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An atomistic modeling survey of the shear strength of twist grain boundaries in aluminum

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A computational survey of the shear strength of 343 unique grain boundaries was performed. For each boundary, the strength was surveyed as a function of shear direction. The results suggest that: (1) the shear strength cannot be comprehensively predicted by common grain boundary descriptors, (2) the shear strength depends significantly and simply on shear direction due to the faceted geometry of boundary planes, and (3) grain boundary shear strengths in an ordinary material can be represented by a simple statistical distribution.

Keywords: Aluminum; Grain boundary structure; Grain boundary sliding; Plastic deformation; Atomistic simulation

It is well known that grain boundaries can significantly influence the mechanical behavior of polycrystalline materials [1,2]. This point has motivated a long-standing effort to better understand the behavior of grain boundaries, with a technological aim of (1) better predicting the deformation and failure of materials and (2) illuminating novel routes for creating improved materials via grain boundary engineering [3].

An important task in the quest to achieve these two goals is to establish a relationship between the geometry and mechanical properties of boundaries. Establishing such a relationship would enable qualitative assessment of the relative performance of materials given microstructure crystallographic data, some of which can be measured using electron backscatter diffraction technologies [4]. Further, more quantitative predictions of material behavior using polycrystal physics-based microstructural models will benefit from an ability to link grain boundary geometry to properties [5–8], as there is currently no rational means of comprehensively assigning grain boundary properties in microstructural models.

Describing the relationship between grain boundary geometry and mechanical properties is a longstanding challenge due to the complexity of the relationship and the vast geometric space in which grain boundaries reside. Previous efforts have examined the connection between grain boundary properties and simplified descriptors of boundary geometry, such as coincident site lattice (CSL) density, boundary energy, and boundary free volume [9–13]. While these efforts have revealed that some rough trends do exist, the trends are not inclusive [14,15].

Following this motivation, this letter reports on the results of a computational survey of the shear strength of a large set of grain boundaries. The survey examined the shear strength as a function of shear direction for 343 unique grain boundary structures, making this study the most extensive of its kind to the authors' knowledge. Results showed (1) no comprehensive relationships between grain boundary shear strength and eight common grain boundary descriptors, (2) a significant and simply describable dependence of shear strength on shear direction, and (3) that the grain boundary shear strengths in an ordinary polycrystalline material can be represented by a simple statistical distribution.

This survey spanned a set of pure twist grain boundaries constructed with the aluminum embedded atom interatomic potential of Mishin et al. [16]. The boundary structures were obtained from the interface structure databank (ISDB) [17] http://www.isdb.cee.cornell.edu/. A detailed account of the generation procedure is given in [17]. The validity of the boundary structures was assessed by comparing boundary energies with literature values where possible, and also by comparing to measured population densities [17,18]. A linear correlation between the boundary energy and free volume was observed consistent with the works of Wolf [19] and Olmsted et al. [14], providing further validation of the grain boundary structures examined here.

An orthorhombic simulation cell was used with the grain boundary plane being parallel to the x and y global

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coordinate directions, as shown in Figure 1. The z direction of the cell then defined both the normal direction to the grain boundary plane and the twist misorientation axis. The cell boundaries in the x and y directions were periodic, and free surfaces were used in the z direction. Thus, the system can be considered an infinitely large bicrystal slab. The size of the simulation cell in the x and y direction was determined by the crystallographic periodicity. The size in the z direction is chosen so that the free surfaces do not artificially influence the grain boundary energy (≈15 nm).

Loading was applied with a prescribed shear velocity $\mathbf{v}$ on the top z surface at 0 K. Atoms within 0.5 nm of the z surfaces were constrained in the shearing plane but remained free in the z direction. The magnitude of $\mathbf{v}$ was chosen to correspond to a strain rate of 10^8 s^{-1}. For each grain boundary geometry, simulations were performed with different $\mathbf{v}$ directions, characterized by the angle θ between the positive x axis and $\mathbf{v}$ (Fig. 1). The range of $0° \leqslant \theta \leqslant 360°$ was tested in increments of 5°, resulting in 72 simulations for each grain boundary geometry (24,696 total). The simulations were performed using the LAMMPS [20] software requiring a total computation time of approximately 250,000 processor hours on a quad core Intel(R) Xeon(R) CPU (X5355, 2.66 GHz).

