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Geometrically necessary dislocation density measurements at a grain boundary due to wedge indentation into an aluminum bicrystal

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ABSTRACT

An aluminum bicrystal with a symmetric tilt $\Sigma 43\,(3\,3\,5)[1\,1\,0]$ coincident site lattice grain boundary was deformed plastically via wedge indentation under conditions that led to a plane strain deformation state. Plastic deformation is induced into both crystals and the initially straight grain boundary developed a significant curvature. The resulting lattice rotation field was measured via Electron Backscatter Diffraction (EBSD). The Nye dislocation density tensor and the associated Geometrically Necessary Dislocation (GND) densities introduced by the plastic deformation were calculated. The grain boundary served as an impediment to plastic deformation as quantified through a smaller lattice rotation magnitude and smaller GND density magnitudes in one of the crystals. There is evidence that the lattice rotations in one grain brought a slip system in that grain into alignment with a slip system in the other grain, upon which the impediment to dislocation transmission across the grain boundary was reduced. This allowed the two slip systems to rotate together in tandem at later stages of the deformation. Finite element crystal plasticity simulations using classical constitutive hardening relationship capture the general features observed in the experiments.

1. Introduction

The motion and multiplication of dislocations are the mechanisms responsible for plastic deformation in most metals at quasistatic deformation rates. The qualitative behavior of dislocations in single crystals or individual grains of a metal is generally understood in terms of the physical mechanisms and interactions of dislocations, although a predictive quantitative understanding remains elusive (e.g. McDowell, 2010). Polycrystalline metals typically have significantly different responses than single crystals due to the presence of grain boundaries. The mechanics and physics of interactions between dislocations and grain boundaries are much more complicated than intragranular dislocation interactions alone. Indeed the qualitative behavior of the various physical mechanisms and interactions of dislocations near grain boundaries is not yet well understood, let alone a quantitative behavior (e.g. Bieler et al., 2014; Spearot and Sangid, 2014).

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In this study we characterize the plastic deformation in an aluminum bicrystal. The mechanical testing of bicrystals to infer the properties of grain boundaries has a long history. Some early work on aluminum bicrystals can be found in Clark and Chalmers (1954), Aust and Chen (1954), Livingston and Chalmers (1957) and Davis et al. (1966) where stress-strain tensile test data are correlated to known orientations of a single grain boundary. Similar tests by Davis et al. (1966), Miura and Saeki (1978), Rey and Zaoui (1980) and Lim and Raj (1985) observed slip lines on the specimen surface close to the grain boundary to investigate grain boundary mechanics. With the introduction of Orientation Imaging Microscopy (OIM) via Electron Backscatter Diffraction (EBSD) with micrometer-scale spatial resolution, the mechanical response can be coupled to the complete determination of crystal orientations. Examples of this technique can be found in Sun et al. (2000), Larson et al. (2004), Okada et al. (2006), Zaeffer et al. (2003) and Ohashi et al. (2009). A recent study of grain boundary properties using nanoindentation can be found in Wang and Ngan (2004), Soer and De Hosson (2005) and Vachhani et al. (2016). Finally, several studies have investigated the behavior of dislocations near the tips of cracks that lie along grain boundaries, including Kysar (2000, 2001a, 2001b) as well as Kysar and Briant (2002).

The specimen employed in this study is a bicrystal of face-centered cubic (FCC) aluminum. The grain boundary has a symmetric tilt character with a shared tilt axis parallel to the [110] direction of both crystals. As will be described in more detail below, the grain boundary abuts a plane from the {335} family of atomic planes in both crystals. If the crystallographic lattice of one crystal were to be extended mathematically into the lattice of the other crystal, 1/43 of the lattice sites would coincide. Hence, this grain boundary is designated as a Coincident Site Lattice (CSL) $\Sigma 43\,(3\,3\,5)[1\,1\,0]$.

