Anti-thermal mobility in the $\Sigma 3$ [111] 60° {11 8 5} grain boundary in nickel: Mechanism and computational considerations

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Abstract

Synthetic driving force molecular dynamics simulations were performed to examine anti-thermal mobility in the incoherent $\Sigma 3$ [111] 60° {11 8 5} grain boundary in a model FCC metal. This boundary is faceted, and motion occurs by the movement of the {110} facets via the glide of sets of three Shockley partial dislocations. We explore several consequences of this motion mechanism, and show how additional factors must be taken into consideration when simulating this boundary.

Keywords: grain boundary structure, grain boundary migration, facets, molecular dynamics (MD), anti-thermal motion

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Although conventional wisdom suggests that metallic microstructures should be stabilized by quenching to low temperatures, there are numerous examples of microstructural evolution, including extensive grain boundary motion, at room temperature and below [1-7]. These observations are at odds with the prevailing models for grain boundary mobility. With the exception of a handful of special boundaries that move by dislocation glide [8], grain boundary motion is widely accepted to occur by thermally activated atomic processes (c.f. [8-11]). In thermally activated grain boundary motion, the mobility follows an Arrhenius relationship with temperature T , such that $M = M_0 \exp(-Q/kT)$ where Q is the activation energy and M_0 is a constant prefactor [12]. For such boundaries, mobility should decrease exponentially with temperature.

Results of a recent computational survey of grain boundary mobilities suggest that boundary motion is more complex than the thermal activation model would predict. For example, a significant fraction of incoherent $\Sigma 3$ boundaries – typically the most prevalent grain boundaries in FCC metals – showed anti-thermal behavior, where mobility increases as temperature decreases, in the range $600\text{K} \leq T \leq 1400\text{K}$ [13, 14].

The boundary survey identified these deviations from thermally activated behavior, but did not attempt to characterize the mechanisms that cause them. Thus, here we investigate an incoherent $\Sigma 3$ boundary that displays anti-thermal behavior, in order to discover whether this behavior persists at low temperatures and to determine the anti-thermal motion mechanism.

To investigate anti-thermal motion in a typical incoherent $\Sigma 3$ boundary, we preferred a boundary that differs from the coherent twin in character, with high mobility, and zero shear coupling. One such boundary is the $\Sigma 3$ [111] 60° boundary with $\{11\bar{8}5\}$ boundary planes. This boundary is of mixed tilt and twist character, has a relatively low boundary energy of 0.384 J/m^2 at 0K, a relatively high mobility of 638 m/s_GPa at 1400K, and is boundary number 366 in the Olmsted survey [14, 15].

To simulate motion in this boundary, we apply the synthetic driving force molecular dynamics (MD) method [14, 16, 17]. Boundary motion is induced via the energy-conserving orientational (ECO) force method recently developed by Ulomek, *et al.* [17]. In this approach, nearest neighbor vectors define the crystallographic orientations of two grains. Each atom is assigned an order parameter χ based on how similar its local crystallographic orientation is to that expected in each grain, such that χ varies from -1 for atoms in the favored grain to 1 for atoms in the unfavored grain. An additional energy is assigned to each atom according to its order parameter, which creates a free energy difference between the grains and results in the boundary moving so as to grow the favored grain at the expense of the unfavored grain. The ECO force has several advantages over previous driving forces, such as the appropriate conservation of added artificial energy near the cutoff distance and increased resolution between the grains at high temperatures or low misorientations. A cutoff radius of 1.1 lattice parameters, which is sufficient to include first and second nearest neighbors, was selected to ensure the thermodynamic driving force remains close to the nominal driving force. The ECO force threshold order parameter was set to $\eta = 0.25$.

