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Multi-scale modeling of dislocation boundaries: Understanding interaction and effect of rotation angle

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ABSTRACT

The formation and evolution of dislocation boundaries during plastic deformation is one of the primary basis for understanding material strength, shaping, texture, re-crystallization properties, and plastic deformation itself. Better understanding of plastic deformation characteristics will provide for enormous benefits in manipulation of manufacturing processes. Although several analytical and numerical studies have been conducted on 2D analysis of simplified configurations of dislocation boundaries, more complex dislocation boundaries have not received much attention. The present paper presents a 3D numerical analysis of a geometrically necessary dislocation boundary using a multi-scale simulation technique: the multi-scale discrete dislocation plasticity (*MDDP*). The characteristics and internal structure of the dislocation boundary are extracted from experimental measurements. Effect of dislocation boundary rotation angle on the generated self-stress field and behavior of multiple dislocation boundaries is investigated.

1. Introduction

Based on dislocation theory, plastic deformation is believed to occur as a result of dislocation motion on certain crystallographic slip planes. This motion causes dislocations to arrange themselves into certain structures and patterns, which therefore, hold the valuable information about the characteristics of the plastic deformation history. These dislocation structures and patterns play an important role in determining the overall response of the material to plastic deformation, and therefore considerable effort (experimental, analytical and numerical [1–19]) has been devoted to characterize the different dislocation structures. One of the important dislocation patterns frequently observed is the formation of dislocation boundaries and cells. Dislocation boundaries are areas with dense dislocation density and cells are areas nearly free of dislocations. Saada [1] and Saada and Bouchaud [2] studied elastic fields associated with dislocation networks, grain boundaries and dislocation boundaries and presented analytical relations for the elastic field of certain dislocation patterns. Rai et al. [3] performed TEM studies on In-doped and undoped GaAs and presented dislocation structures observed between 700 and 1100 °C. Lubarda et al. [4] analyzed the equilibrium arrangement of collections of edge dislocations under plane strain conditions. Nazarov and Romanov [5] and Nazarov et al. [6] studied elastic fields for finite walls with disordered dislocation arrays. MacLaren and Aindow [7] analyzed dislocation networks at a low-angle near twist boundary in zinc using TEM. The experimental work done by Mughrabi [8,9] and Ungar et al. [10] shows that dislocation boundaries and cell structures produce long-range internal stresses. A composite model, developed by Mughrabi [8,9] explains the origin of the long-range internal stresses based on the heterogeneity of the dislocation structure. It is suggested that long-range internal stresses develop as a result of compatibility requirement between hard (dislocation boundary) and soft (cell) materials. Another theory to explain the formation and characteristics of dislocation boundaries is developed by Kuhlmann-Wilsdorf [11–13] and is referred to as the Low Energy Dislocation Structures (LEDS) theory. As the name implies, among those structures that are accessible to the dislocations, dislocations tend to form a structure that minimizes the free energy per unit length of the dislocation line. Hughes and Hansen and collaborators [14–17] have carried out rigorous experimental studies of micro-structural evolution in various metals and alloys. They have performed a comprehensive statistical study of dislocation boundaries, cell structures and shear bands formation in various deformed metals. Recently, the effect of dislocations and dislocation structures on other material properties has been studied. Zhu et al. [18] studied the interaction behavior between dislocation networks and matrix dislocation in Ni-based single crystal alloy. Liu et al. [19] analyzed the effect of deviation from the equilibrium state of grain boundaries on mechanical properties of ultrafine grained titanium with

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different properties and fractions of the grain boundary by simulating tensile tests in a finite element model. Since the evolution of the microstructure is to a large extent determined by various dislocation motion mechanisms (e.g., easy glide, cross-slip), which are three-dimensional in nature, therefore the resulting dislocation microstructure carries three-dimensional characteristics. The above discussion calls for a 3D analysis of dislocation boundaries for better understanding of these dislocation structures. Multi-scale discrete dislocation plasticity has emerged as an excellent numerical simulation technique for investigating various dislocation structures [20]. A detailed 3D multi-scale discrete dislocation plasticity analysis of experimentally observed dislocation boundaries was performed earlier [21], and results were presented on self-stress field and dynamic stability of a single dislocation boundary. In the present study, the effect of dislocation boundary rotation angle on the generated self-stress field of the dislocation boundary and interaction behavior of multiple dislocation boundaries will be investigated. In addition, the concept of shear stress on various intersecting slip systems resolved from the self-stress field of dislocation boundaries will be analyzed.

2. Multi-scale discrete dislocation plasticity

Multi-scale discrete dislocation plasticity (*MDDP*) has emerged as a powerful tool to analyze various dislocation structures and mechanisms. The core of *MDDP* lies in coupling two lengths scales: micro (discrete dislocation dynamics analysis) and macro (continuum elasto-viscoplasticity finite element analysis). The description of the *MDDP* code used in the present studies is as follows.

