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On migration and faceting of low-angle grain boundaries: Experimental and computational study

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Abstract

The motion and faceting behavior of low-angle ⟨100⟩ tilt and mixed tilt–twist boundaries was investigated. The experiments were conducted on high-purity (99.999%) aluminum bicrystals by utilizing an in situ technique for the observation and continuous recording of boundary migration. In contrast to pure tilt boundaries, the mixed boundaries were found to readily assume a curved shape and steadily move under the capillary driving force. This behavior is associated with the inclination dependence of boundary energy, which was determined for tilt and mixed boundaries by molecular statics simulations. The shape evolution and shrinkage kinetics of cylindrical grains with different tilt and mixed boundaries were studied by molecular dynamics simulations. The mobility of low-angle ⟨100⟩ boundaries with misorientation angle >10°, obtained by both the experiments and simulations, does not differ from that of the high-angle boundaries, but decreases essentially with the further decrease of misorientation. The shape evolution of the embedded grains was found to relate directly to results of the energy computations. Further simulation results revealed that the shrinkage of grains with pure tilt boundaries is accompanied by grain rotation. In contrast, grains with the tilt–twist boundaries composed of dislocations with the mixed edge–screw character do not rotate as they shrink.

Keywords: Grain boundary migration; Grain boundary energy; Inclination; Grain rotation

1. Introduction

It is well known that grain boundary energy depends essentially on misorientation between adjacent grains and, for a given grain misorientation, on the inclination of the boundary plane [1]. An inclinational anisotropy of grain boundary energy results in the formation of low-energy grain boundary facets [2–11]. In turn, grain boundary faceting can substantially affect grain boundary motion [12–16] and, therefore, be crucial for grain growth in polycrystals [17–21].

Most reported observations of grain boundary faceting relate to high-angle boundaries with misorientations close to low Σ coincident site lattice orientation relationships [2–6]. The inclinational anisotropy of grain boundary energy, however, is not confined to these "special" boundaries only, but also applies to low-angle tilt grain boundaries with low-index rotation axes [22–24]. As was found in experiments on aluminium bicrystals with ⟨100⟩ and ⟨111⟩ tilt grain boundaries, the low-angle tilt boundaries with misorientation angles $\theta < 10°$ do not assume an expected curved shape during annealing at elevated temperatures [25,26] and, accordingly, do not move under a capillary/curvature driving force. With increasing misorientation the tilt boundary behavior changes – boundaries with misorientations $10° < \theta < 15°$ were observed to form a single facet, which meets the initial boundary at a sharp edge and remains immobile during annealing at constant temperature. The experiments revealed that only the

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boundaries with $\theta > 15°$ can easily assume a curved shape and steadily move under a curvature driving force. The observed faceting behavior of $\langle 1\,0\,0\rangle$ and $\langle 1\,1\,1\rangle$ tilt boundaries and its change with increasing misorientation was attributed to the dependence of grain boundary energy on inclination [22,23]. Computational analysis proved that the inclinational anisotropy of grain boundary energy is especially pronounced for low-angle tilt boundaries, where the energy is minimal for specific symmetric configurations. The energy anisotropy diminishes with increasing misorientation angle [23], such that for originally flat tilt boundaries with higher misorientations it becomes energetically preferable to form a curved segment composed of a continuous set of differently inclined boundary sections in order to reduce the boundary area/energy and, therefore, to move under the curvature force. The remaining energy cusp at an inclination $\psi = 0$ (symmetric boundary position), however, can cause the formation of a mobile facet combined with a curved boundary section [16].

A geometrically pure tilt grain boundary, which is composed of only one set of edge dislocations with Burgers vector nearly perpendicular to the boundary plane, represents a model case. Most previous experimental and modeling studies of grain boundary kinetics and thermodynamics are performed on tilt boundaries [1], since they are easier to fabricate/produce in both experiment and simulations. In a real polycrystal, however, most boundaries are of general type. The migration and faceting behavior of random/non-tilt grain boundaries can be expected to differ substantially from that of pure tilt boundaries. It is thus important to push the experimental and modeling efforts toward random boundaries with more complex structure. Therefore, in the current experimental and computational study the behavior of the mixed tilt–twist low-angle boundaries in bicrystals of different geometry was addressed and the present paper reports on the results of the respective measurements and simulations.