All simulations were carried out using the LAMMPS molecular dynamics package [18, 19], using the EAM potential for nickel developed by Foiles and Hoyt [20]. We note that we would not expect this interatomic potential to quantitatively reproduce grain boundary mobilities for nickel, but it has been shown to capture qualitative trends for both simulated and real FCC grain boundaries [21-23]. The system was maintained at the target temperature by a Nose-Hoover thermostat, and a timestep of 3 fs was used. The simulation cell is periodic in all three Cartesian directions, creating two grain boundaries in the bicrystal. In all simulations reported here, the length of the simulation cell normal to the boundaries was 218.6 Å; the dimensions in the plane of the boundary and the magnitude of ECO force varied as described later. Construction of the simulation cell was aided by GBpy, a Python package for calculating the geometric properties of bicrystals [24]. Visualization of the simulation results was performed with the OVITO software [25].

To determine grain boundary mobility, the simulation box was divided in half at the midpoint, and the position of each boundary was tracked independently. In each half of the simulation cell, the displacement Δx of the boundary was calculated as $\Delta x = L_x (\Delta \bar{\chi} + 1)/4$ where L_x is the length of the simulation normal to the grain boundaries and $\bar{\chi}$ is the average order parameter. As previous studies of boundary migration have pointed out, the definition of grain boundary position is somewhat arbitrary [15], but because we are principally interested in tracking the change in position over time, any self-consistent method for defining boundary position should yield reasonable results, so long as boundary motion is self-similar. From the displacement vs. time data for each boundary, we then calculate a mean and standard deviation for the boundary position using the bootstrap resampling technique described by Race [26], with a smoothing length of 5 ps and a block length of 100 ps. It should be noted, as Race did, that such techniques systematically underestimate the standard deviation, but that they allow for accurate estimation of grain boundary mobilities with comparatively little computational cost.

As shown in Figure 1(a), the $\Sigma 3$ [111] 60° {11 8 5} boundary adopts a fully faceted structure, with {111} coherent twin facets alternating with {110} facets. When referring to crystallographic directions or planes, we will use the lattice of grain 1 (marked red in Figure 1(a)) as a reference, but we note that the boundary is symmetric. This pattern of grain boundaries faceting along low-index planes – namely, {111}, {110}, and {112} – that represent local energy minima in the grain boundary energy landscape has been observed previously in both experimental and computational studies [14, 27-32], and recent work by Banadaki and Patala suggests that this behavior is common to all $\Sigma 3$ grain boundaries [27].

As would be expected, the overall motion of the boundary occurs not by movement of the sections of coherent twin boundary, but by the movement of the much more mobile {110} facets. (Animations of boundary motion at 700K are included in the online supplemental materials.) At these {110} facets, the misfit between the two crystals is accommodated by sets of three Shockley partial dislocations on each trio of {111}

planes, as illustrated in Figure 1(b), where the sum of the Burgers vectors for each set of dislocations is zero. The collective glide of this set of three partial dislocations has the net effect of exchanging the FCC stacking order of the $\{111\}$ planes that are not in registry across the $\{110\}$ facet, thus converting the crystallographic orientation of the atoms from that of one grain to that of the other. This is directly analogous to the motion of the $\{112\}$ incoherent twin boundary, which has been studied extensively for its role in twinning and detwinning processes [31, 33-37].

This structure and motion mechanism sharply contrast those seen in typical high-angle grain boundaries, which contain no structure too large to be captured at the scale of the coincident site lattice (CSL) unit cell, and which are assumed to move via uncoordinated diffusive atomic hops. Thus, these features produce complications that are not present in simulations of general high-angle boundaries, but that must be accounted for to ensure physically accurate simulations of grain boundary motion. We consider three important factors here: the two dimensions of the simulation in the plane of the grain boundary, and the magnitude of the force used to drive grain boundary motion.

