Grain boundary mobility has been measured in high-purity aluminum alloyed with 0.03 wt.% Zr using energy stored during plastic deformation as a driving force. In general, the dependence of mobility on grain boundary character was similar to that observed by previous authors with a maximum in mobility in the vicinity of the $\Sigma 7$ type ($38^\circ<111>$). The exact location of the mobility maximum varied, however, with temperature in a manner similar to that observed for curvature-driven mobility measurements. Although $<111>$ tilt boundaries exhibit high mobilities in general, the single peak at the $\Sigma 7$ position at low temperatures changes to a double peak at high temperatures with a local minimum at $\Sigma 7$. The combination of mobility variation and the thermal activation analysis of the results points to a compensation temperature effect. All these results suggest that grain boundary mobility is a true material property.

**Keywords:** Grain Boundary; Mobility; Stored Energy; Driving Force; Curvature

### 1. Introduction

The purpose of this paper is to present evidence that grain boundary mobility is a true material property and obeys the same rules regardless of driving force. An initial investigation into the subject of boundary mobility might suggest a lack of consistency between the various measurements. The literature stretches back into the 1940s and a casual reading suggests that in fcc metals, at least, there is a maximum in mobility in the vicinity of the lattice misorientation characterized by a $40^\circ$ rotation about a $<111>$ axis [1, 2]. This was further linked to the presence of a special coincident site lattice (CSL) boundary type, the $\Sigma 7$ at about $38^\circ<111>$. This view has persisted in the recrystallization literature and has been much discussed in the context of the development of recrystallization textures because certain plane strain texture components possess this misorientation with the cube texture component, which is often present at high fractions after annealing. The evidence for this comes from experiments in which the driving force is a stored energy from plastic deformation [3, 4], i.e. recrystallization experiments. The results are somewhat statistical in nature because each experiment produces many new grains, and the migration rate of the boundary between each new recrystallizing grain and the deformed matrix is taken as representative of its mobility. In the recent literature on boundary mobility, however, it is typical to use boundary curvature as a driving force. Each experiment is based on an individual manufactured bicrystal and therefore there is more control over the experiments. The results reveal a widely varying mobility as a function of boundary type. The main features of mobility in aluminum are as follows.

- The highest mobilities are observed in the vicinity of boundaries with a misorientation of $38^\circ-40^\circ<111>$ [5].
- The exact position of the mobility maximum varies with temperature: at lower temperatures, the maximum is close to $38^\circ<111>$, whereas at high temperatures, the maximum shifts to around $40^\circ<111>$ [5].
- Evaluation of activation enthalpies reveals a compensation temperature effect such that there is a proportionality between the enthalpy and the prefactor, giving rise to a temperature at which the variation in mobility between boundary types is minimized.
- There are substantial variations in activation enthalpy with $<110>$ tilt boundaries exhibiting values substantially greater than those associated with bulk diffusion of solutes, for example.
- Solutes are a powerful retardant on mobility. Solute concentrations above the 1 ppm level result in measurable decreases in mobility. Transition metal solutes such as iron exert the strongest retardation effect [6].

This paper makes the case that many of the same trends are apparent when a sufficiently detailed examination is conducted of mobility measurements that use a stored energy driving force.

### 2. Experimental

Samples of Al-0.03 wt.% Zr alloys were provided by the Alcoa Technical Center with additions to represent the composition of commercial purity aluminum. After breakdown forging, high-temperature anneals were performed to develop coarse grain structures from which single-crystal specimens were cut. The deformation was applied by 30% reduction in cold rolling to generate appropriate stored en-
ergy levels. [7 – 10]. Each specimen was scratched followed by annealing to nucleate new, recrystallizing grains that grew into the deformed regions. The migration rates were derived from the boundary positions and misorientations were measured from automated electron back-scatter diffraction (EBSD) scans. Serial sectioning was performed on certain specimens to examine inclination angles and morphology of highly mobile boundaries. Samples were annealed at several different temperatures. In these recrystallization experiments, migrating boundaries encounter variations in orientation of up to 2° observed within the deformed matrix.

3. Results

3.1. Observations of migrating boundaries

Figure 1 illustrates an example of the observations of growing grains. A range of migration rates was observed for different grain boundary types. At low temperatures, the fastest growing grains were always associated with boundaries near 38°<111>. Detailed analysis of the dependence on boundary type is presented in the next section. The morphology of the growing grains showed that the fastest growing grains were often faceted at low annealing temperatures whereas at high temperatures, no faceting was observed, suggesting the presence of a faceting–defaceting transition. The long, immobile facets were consistent with pure twist character whereas the mobile portion of the boundary appeared to be consistently pure tilt.