2. Applied methods

2.1. Experimental specimens and techniques

The experiments were conducted on high-purity (99.9995%) aluminum bicrystals grown by the *vertical Bridgman method*. The orientation of the grains in the grown bicrystals was measured via X-ray diffraction by the Laue technique. Details of the Laue setup are given elsewhere [27]. The measured orientations of the adjacent crystals in the investigated bicrystals and misorientations across the boundary are given in Table 1.

For measurement of grain boundary migration the well-approved technique with a constant driving force p provided by the boundary energy γ, $p = \gamma/a$ (Fig. 1) [28–33], was applied. Specimens 2 mm thick were fabricated from grown bicrystals by electrical discharge machining so that the initial straight grain boundary separates an ~400 μm wide grain with orientation "2" (shrinking during boundary migration) from a 2 mm wide grain with orientation "1" and meets the surface of the bicrystal at one side under a sharp angle (Fig. 1). Grain boundaries with various rotation angles around a $\langle 1\,0\,0\rangle$ axis and different orientation of this axis with respect to the boundary plane and sheet normal were examined. The investigated mixed grain boundaries are defined by a rotation angle θ around a common [0 0 1], which is inclined from the boundary plane by an angle $\xi \approx 20°$ in the direction of the boundary normal (Fig. 1a). The angle ξ, therefore, specifies a twist component of a mixed grain boundary, i.e. $\xi = 0°$ complies with a purely tilt, and $\xi = 90°$ with a purely twist boundary geometry. Specifically, four [0 0 1] boundaries with the geometry shown in Fig. 1a and misorientation angles 4.9°, 9.1°, 12.3° and 20.9° ("mixed I" in Table 1) were investigated. For comparison the behavior of a symmetric 9.1° [0 0 1] pure tilt boundary, i.e. with $\xi = 0°$ and $\psi = 0°$ ("tilt I" in Table 1), was also examined. In the two further investigated bicrystals with 7.0° and 11.4° [$\bar{1}$ 0 0] boundaries a common rotation axis of the adjacent grains was parallel to the bicrystal surface as shown in Fig. 1b. The initial inclination of a 7.0° [$\bar{1}$ 0 0] boundary was parallel to the growth (x) axis of the bicrystal, i.e. this boundary had a tilt geometry ("tilt II" in Table 1). The plane of the 11.4° [$\bar{1}$ 0 0] boundary was initially inclined from the pure tilt position by ~6° (rotated around z-axis), i.e. it was of a mixed geometry with a twist component $\xi = 6°$ ("mixed II" in Table 1).

The measurements of grain boundary shape and motion in the temperature range from 390 to 640 °C were performed by an in situ technique in a scanning electron microscope equipped with a specially designed heating stage [34]. The grain boundary shape and location were determined utilizing the orientation contrast revealed by an electron backscatter detector (Figs. 2 and 4). The measuring procedure is described in Refs. [22,23].

2.2. Molecular statics simulations

Molecular statics (MS) simulations were performed to compute the atomic structure of boundaries with similar geometries and misorientations in Al as investigated experimentally, i.e. low-angle $\langle 1\,0\,0\rangle$ mixed tilt–twist and pure tilt, in order to determine the boundary energy and its dependence on the boundary inclination. The computation procedure proposed by Lee and Choi [35] was applied. The advantage of this method is that it does not require periodic boundary conditions, typically assigned to the simulation sample in the two directions parallel to the boundary [36], and therefore can be utilized for computing grain boundary structure and energy for any misorientation and inclination angle.

For creating a θ[0 0 1] tilt grain boundary in our simulations the original spherical single crystals (with orientation [1 0 0]$\|x$, [0 1 0]$\|y$, [0 0 1]$\|z$), which were used to construct the bicrystal [35], were rotated by an angle of $\theta/2$ and $-\theta/2$ about the z-axis or the x-axis (to create the boundary with the tilt axis parallel to the bicrystal surface as shown in