Faceting of the boundary along the $\{111\}$ and $\{110\}$ planes requires us to consider how the size of our simulations along the $[6\bar{2}\bar{10}]$ faceting direction may affect the motion of the boundary. Hamilton et al. examined the grain boundary faceting via a continuum elastic model, and based on the dislocation-like interaction between facet junctions, they determined that the energy of interaction between facet junctions E varies as

$E = (A \log L + B)/L$ where L is the facet spacing and A and B are constants related to grain boundary properties and the elastic constants of the material [38]. This dependence was corroborated by molecular statics calculations; we find a similarly good fit to molecular statics calculations for our boundary. The interaction between facet junctions sets the simulation length scale in the $[6\bar{2}\bar{10}]$ faceting direction; if this length is too small, the facet will interact with its own duplicates in neighboring periodic images, which may change the dynamics of the moving boundary. To ensure that the simulation captures realistic facet interactions in this direction, we determined boundary mobility using simulations with varying lengths along the $[6\bar{2}\bar{10}]$ direction, as shown in Figure

2(a). For system sizes below 5 – 6 repeats of the boundary period, interactions between facet junctions produce a significant, systematic variation in boundary mobility. Because the grain boundary mobility survey by Olmsted et al. used a system size of 46.4 Å [15], or two repeats of the boundary period in this direction, it operated in a regime in which facet junction interactions markedly change the calculated mobilities. In contrast, though there is some fluctuation in mobility above 5 – 6 repeats, there is no systematic variation, and the mobilities do not differ outside the bounds of simulation error estimates.

Next, we must consider the size of the simulation along the high-symmetry tilt axis of the boundary, i.e. the $[1 \bar{2} 1]$ direction in the crystal. The mechanism of motion depends on the glide of partial dislocations with sense vectors that point in this direction, and so we must ensure that any simulation is large enough to accurately capture the behavior of these dislocations. An additional complication arises because the $\{110\}$ boundary prefers, below a certain temperature, to form a series of facets with $\{112\}$ orientations rather than a flat boundary of $\{110\}$ orientation. This faceting transition occurs because in FCC metals $\{112\}$ boundaries have lower energy than $\{110\}$ boundaries, and a $\{110\}$ boundary may facet into $\{112\}$ sections by rotating about the $\langle 111 \rangle$ tilt axis common to both boundaries. This behavior has been observed experimentally by Hsieh and Balluffi as the reversible faceting/de-faceting transition of a $\{110\}$ boundary in Al [29], and has been examined in more detail by Daruka and Hamilton using a combination of MD and Monte Carlo techniques [28]. The length of the simulation box along the $[1 \bar{2} 1]$ tilt axis of the bicrystal imposes an upper limit on the $\{112\}$ facet length. If this length is too small, interactions between the facet junctions will artificially raise the energy of the faceted boundary relative to its unfaceted form. This, in turn, lowers the temperature at which the boundary undergoes the faceting transition.

To estimate the effect of the simulation size in the $[1 \bar{2} 1]$ direction, we attempted to observe the faceting/defaceting transition in a manner similar to Hamilton and Deruka by creating a planar $\{110\}$ boundary, cooling it below the presumed faceting transition temperature, heating above said temperature, and observing the faceting transition. However, when we cooled a planar $\{110\}$ boundary of Foiles-Hoyt nickel, we observed

no faceting even at 100K, far below the presumed transition temperature. We hypothesize that this is caused by a material-dependent difference in the energy barrier for the faceting transition. Moreover, calculations by Olmsted et al. using the Foiles-Hoyt potential indicate that the faceted and unfaceted forms of the boundary are close in energy [15], which may contribute to the difficulty of nucleating the $\{112\}$ facets.

Working under the assumption that the unfaceted-to-faceted transition is more difficult than the faceted-to-unfaceted transition, we then generated bicrystals containing boundaries with average orientations of $\{110\}$, but which were faceted along $\{112\}$ planes with as large a facet length as the simulation box could accommodate. These boundaries were checked for defaceting after 1 ns at a constant temperature. We operationally defined the faceting transition temperature as the lowest temperature at which at least one grain boundary transitions from faceted to defaceted. It should be emphasized that this is in no way a rigorous definition of the faceting transition temperature, but rather is an upper bound on it. At each system size and temperature, it is possible that defaceting might occur if the system were simulated for a longer time. However, in acknowledgement of computational limitations, we approximate the faceting temperature as the limit of the transition temperatures as the system size along the $[1\bar{2}1]$ direction increases. As seen in Figure 2(b), this limit appears to be approximately 600K.