2.1. Discrete dislocation dynamics

In *discrete dislocation dynamics* (*DD*) simulations, the plastic deformation of a single crystal is obtained by explicitly accounting for the evolution of a multitude of dislocation loops and curves. The dislocations are discretized into segments of mixed character. The Peach–Koehler force acting on a dislocation segment is calculated from the stress field of all other dislocations and the applied stress. For a dislocation segment bounded by j and $j+1$, the Peach Koehler force $\mathbf{F}_{jj+1}$ on the segment is obtained by integration over the entire segment length L, such that:

$$\mathbf{F}_{jj+1} = \left(\sum_{i=1}^{N-1} \frac{1}{L} \int_L (\sigma^D_{i,i+1}(p) + \sigma^a(p)) \cdot \mathbf{b}_{jj+1} \right) \times \xi_{jj+1} dl + \mathbf{F}_{jj+1\text{-self}} \tag{1}$$

where p is a field point on the dislocation segment $j, j+1$, N is the total number of nodes, $\sigma^D_{i,i+1}(p)$ is the stress from a remote dislocation segment bounded by i and $i+1$, $\sigma^a(p)$ is any other externally applied stress plus internal friction (if any) and stress induced by other defects, $\mathbf{b}_{jj+1}$ is the Burgers vector, ξ_{jj+1} is the line sense vector, and $\mathbf{F}_{jj+1\text{-self}}$ is the Peach Koehler force corresponding to local interaction between the segment adjacent to $j, j+1$. Then, following standard finite element procedure and using linear interpolation shape functions over the segment, the Peach Koehler force per unit length $\mathbf{F}_{jj+1}$ is distributed equally to the nodes j and $j+1$. Thus, once all the forces are assembled, the net force on each node would have contributions from all the segments connected to it. The N dislocation nodes move simultaneously in the glide direction over a characteristic time corresponding to the least time increment required for an interaction to take place. The governing equation of glide motion for each dislocation node is nonlinear and given as:

$$m^*_i \dot{\boldsymbol{v}}_i + \frac{1}{M_i(T,P)} \boldsymbol{v}_i = \mathbf{F}_{i\,\text{glide-component}} \tag{2}$$

where m^* is the effective mass per unit dislocation length, M is the dislocation mobility which could depend on both temperature T and pressure P, $\boldsymbol{v}_i$ is the velocity of node i, $\dot{\boldsymbol{v}}_i$ is the acceleration, and $\mathbf{F}_{\mathbf{i\,glide\text{-}component}}$ is the glide component of the Peach–Koehler force. Thus, the motion and interaction of an ensemble of dislocations in a 3-D crystal is integrated over time yielding macroscopic plastic distortion, which is defined as:

$$\dot{\boldsymbol{\varepsilon}}^p = \sum_{i=1}^{K} \frac{l_i v_{gi}}{2V} (\mathbf{n}_i \otimes \mathbf{b}_i + \mathbf{b}_i \otimes \mathbf{n}_i) \tag{3}$$

where l_i is the segment length, $\mathbf{n}_i$ is a unit normal to the slip plane, v_{gi} is the magnitude of the glide velocity, K is the total number of segments and V is the volume of the representative volume element (*RVE*). For further details of the *DD* code, please see Zbib et al. [22,23] and Rhee et al. [24].

2.2. Integrating multi-scale approach

Using *DD* for infinite domain problems, the computational cell as a whole is considered as an *RVE*, with either reflection boundary conditions (ensuring the continuity of the dislocation curve) or periodic boundary conditions (ensuring conservation of the dislocation flux across boundaries as well as continuity). However, for the simulation of a unit cell representing, say a grain or for finite domain problems, these models are no longer valid and a more rigorous treatment of boundary conditions is required to account for dislocation image stresses. This issue has been addressed by developing a *3-D multi-scale model* that couples the microscale *DD* analysis with the continuum scale via a viscoplasticity model. In this model, the governing equations for the continuum scale are based on an *RVE* over which the deformation field is assumed to be homogeneous. On the macroscale, the material obeys the law of conservation of linear momentum:

$$\mathbf{div}\,\mathbf{S} = \ddot{\boldsymbol{u}}\rho \tag{4}$$

and the energy equation:

$$\rho c_v \dot{T} = k\nabla^2 T + \mathbf{S} \cdot \dot{\boldsymbol{\varepsilon}}^p \tag{5}$$

where $\mathbf{S}$ is the stress tensor, $\boldsymbol{u}$ is the particle displacement, ρ, c_v and k are the mass density, specific heat and thermal conductivity respectively. For elasto-viscoplastic behavior, the strain rate tensor $\dot{\boldsymbol{\varepsilon}}$ is decomposed into an elastic part $\dot{\boldsymbol{\varepsilon}}^e$ and a plastic part $\dot{\boldsymbol{\varepsilon}}^p$ such that:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^e + \dot{\boldsymbol{\varepsilon}}^p \tag{6}$$

For most metals, the incremental form of Hooke's law can be used to express the elastic response for large deformation and material rotation such that:

$$\overset{\circ}{\mathbf{S}} = [\mathbf{C}^e]\dot{\boldsymbol{\varepsilon}}^e, \quad \overset{\circ}{\mathbf{S}} = \dot{\mathbf{S}} - \omega\mathbf{S} + \mathbf{S}\omega, \quad \omega = \mathbf{W} - \mathbf{W}^p \tag{7}$$

where $\mathbf{C}^e$ is a fourth order tensor, ω is the spin of the substructure and is given as the difference between the material spin $\mathbf{W}$ and plastic spin $\mathbf{W}^p$. Combining Eqs. (6) and (7) leads to:

$$\overset{\circ}{\mathbf{S}} = [\mathbf{C}^e][\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}^p] \tag{8}$$

When coupling *DD* with FE, the principle of superposition is employed to correct for the actual boundary conditions, for both finite domain and homogeneous materials. The dislocations contained within the *RVE* give rise to an internal stress $\mathbf{S^D}$ (homogenized over the element) and the effective total stress within the *RVE* is the sum of the stresses by all external agencies and the internal stress $\mathbf{S^D}$. This way, the long-range stress is treated as internal variables, yielding an efficient numerical scheme. $\mathbf{S^D}$ is responsible for the energy stored in the material by virtue of presence of dislocations. With this approach, one can deal with mixed