3.2. Dependence of mobility on misorientation type

The misorientation dependence of the mobility of the migrating grain boundaries is plotted for each boundary versus misorientation angle (regardless of axis) in Fig. 2. The results show a well-defined peak in mobility at 38° at the lower annealing temperature, 350 °C. At the higher annealing temperature of 485 °C, however, this same boundary type becomes a (local) minimum. There are two maxima, of which one is close to the classical 40° and the other is in the vicinity of 35° (in misorientation).

In order to characterize the dependence on the full misorientation character, the same data were plotted in Rodrigues–Frank space, Fig. 3, where white represents high mobility; some smoothing has been applied to the data for readability. These plots show that 38°<111> boundaries are the most mobile at 350 °C (maximum in the lower left corner of the $R_3 = 0.2$ section), whereas at 485 °C, many other boundary types are also mobile, which corresponds

![Fig. 1. Al-0.03 Zr annealed at (a) 350 °C and (b) 485 °C showing faceted grains at low temperature but unfaceted grains at the higher temperature. In (a) the scratch from which grains nucleated is at the right hand edge of the figure, whereas in (b), it is in the center of the image.](image1)

![Fig. 2. Mobility for all boundaries as a function of misorientation angle for samples isothermally annealed at (a) 350 °C and (b) 485 °C.](image2)
to the shift in maxima in the misorientation angle plots. Note that a few low-angle boundaries were mobile at the higher temperature.

The mobility of all boundaries within 12.5° of a <111> misorientation axis at several annealing temperatures (350°C, 460°C and 485°C) is plotted in Fig. 4. Note that the location of the maximum mobility changes from 38° to 47°, going from the lowest temperature to the highest. Also the shape of the maximum broadens slightly.

3.3. Boundary normal dependence

In order to identify the tilt twist character of moving grain boundaries, pole figure analysis was performed on subsets of the EBSD scans. A section of the moving boundary on its leading edge was isolated, together with a portion of the (nearly) sessile side-flank, as shown in Fig. 5. A {111} pole figure from such a section of a highly mobile faceted grain from the 350°C anneal shows a common 111 pole between the growing grain and its adjacent matrix; given that the misorientation was measured to be 38°<111>, this common pole must be the misorientation axis. The geometry is such that this pole could be perpendicular to the nearly sessile side-flank of the growing grain, which suggests that the side-flank is in twist configuration (misorientation parallel to the boundary normal). The misorientation axis is approximately perpendicular to the normal of the mobile edge which means that this is likely to be a tilt boundary. At the highest annealing temperature (485°C), however, the same pole figure analysis fails to reveal such a tilt twist relationship for any of the mobile grains. This observation is consistent with the disappearance of faceted grains between 385°C and 425°C.

3.4. Activation analysis of mobility

The activation energy of boundaries close to <111> as a function of misorientation angle was calculated. Figure 6 shows an example of an Arrhenius plot for all boundaries within 12.5° of the 38°<111> type for the HPAI + Zr, and an activation energy was calculated form the slope of the logarithm of the mobility versus temperature.

For boundaries whose misorientation axis was within 12.5° of <111>, the mobilities were sorted by misorientation angle and activation energies calculated for each type. The results are plotted in Fig. 7, along with literature results for curvature driven boundary migration [11, 12]. For both the stored-energy and curvature-driven migration, there is a minimum in activation energy for the near Σ7 type CSL boundaries (~ 38°<111>). The comparison also shows good agreement in terms of a minimum near 45°, a maximum between 50 and 60°, and a rising tendency at small misorientations (approaching the low-angle regime).

4. Discussion

Most of the older literature on grain boundary mobility sought to define a general rule for the variation in mobility with boundary type. For fcc metals, the results have been typically summarized in terms of a maximum in mobility for boundaries with a misorientation close to the Σ7, 38°<111>, type, although the exact location of the maximum has been uncertain within the range of 35–45°. The results presented here support this basic understanding to
Fig. 5. Inverse pole figure maps with $\{111\}$ pole figures of selected areas from (a) a faceted grain in 350°C anneal; (b) nearly faceted grain in 485°C anneal. In (a), one of the 111 poles overlaps between the two grains whereas in (b), none of the four $\{111\}$ poles overlaps.