The secondary faceting of this boundary has a drastic effect on the boundary's mobility, because $\{112\}$ facets have lower mobility than $\{110\}$ facets. The reasons for this difference in mobility, despite the similarity of the dislocation structures of the facets, are outside the scope of this report, but the difference has been observed previously [31]. Clearly, the high mobility $\{110\}$ faceted boundary will be the principal form of the boundary above the $\{110\}$ faceting transition temperature. However, the combination of the driving force for boundary migration and fluctuations at the $\{112\}$ facet junctions can extend this regime by causing kinetically-driven defaceting even below the nominal faceting transition temperature; thus, we will also report the mobilities of the $\{110\}$ faceted boundary for temperatures down to 400 K. Because the activation energy for motion of the $\{112\}$ facets is relatively large and the relevant temperatures are low, the

mobility of the $\{112\}$ faceted boundary is very small and cannot be resolved on MD time scales.

Finally, we must consider the effect of the magnitude of the ECO force used to drive the motion of the boundary. Because most boundaries move by a thermally activated mechanism, MD driving forces are generally several orders of magnitude larger than typical experimental driving forces in order to achieve significant motion within the MD timeframe. In this case, however, the boundary motion mechanism is the glide of partial dislocations on $\{111\}$ planes, and so the energy barrier is expected to be very low. Thus, the driving force can and should be considerably smaller than that used in typical MD simulations to avoid overdriving the boundary. This motivates us to test the nominal mobility calculated for this boundary as a function of the ECO driving force applied. Figure 3 compares these mobilities to the boundary mobility in the zero-driving-force limit calculated from fluctuation-based methods [39].

At driving forces below 0.25 meV/atom, the boundary moves such a small amount during the simulation and the thermal noise becomes so significant that the calculated mobility becomes increasingly inaccurate. In contrast, for driving forces above 2.5 meV/atom, mobility falls below the zero driving force value and decreases as driving force increases. It should be noted that this high driving force regime is standard for MD simulations of grain boundary motion, and includes the driving forces used in the boundary survey by Olmsted, et al. [14] Because overdriving the boundary essentially reduces the energy barrier for forward motion to near zero, the forward motion of an overdriven boundary does not depend on temperature. Backward motion, however, remains an activated process. Thus at low temperatures where thermal fluctuations are insufficient to overcome the activation energy for backward motion, the overdriven boundary mobility is dominated by forward motion and appears not to vary with temperature, i.e. athermal mobility. In contrast, as temperature increases, forward motion remains constant while thermal fluctuations enable an increasing amount of backward motion, causing the overall mobility to decrease, i.e. antithermal mobility. The result is that driving forces that are too small or too large do not allow the accurate calculation of mobility, as

defined in the limit of low driving force. Between the extremes, though, there is a region of driving forces for which the nominal mobilities agree with the true mobility calculated by fluctuation simulations. This indicates that physically accurate mobilities can be obtained from simulations of driven boundaries at less computational cost than fluctuation-based methods. Furthermore, the driving forces in this regime approach the upper end of experimentally achievable driving forces, as driving forces on the order of 10 MPa are possible during recrystallization. It should be noted, however, that the defect structures that produce this driving force might interfere with coordinated dislocation glide, and thus be likely to alter the mechanism of boundary motion.

Based on the factors discussed above, we selected a system size of 86.3 Å (ten repeats of the boundary period) in the $[1\bar{2}1]$ direction, 104.5 Å (five repeats of the boundary period) in the $[6\bar{2}\bar{1}0]$ direction, and a synthetic driving force of 1 meV/atom (14.7 MPa) to simulate the motion of the $\Sigma 3 \{11\bar{8}5\}$ grain boundary over the temperature range $400\text{K} \leq T \leq 1400\text{K}$. The results are shown in Figure 4. As has been seen in previous studies [13, 14], the boundary mobility is high in an absolute sense and decreases as temperature increases in an antithermal manner. However, thermally damped behavior, in which the mobility scales inversely with temperature, is not observed. This is to be expected, since thermally damped motion is typical of the phonon-damped glide of isolated dislocations. In contrast, the mechanism of concerted glide of successive triplets of Shockley partial dislocations does not necessarily dictate that the boundary as a whole will move as would a lone dislocation. Nonetheless, the low energy barrier to the glide of these Shockley partial triplets implies that the mobility of the boundary should certainly be large and should decrease with increasing temperature, as we see here.

