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Effect of inclination dependence of grain boundary energy on the mobility of tilt and non-tilt low-angle grain boundaries

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In contrast to a 9.1° <1 0 0> tilt grain boundary, which remains straight and immobile at elevated temperatures, a 9.1° <1 0 0> mixed boundary easily assumes a curved shape and steadily moves under a capillary force. Molecular statics simulations suggest that this is due to the inclination dependence of grain boundary energy, which in turn depends on boundary geometry. The energy of a tilt boundary was found to change, whereas that of a mixed boundary was found not to change with boundary inclination.

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

According to recent experimental, theoretical and computer simulation efforts it has been recognized that the anisotropy of grain boundary energy, which is reflected by the formation of grain boundary facets, can be crucial for processes of microstructure evolution in polycrystals, such as recrystallization, grain growth and sintering [1–5]. Although practically all reported observations of grain boundary faceting relate to high-angle boundaries with misorientations close to low Σ CSL orientation relationships [6–9], the inclinational anisotropy of grain boundary energy applies not only to these "special" boundaries (e.g. [10]).

Our previous experiments on aluminum bicrystals with <1 0 0> and <1 1 1> tilt grain boundaries with misorientation angles θ in the transition range from low to high angles revealed that, in contrast to expectations for the used bicrystal geometry (Fig. 1), low-angle boundaries ($\theta < 13°$) do not assume a continuously curved shape [16] and, correspondingly, do not move under a capillary driving force [17,18]. For the entire investigated temperature range they remain flat or form facets which are inclined to the initial boundary orientation and meet the initial boundary at a sharp edge (e.g. Figs. 4 and 5 of Ref. [18]). Computational analysis provided evidence that the observed behavior of low-angle boundaries is associated with the anisotropy of grain boundary energy with respect to boundary inclination [18].

It is worth noting, however, that a pure tilt boundary with low index rotation axis, composed of edge dislocations, is a very specific model case, whereas in a real polycrystal most boundaries are of general type. Their structure is more complex and, thus, their faceting behavior and kinetics can be expected to differ from that of pure tilt low-angle boundaries.

In the current paper we report and compare results of experiments and simulations obtained for pure tilt and mixed low-angle boundaries with similar misorientations around the same rotation axis.

The experiments were carried out on bicrystalline specimens (Fig. 1) fabricated by electrodischarge machining from high-purity Al bicrystals (99.9995%) grown by the vertical Bridgman technique. An investigated mixed grain boundary was composed of a rotation angle $\theta = 9.1°$ around a common [0 0 1] axis and grain boundary plane rotated 20° with respect to the tilt boundary plane, i.e. with a twist component $\xi = 20°$ (Fig. 1). For comparison the behavior of a 9.1° [0 0 1] pure tilt boundary, i.e. with a [0 0 1] rotation axis normal to the bicrystal surface (z-axis in Fig. 1), was examined. Details of crystal growth, bicrystal characterization and sample preparation are given elsewhere [17–19]. The measured orientations of the adjacent crystals in the grown bicrystals and misorientations across the boundary are given in Table 1.

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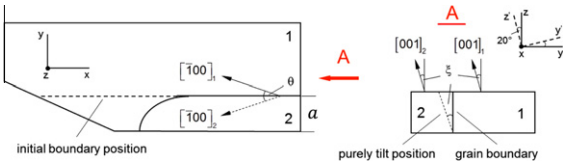

Figure 1. Bicrystal technique for measuring grain boundary migration under a constant curvature driving force p provided by the boundary energy γ, $p = \gamma/a$, repeatedly utilized for investigations of high-angle grain boundary motion in different metals [11–15]. The depicted boundary geometry corresponds to a θ <100> grain boundary with a twist component ξ. In the current experiment a boundary with $\theta = 9.1°$ and $\xi = 20°$ was investigated. In the bicrystal with a 9.1° <100> pure tilt boundary, which was also investigated in the current study, the [001] rotation axis was parallel to the sheet normal (not shown).

The shape evolution and migration of the investigated boundaries during annealing in the temperature range between 390 and 640 °C was measured in-situ in a scanning electron microscope equipped with a specially designed heating stage [20]. The shape of the grain boundaries was observed utilizing the orientation contrast revealed by an electron backscatter detector (Fig. 2). The procedure for measuring the boundary migration is described in Ref. [18].

