustrate the effects of the presence of GB interfacial regions. The material properties that are used here are representative of polycrystalline copper [2]. Grain bulk and GB properties are given in Table (1). The initial mobile and immobile dislocation densities within GB interfacial regions were varied randomly as a function of GB misorientation (for further details, see [7]). Using the method outlined in [6], the saturated immobile dislocation density, $\overline{\rho}_{ims}$, was calculated as 10^{14} m^{-2} and the

saturated mobile dislocation density, $\overline{\rho}_{ms}$, was calculated as $4.3\text{x}10^{13}$ m^{-2}. Using these values, the coefficient values and the enthalpy, needed for the evolution of the immobile and mobile density equations (6-7), are calculated as

$$g_{minter} = 5.53,\ g_{recov} = 6.67,\ g_{immob} = 0.0127,\ g_{sour} = 2.76\text{x}10^{-5},\ \text{H/k} = 3.289\text{x}10^{3}\ ^{0}\text{K}. \qquad (7)$$

All twelve-slip systems were assumed to be potentially active in each grain and GB region.

The effects of the GB interfacial region on the evolution of the total dislocation density can be clearly seen in the contours shown in Fig. 1a-b. These contours correspond to a nominal strain of 20%. for a Σ3 bicrystal. Accumulated plastic strains, which correspond to all the active slip-systems, have localized and accumulated within some of the grains and at the GB regions (Fig. 1b). These contours show the accumulation of dislocation density activity within the GB region. If GB effects had been ignored, these dislocation density activities would not have evolved. It should also be noted (Fig. 1b) that accumulated plastic strains, are concentrated in regions corresponding with high dislocation-density activity adjacent to GB interfacial region.



(a) (b)

Figure 1. (a) Dislocation density (b) Accumulated plastic strains for a Σ3 bicrystal

SUMMARY AND CONCLUSIONS

A multiple-slip crystal plasticity constitutive formulation that is coupled to the temperature dependent evolution of mobile and immobile dislocation densities has been developed for a detailed understanding and prediction of the ductile failure modes, which are associated with void growth and interaction, in polycrystalline aggregates with GB effects. The predictive capabilities and accuracy of the constitutive formulation and the specialized finite-element computational scheme have been used to investigate the effects of random GB orientations on failure initiation and growth in polycrystalline copper. The overall behavior of polycrystalline aggregates has been shown to be directly related to GB orientation, distribution, and structure. In future investigations, the dislocation-density constitutive formulation and the computational

schemes will be used to investigate how wave propagation affects subgrain formation and failure initiation in aggregates subjected to dynamic loading conditions.

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