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Disclination mediated plasticity in shear-coupled boundary migration

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ABSTRACT

The shear-coupled boundary migration of ⟨001⟩ symmetric tilt boundaries is investigated within the framework of an elasto-plastic theory of disclination and dislocation fields. The tilt boundaries are built from periodic partial wedge-disclination dipole arrays, on the basis of their atomistic topography. Non-locality of the elastic response of the adjacent crystals stems from the defected structure of their boundary. Upon applying a shear strain to the bicrystal, couple stresses are generated, which set the disclination dipole array into motion normal to the boundary. In the process, edge dislocation densities with partial Burgers vector lying along the boundary are nucleated, whose glide parallel to the boundary and annihilation produces plastic shear. The misorientation dependence of the shear coupling factor predicted by the model is in full agreement with data from atomistic simulations and experiments. It is found to depend on the polarity and the magnitude of the wedge disclination dipoles composing the grain boundary.

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1. Introduction

Plasticity in polycrystalline media is mediated by a vast diversity of defect nucleation and motion mechanisms (e.g. dislocation glide, vacancy diffusion, dislocation climb, grain boundary migration, grain boundary sliding, etc.). At fixed chemistry, the relative contribution of each mechanism depends on temperature, strain rate, grain size, texture, etc. For example, when the grain size is in the range of tens of nanometers, the role of grain boundaries and triple junctions in so-called nanocrystalline materials become predominant (Gurtin and Anand, 2008). Triple junction and grain boundary migrations are readily activated at moderate temperatures (Mompiou et al., 2009). To deconvolute the role of triple junction motion from that of grain boundary migration, several experimental and theoretical studies have focused on bicrystals (Winning et al., 2001; Cahn et al., 2006; Gorkaya et al., 2009; Berbenni et al., 2013). When a shear stress is applied to a bicrystal, the grain boundary can migrate normal to its axis of symmetry and relax stresses by producing plastic shear. In this process, one crystal grows at the expense of the other by the normal motion (migration) of the grain boundary, and shear/rotation of the material traversed by the grain boundary occurs. Shearing of this region results in the relative motion of the two crystals, parallel to the grain boundary. This essentially non-diffusive mechanism was observed experimentally and modeled for ⟨001⟩ symmetric tilt boundaries in Cu bicrystals by using molecular dynamics methods (Cahn et al., 2006). The coupling of the displacements parallel and normal to the boundary is quantified by a geometrical factor β defined from pure interfacial kinematics considerations (Berbenni et al., 2013). If $u_\perp$ and $u_{//}$ denote the distance of normal migration of the grain boundary and the relative displacement of the two crystals produced by shear, respectively, the shear coupling factor is measured by the ratio $\beta = u_{//}/u_\perp$. Interestingly, β increases in absolute value with misorientations relative to 0° and 90°, and follows two

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branches of opposite sign, with a sharp switch around 37° (Cahn et al., 2006). This misorientation dependence was retrieved experimentally for ⟨001⟩ symmetric tilt boundaries in Al bicrystals (Gorkaya et al., 2009). Using surface-dislocation-based models of grain boundaries (Frank, 1950; Bilby, 1955), the coupling factor β may be simply obtained from the Burgers vector's content of the interface as a function of the misorientation (Cahn et al., 2006). However, this approach fails to account for the structure and energy of high-angle grain boundaries, because it overlooks their core properties.

In the present paper, we intend to analyze shear coupled boundary migration within the framework of a recently developed elasto-plastic theory of dislocation and disclination fields (Fressengeas et al., 2011). In this approach, the internal stress and couple-stress fields arising from the presence of crystal defects (dislocations and disclinations) are accounted for. Further, nonlocal elastic response in the presence of dislocations and disclinations is assumed, consistent with previous findings (Upadhyay et al., 2013). A field description of the crystal displacements and of its defects through their densities at inter-atomic resolution length scale then allows describing the structure and core energy of grain boundaries, in excellent agreement with atomistic simulations and experiments (Taupin et al., 2013; Fressengeas et al., 2013). Plasticity derives from the transport of dislocation and disclination densities through the material. Interestingly, the transport equations provide an undisputable kinematic structure for the spatio-temporal evolution of the crystal defect densities. Thermodynamical guidelines allow substantiating this structure with appropriate constitutive relationships for plasticity in terms of driving forces vs. dislocation/disclination velocities (Fressengeas et al., 2011). The theory is used to model the symmetric ⟨001⟩ tilt boundaries in Cu bicrystals previously considered (Fressengeas et al., 2013). Our main objective is to analyze the boundary migration mechanisms in terms of the coupled disclination and dislocation dynamics, and to provide tools for further studies of grain boundary-mediated plasticity. However, other potential mechanisms, such as grain boundary sliding or dislocation emission/absorption, will not be treated in the present paper. The predictions of our theory will be compared with experimental data and other existing approaches, mainly atomistic simulations (Cahn et al., 2006; Farkas et al., 2006; Tucker et al., 2010) and surface-dislocation-based models (Cahn et al., 2006; Berbenni et al., 2013).