The mechanical loading on the bicrystal, the orientation of the grain boundary, the specimen configuration, and the crystallographic orientations of the grains are chosen or prescribed to induce a plane strain elastic-plastic deformation state in the material near and within the grain boundary. Plastic slip occurs on three pairs of active slip systems in each crystal; two are coplanar pairs and the third is a collinear pair. Each pair of slip systems together acts as an effective in-plane (i.e. plane strain) slip system. In the sequel we discuss the plastic deformation in terms of the three effective in-plane slip systems. The plane strain plastic deformation is induced in the specimen via a wedge indenter with a 90° included angle. The plastically deforming zone straddles the grain boundary and extends into both grains. Thus our experimental measurements are designed to give insight into how dislocations interact with the grain boundary during plastic deformation under plane strain conditions.

We measure the crystal lattice rotation induced by the plane strain plastic deformation via the method of Electron Backscatter Diffraction (EBSD) in a Scanning Electron Microscope (SEM). From these measurements, we calculate the Nye dislocation density tensor as well as the Geometrically Necessary Dislocation (GND) density on each of the three effective in-plane plastic slip systems using methods developed in Kysar et al. (2010) and Dahlberg et al. (2014).

The stress and deformation states associated with wedge indentation into single crystals have been analyzed in detail both with analytical and numerical methods in Saito and Kysar (2011), Saito et al. (2012) and Dahlberg et al. (2014). In this study we extend those analyses to wedge indentation into bicrystals via detailed single crystal plasticity finite element simulations.

The lattice rotation field predicted from the simulations is largely consistent with experimental measurements. We focus attention on a pair of coplanar slip systems that exist in each grain and intersect at the grain boundary; the two slip planes are nearly parallel prior to deformation. The GND density measurements suggest that the grain boundary impeded dislocation motion causing dislocations to pile up against the grain boundary at the initial stages of the deformation. However as deformation proceeds, lattice rotation in one grain brings the coplanar slip system in that grain into alignment with the coplanar slip system in the other grain, upon which the impediment to dislocation transmission across the grain boundary diminishes. As further deformation occurs, the two coplanar pairs of slip systems rotate in tandem suggesting that the grain boundary becomes largely transparent to the transmission of dislocations.

The paper is organized as follows. Section 2 reviews the geometry and relevant variables associated with plastic slip transmission across a grain boundary. In addition, the various proposed mechanisms and criteria of plastic slip transmission across a grain boundary are reviewed. Section 3 discusses the test specimen, the experimental procedures, data collection and data processing. In Section 4 the experimental results are presented and analyzed with respect to lattice rotations and densities of geometrically necessary dislocations. Section 5 discusses detailed finite element method crystal plasticity simulations of the experiment. The simulation results are compared to the experimental results both qualitatively and quantitatively. The results are discussed in Section 6 and conclusions are drawn in Section 7.

2. Background

We now review the geometry and notation for general grain boundaries and plastic slip systems. The idealized geometry of a grain boundary and its two adjoining crystals (also referred to as grains) is shown in Fig. 1. Adopting the terminology of Mercier et al. (2016), the *incoming slip plane* in crystal #1 has unit normal vector $\boldsymbol{n}_{\mathrm{in}}$ with Burgers vector $\boldsymbol{b}_{\mathrm{in}}$. The *outgoing slip plane* in crystal #2 has unit normal vector $\boldsymbol{n}_{\mathrm{out}}$ with Burgers vector $\boldsymbol{b}_{\mathrm{out}}$. The angle between $\boldsymbol{n}_{\mathrm{in}}$ and $\boldsymbol{n}_{\mathrm{out}}$ is denoted by ψ. The intersection of the incoming slip plane and the grain boundary plane is denoted by the line $\boldsymbol{l}_{\mathrm{in}}$ and the intersection of the outgoing slip plane and the grain boundary is denoted by the line $\boldsymbol{l}_{\mathrm{out}}$. In general $\boldsymbol{l}_{\mathrm{in}}$ and $\boldsymbol{l}_{\mathrm{out}}$ meet at one point and the angle between them is denoted as θ. The unit vector $\boldsymbol{d}_{\mathrm{in}}$ indicates the direction of the prolongation of $\boldsymbol{b}_{\mathrm{in}}$ from crystal #1 (through the intersection of $\boldsymbol{l}_{\mathrm{in}}$ and $\boldsymbol{l}_{\mathrm{out}}$) into crystal #2. For consistency, the unit vector $\boldsymbol{d}_{\mathrm{out}}$ indicates the direction of