IMPACT OF GRAIN BOUNDARY CHARACTER ON FACETING AND MIGRATION OF LOW ANGLE BOUNDARIES AND GRAIN ROTATION: EXPERIMENTS AND SIMULATIONS

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Abstract

The migration and faceting behavior of low angle <100> tilt and mixed grain boundaries was investigated. For measurements on high purity aluminum bicrystals an in-situ technique based on orientation contrast imaging was applied. In contrast to the pure tilt boundaries, the mixed boundaries readily assumed a curved shape and steadily moved under the capillary force. Computational analysis revealed that this behavior is due to the inclinational anisotropy of grain boundary energy, which in turn depends on boundary geometry. The shape evolution and shrinkage kinetics of cylindrical grains with different tilt and mixed boundaries were studied by molecular dynamics simulations.

Introduction

It is well established that both grain boundary energy and mobility depend on misorientation between adjacent grains and, for a given grain misorientation, on inclination of the boundary plane [1]. A dependence of grain boundary energy on inclination can result in the formation of low energy grain boundary facets [2-9], which in turn can substantially affect grain boundary motion [10-14] and, therefore, be crucial for processes of microstructure evolution in polycrystals, such as recrystallization, grain growth and sintering [15-19]. Although practically all reported observations of grain boundary faceting relate to high angle boundaries with misorientations close to ORZȈ&6/RULHQWDWLRQUHODWLRQUHODWLRQVKLSV>, the inclinational anisotropy of grain boundary energy is not confined to these “special” boundaries only, but also applies to low angle tilt grain boundaries with low index rotation axis [20-23]. In experiments on aluminum bicrystals with <100> and <111> tilt grain boundaries with misorientation angles θ in the transition range from low to high angles was found that the boundaries with misorientation angles θ < 10° do not assume an expected curved shape during annealing at elevated temperatures [20,21] and, correspondingly, do not move under a curvature driving force. Boundaries with misorientations 10° < θ < 15° were observed to form a single facet, which meets the initial boundary at a sharp edge and remain immobile during annealing at constant temperature, and only boundaries with misorientation angles larger than 15° were found to assume a curved shape and steadily move under a capillary driving force. The observed faceting behavior of low angle tilt boundaries and its change with increasing misorientation was attributed to the dependence of grain boundary energy on inclination [20,21]. It is important to note, however, that a geometrically pure tilt grain boundary with low index rotation axis, composed of edge dislocations, is a specific model case. In a real polycrystal most boundaries are of general type. The migration and faceting behavior of random grain boundaries can be expected to differ substantially from that of pure tilt boundaries. It is therefore important to push the study efforts toward random boundaries with more complex structure. In the current
paper we report on the results of experiments and simulations obtained for non-tilt, i.e. mixed tilt-twist low angle boundaries.

**Experimental**

The experiments were conducted on specimens (Fig. 1) fabricated by electro-discharge machining from high purity Al bicrystals (99.9995%) grown by the vertical Bridgman technique. Details of crystal growth, bicrystal characterization and sample preparation are given elsewhere [20,21,26]. The well approved experimental technique [20-24,27-34] for measuring grain boundary migration under a constant curvature driving force \( p \) provided by the boundary energy \( \gamma \), \( p = \gamma / a \) (Fig. 1) was applied. Grain boundaries with various rotation angles around a <100> axis and different orientation of this axis with respect to the boundary plane and sheet normal were examined. The investigated mixed tilt-twist grain boundaries were composed of a rotation angle \( \theta \) around a common [001] axis and grain boundary plane rotated by an angle \( \xi \approx 20^\circ \) with respect to the tilt boundary plane (Fig. 1a). The angle \( \xi \), therefore, specifies a twist component of a mixed grain boundary. In particular, three <100> mixed low angle boundaries with misorientations 4.9°, 9.1°, 12.3° and 20.9° were investigated. For comparison the behavior of a 9.1° [001] pure tilt boundary, i.e. with \( \xi = 0^\circ \), was also examined. In the two further investigated bicrystals with 7.0° and 11.4° [100] 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° [100] boundary was parallel to the growth (x-) axis of the bicrystal, i.e. this boundary had tilt geometry. The plane of the 11.4° [100] boundary was initially inclined from the pure tilt position by about 6° (rotated around z-axis), i.e. it was of a mixed geometry with a twist component \( \xi = 6^\circ \).

![Figure 1. Bicrystal geometries for measuring the grain boundary migration. (a) Bicrystal with a \( \theta <100> \) tilt-twist grain boundary (\( \xi \) is a twist component); (b) bicrystal with a \( \theta <100> \) tilt boundary with a rotation axis parallel to the specimen surface.](image)

The measurements of grain boundary shape and motion in the temperature range between 390°C and 640°C were performed by an in-situ technique in a SEM equipped with a specially designed heating stage [35]. The grain boundary shape and location were determined utilizing the orientation contrast revealed by an electron back scatter detector (Fig. 3). The measuring procedure is described in Refs. [20,21].

**Applied modeling techniques**

In order to determine the grain boundary energy of both the <100> tilt and mixed grain boundaries the computation procedure proposed by Lee and Choi [36] was applied. The method