The paper is organized as follows. In Section 2, the elasto-plastic theory of disclination and dislocation fields is briefly recalled. More details can be found in reference (Fressengeas et al., 2011) and in the pioneering work of deWit (deWit, 1970). In Section 3, the construction of tilt boundaries with wedge disclination dipoles introduced (Fressengeas et al., 2013), is recalled for completeness. Then, nonlocal elastic constitutive laws are derived, and our results on shear-coupled boundary migration are presented and discussed by comparison with experiments and other modeling approaches. Conclusions follow in Section 4.

2. Elasto-plastic theory of disclination and dislocation fields

2.1. Notations

A bold symbol denotes a tensor. When there may be ambiguity, an arrow is superposed to represent a vector: $\vec{\mathbf{V}}$. The symmetric part of tensor $\mathbf{A}$ is denoted $\mathbf{A}^{sym}$. Its skew-symmetric and deviatoric parts are $\mathbf{A}^{skew}$ and $\mathbf{A}^{dev}$ respectively. The tensor $\mathbf{A}\cdot\mathbf{B}$, with rectangular Cartesian components $A_{ik}B_{kj}$, results from the dot product of tensors $\mathbf{A}$ and $\mathbf{B}$, and $\mathbf{A}\otimes\mathbf{B}$ is their tensorial product, with components $A_{ij}B_{kl}$. The vector $\mathbf{A}\cdot\mathbf{V}$, with rectangular Cartesian components $A_{ij}V_j$, results from the dot product of tensor $\mathbf{A}$ and vector $\mathbf{V}$. A : represents the trace inner product of the two second order tensors $\mathbf{A}:\mathbf{B} = A_{ij}B_{ij}$, in rectangular Cartesian components, or the product of a higher order tensor with a second order tensor, e.g., $\mathbf{A}:\mathbf{B} = A_{ijkl}B_{kl}$. The cross product of a second-order tensor $\mathbf{A}$ and a vector $\mathbf{V}$, the **div** and **curl** operations for second-order tensors are defined row by row, in analogy with the vectorial case. For any base vector $\mathbf{e}_i$ of the reference frame:

$$(\mathbf{A}\times\mathbf{V})^t\cdot\mathbf{e}_i = (\mathbf{A}^t\cdot\mathbf{e}_i)\times\mathbf{V} \tag{1}$$

$$(\mathbf{div}\,\mathbf{A})^t\cdot\mathbf{e}_i = \mathbf{div}\,(\mathbf{A}^t\cdot\mathbf{e}_i) \tag{2}$$

$$(\mathbf{curl}\,\mathbf{A})^t\cdot\mathbf{e}_i = \mathbf{curl}\,(\mathbf{A}^t\cdot\mathbf{e}_i). \tag{3}$$

In rectangular Cartesian components:

$$(\mathbf{A}\times\mathbf{V})_{ij} = e_{jkl}A_{ik}V_l \tag{4}$$

$$(\mathbf{div}\,\mathbf{A})_i = A_{ij,j} \tag{5}$$

$$(\mathbf{curl}\,\mathbf{A})_{ij} = e_{jkl}A_{il,k}. \tag{6}$$

where e_{jkl} is a component of the third-order alternating Levi–Civita tensor $\mathbf{X}$. A vector $\vec{\mathbf{A}}$ is associated with tensor $\mathbf{A}$ by using its trace inner product with tensor $\mathbf{X}$:

$$(\vec{\mathbf{A}})_k = -\frac{1}{2}(\mathbf{A}:\mathbf{X})_k = -\frac{1}{2}e_{ijk}A_{ij}. \tag{7}$$

In the component representation, the spatial derivative with respect to a Cartesian coordinate is indicated by a comma followed by the component index. A superposed dot represents a material time derivative.

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