Fig. 6. Arrhenius plot for 38°<111> boundary migration in HPAI + Zr.

Fig. 7. Activation energy of <111> boundaries in Al as a function of misorientation angle. Data after Molodov et al. [11] and Gottstein et al. [5] is for curvature-driven migration experiments, in contrast to this work, which is stored-energy driven.
first order. Examined in more detail, however, it is apparent that the location of the maximum mobility varies with temperature. As the temperature at which the experiments are conducted is raised, the maximum shifts away from 38°<111> to higher misorientation angles. In fact the variation in mobility with angle changes from exhibiting a single peak at the Σ7 type to a double peak with a local minimum at this position. This behavior is strikingly similar to that observed for experiments on manufactured bicrystals in which curvature is the driving force, rather than the stored energy used here. The absolute values of mobility are different because of the sensitivity to solute content via the solute drag effect but the anisotropy with respect to boundary type. Furthermore, a thermal activation analysis for boundaries close to a <111> misorientation axis shows that the activation enthalpy of boundary migration is lowest for the Σ7 boundary type. This, and the overall variation of the activation energy with angle, is also in agreement with the curvature driving force results.

The faceting behavior that was observed for the most mobile Σ7 boundaries at low temperature is consistent with the highly elongated grain shapes observed by the Aachen group [5]. In the latter case, however, a different experimental configuration was used and all boundaries exhibited some degree of tilt versus twist anisotropy. The smallest elongations were observed for boundaries close to 38°<111>. These experiments were performed at high annealing temperatures, however, so the faceting – defaceting transition observed here may be a new result for stored-energy-driven migration. Grain boundaries are known to exhibit faceting – defaceting transitions with respect to their local shape, as reviewed by Sutton & Balluffi [13]. By contrast to the dependence on boundary normal identified here, a recent investigation using curvature found no dependence of mobility on the boundary normal, both for different <111> tilt boundaries near 38° and for mixed tilt-twist types [14]. These same experiments confirmed previous findings of a minimum of activation enthalpy and pre-factor in the vicinity of the Σ7 type. This discrepancy may, however, be related to the fact that the driving force for boundaries moving in response to curvature contains the interface stiffness such that dependence of the grain boundary energy on the normal (i.e. the torque term) can affect the behavior.

The results presented here also show that the range of boundary types that are mobile enough to be observed in this type of experiment broadens with increasing temperature. Other results, to be presented in a later publication, indicate that increasing solute levels have a similar effect. Direct comparison to the curvature-driven results is not possible because the latter have been obtained for specific series of tilt boundaries, even in the most thoroughly investigated case of aluminum [11, 5]. Gottstein and Shvindlerman suggest, however, that in broad outline the anisotropy of mobility decreases with increasing temperature. Other investigations of stored-energy-driven migration have also observed broad peaks similar to those found in the present work [15, 16]. These broad peaks, when compared to the curvature-driven results, have been speculated to be caused by the higher density of defects in deformed metals [15, 16]. The absorption of defects by the migrating boundary is expected to raise mobility [17] and result in less specificity of mobility by boundary type. Specific evidence to support this hypothesis is lacking, however.

5. Summary

The main conclusions are as follows.

– Grain boundary mobility using stored energy as a driving force has been investigated in an alloy of high purity aluminum with 0.03 % Zr by weight.
– The highest mobility is observed for a 38°<111> boundary type at low temperatures and <111> high angle boundaries are the most mobile in general.
– At high temperatures, a more diffuse maximum is observed and the mobility at 38°<111> becomes a local minimum.
– Faceting of the highly mobile 38°<111> boundaries is observed at low temperatures but not at high temperatures.
– A minimum in activation energy for boundary migration is observed for the 38°<111> boundary type, in good agreement with mobility measurements using curvature as a driving force, although the energies are generally smaller for the stored energy case.
– The similarities of grain boundary mobility using stored energy as a driving force when compared to curvature-based measurements suggests that mobility is indeed a material property.

References


(Rceived ■; accepted ■)

Correspondence address

Prof. Anthony Rollett
Roberts Hall 148, Carnegie Mellon University
5000 Forbes Av., Pittsburgh, PA 15213, USA
Tel.: +1 412 268 3177
Fax: +1 412 268 7596
E-mail: Rollett@andrew.cmu.edu