At low temperatures ($T < 400\text{-}600\text{K}$) we expect the boundary to adopt a structure that includes low mobility $\{112\}$ facets. At this point, rather than continuing the trend seen in Figure 4, we expect mobility to drop abruptly and become thermally activated such that mobility decreases as temperature decreases. However, as discussed above, we were not able to observe this transition within the constraints of the MD simulation.

In this work we have described the structure and motion mechanism of the $\Sigma 3$ [111] 60° {11 8 5} grain boundary in a model FCC metal, and how MD simulations must take these factors into account. The motion mechanism via coordinated glide of Shockley partial dislocation triplets explains the large absolute mobilities observed, as well as the antithermal variation of boundary mobility with temperature. The faceting transition of the mobile {110} facet limits the temperature range for antithermal mobility. We note that boundaries with very large mobilities can drastically influence microstructural evolution. Thus, this characterization of the motion of this incoherent $\Sigma 3$ boundary, which illustrates how a certain type of boundary may move rapidly at relatively low temperatures, provides key parameters required for accurate mesoscale models of microstructural evolution.

Acknowledgements

This work was supported by the National Science Foundation under Award Number DMR-1307138. The authors wish to acknowledge the contributions of Taichong Ma, whose initial simulations revealed that the system dimensions can interact with boundary motion in a significant manner. JH would like to thank Dr. D. L. Medlin for fruitful discussions on the topic of grain boundary faceting.

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Figures

Figure 1. Two illustrations of the structure of the $\Sigma 3$ $[111]$ 60° $\{11\ 8\ 5\}$ incoherent twin boundary. (a) A snapshot from a simulation showing the formation of the coherent twin $\{111\}$ and $\{110\}$ facets. Atoms are colored by the ECO order parameter, where the red atoms represent the reference orientation. (b) A dichromatic pattern similar to those used by Wang, et al. [34] illustrating that the fundamental unit of the $\{110\}$ facet consists of three Shockley partial dislocations with Burgers vectors $\mathbf{b}_1 = \frac{1}{6}[\bar{1}1\bar{2}]$, $\mathbf{b}_2 = \frac{1}{6}[1\bar{2}1]$, and $\mathbf{b}_3 = \frac{1}{6}[\bar{2}11]$. Filled symbols represent atoms in one crystal, empty symbols represent atoms in the other, and triangles and circles are used to distinguish atoms in different $\{112\}$ planes.

Figure 2. Boundary properties as a function of simulation size in the plane of the grain boundary. (a) The variation in calculated mobility at $T = 700\text{K}$ with the system size in the faceting direction. (b) The variation in the temperature at which the $\{110\}$ boundary undergoes a defaceting transition with the system size along the tilt axis. Insets show examples of boundary structure above (left) and below (right) the defaceting temperature; the crystallographic directions shown are for the center grain. In both plots, the dashed vertical line indicates the system size used in the original study by Olmsted, et al. [14]

Figure 3. The variation in calculated mobility with applied ECO driving force at $T = 700\text{K}$. The dashed horizontal line is the true mobility calculated from zero-driving-force fluctuation simulations using the AIRWALK method [39].

Figure 4. Mobility as a function of temperature for the $\Sigma 3$ [111] 60° boundary with $\{11\bar{8}5\}$ boundary planes. System size (86.3 x 104.5 x 218.6 Å) and driving force (1 meV/atom) were selected to give optimal results as described in the text. Note that below the $\{112\}$ defaceting temperature ($T \sim 400$ -600K), the mobility will drop abruptly to a value smaller than can be resolved in MD simulations.