For determining the grain boundary energy of both the <100> tilt and mixed grain boundaries the computation procedure proposed by Lee and Choi [21] was applied. This method does not require periodic boundary conditions, typically assigned to the simulation sample in the two directions parallel to the boundary [22], and thus can be utilized for computing grain boundary energy for any misorientation and inclination angle. Two spherical crystals were used to construct the bicrystal. The spheres were oriented in such a way that the orientation relationship between them corresponded to the required boundary misorientation. These spherical samples were then cut radially along preassigned crystallographic planes into two parts of equal size. Joining the opposite hemispheres to a new sphere yielded a spherical bicrystal with the desired boundary. The interaction between atoms in the applied procedure was described by the second nearest-neighbor modified embedded atom method (2NN MEAM) potential developed by Lee et al. [23,24]. With the model parameters for Al the 2NN MEAM potential reproduces excellently the fundamental physical properties of Al [21,25]. The energy of the created bicrystal sample was subsequently minimized by application of 0 K molecular statics. Then the grain boundary energy was determined as the difference between the computed potential energies of the bicrystal and the original single-crystal sphere.

In order to create a θ [001] tilt grain boundary in our simulations the original spherical single crystals (with orientation [100] ∥ x, [010] ∥ y, [001] ∥ z) were rotated by an angle of $\theta/2$ and $-\theta/2$ about the z-axis. The cutting plane, which was effectively the grain boundary plane, was defined in the sample coordinate system by the cross-product of the z-axis with the vector <sin ψ, cos ψ, 0>, where ψ denotes the inclination angle. The boundary inclination was defined such that $\psi = 0$ corresponded to the symmetrical boundary position with regard to the <100> crystallographic directions in the neighboring grains. The θ [001] mixed grain boundaries with twist component ξ were created in a similar manner but the spherical single crystals were additionally rotated by the angle ξ about the x-axis. In the current paper the computational results of grain boundary energy and its inclination dependence for 10.4° <100> tilt and mixed ($\xi = 20°$) boundaries are reported.

The current experiments with the 9.1° <100> tilt grain boundary revealed that, similarly to the 8.4° <100> tilt boundary investigated in Ref. [17], this boundary did not assume a curved shape. It remained planar in its initial position shown in Figure 1, and thus did not move during heating at elevated temperatures up to 640 °C. By contrast, the investigated 9.1° <100> mixed boundary easily assumed a continuously curved shape (Fig. 2), and while migrating retained its shape in the temperature range between 390 and 480 °C. Figure 3a shows the displacement of this boundary vs. annealing time at various temperatures. As can be seen, the boundary moved steadily at each constant temperature. Correspondingly, the velocity v for each temperature could be calculated. The reduced boundary mobility A was determined as $A = v \cdot a$, where a is the width of the shrinking grain (Fig. 1); Figure 3b depicts the temperature dependence of A.

The results of computer simulations, i.e. the computed dependence of grain boundary energy γ on boundary inclination ψ for both the simulated 10.4° <100> tilt and mixed tilt–twist boundaries are shown in Figure 4. Due to the fourfold symmetry of the <100> tilt boundary plane normal, it is sufficient to represent the respective dependence γ (ψ) in the inclination range from 0° to 45°; a 90° inclination for a [001] tilt boundary restores the symmetrical boundary position with $\psi = 0°$.

The results of the performed computations (Fig. 4) provide further evidence that the experimentally observed shape of low-angle boundaries and their ability to move under a capillary driving force are essentially affected by the inclination anisotropy of grain boundary energy.

Experimental observations on a bicrystal with a 9.1 <100> tilt boundary are consistent with the results of previous experiments on low-angle <100> and <111> tilt boundaries [17,18]: the boundary remained flat and did not move under the driving force provided by its energy. Apparently, this is due to the anisotropy of its energy with respect to boundary inclination (Fig. 4). In its original position the 9.1° <100> tilt boundary has a local minimum energy at the symmetrical configuration with $\psi = 0°$. This boundary cannot start to move even at the location where the boundary meets the external surface at a sharp angle (Fig. 1), i.e. where the driving force for its motion is the highest, since any local change in the boundary inclination would result in an increase in its energy that cannot be compensated by a decrease in the boundary length/area. Furthermore, any deviation of the inclination of the grain boundary from the energy minima causes a torque $M = -d\gamma/d\psi$ that forces the boundary to assume only the most stable inclination values, i.e. where $M = 0$. As the inclination dependency of grain boundary energy decreases, e.g. with increasing misorientation angle [18], the torque M becomes less important which results in a more continuously curved