The simulations were conducted to a maximum engineering shear strain of 0.15. The shear stress in the direction of loading was recorded giving the stress–strain responses of the bicrystal specimen. The shear strength of the boundary was taken as the yield stress, σ_y, of the bicrystal simulation and is defined here as the maximum shear stress obtained in the direction of loading prior to 0.002 plastic strain (a stress relaxation of roughly 52 MPa from the initial elastic response). It is noted that in the cases examined, σ_y was often equivalent to the maximum shear stress observed over the entire simulation. The loading procedure was validated by reproducing the shear strength result of Sansoz and Molinari [10] for a Σ9(2 1 1) Cu boundary.

The strengths of the boundaries were found to vary significantly, with grain boundary geometry and the shear direction. Considering all of the simulations performed, the yield strengths ranged from 0.0042 to 4.9 GPa with a mean and median of 0.857 and 0.765 GPa, respectively. The inspection of 25 random simulations revealed grain boundary sliding and migration as prevalent deformation mechanisms. No instances of dislocation emission from gain boundaries were observed, noting that this mechanism would be expected for some particular orientations and can be inhibited by the boundaries of the simulation cell [10].

On the whole, the grain boundary crystallographic plane was not found to significantly influence the average shear strength of a boundary (with respect to shear direction). However, there were two very substantial exceptions (Fig. 2). Grain boundaries on the (1 1 1) and (1 0 0) planes were observed to be much weaker than grain boundaries on all other planes. This observation is attributed to the structure of the (1 1 1) and (1 0 0) boundaries. Boundaries on these planes are very flat, while most other boundaries are faceted, having an asymmetrical 2-dimensional zig-zag feature that inhibits sliding along a particular direction (see the Σ7(3 2 0) boundary in Fig. 1).

This point is illustrated with two example boundaries, the Σ91(1 1 1) and the Σ7(3 2 0) (Fig. 1). For the Σ7(3 2 0) boundary, when the direction of shear aligns with the zig-zags ($\theta = 0, 180$), the highest yield strengths were observed. Contrastingly, when the direction of shear is perpendicular to the direction of the zig-zags, which is nearly flat, the lowest shear strengths were observed. The flat structured Σ91(1 1 1) boundary has a much lower shear strength in all directions and has 60° symmetry, consistent with the boundary plane. Likewise, (1 0 0) boundaries were observed to have 90° symmetry. The large interatomic spacing and small burgers vector in the (1 1 1) and (1 0 0) planes are also likely to contribute to the low shear strength, consistent with these planes being the preferred dislocation glide planes in fcc metals.

On the whole, the average shear strength (with respect to shear direction) was found to be higher for grain boundaries with more coincident lattice sites, a finding that is consistent with current thoughts on atomic scale friction [21].

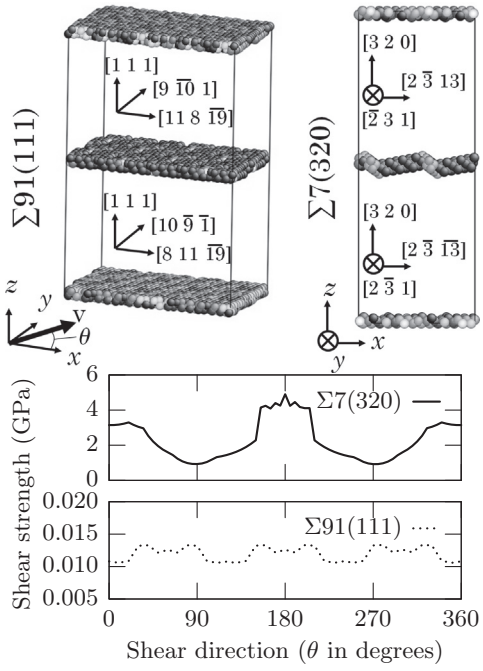

Figure 1. Comparison of a weak and strong grain boundary. The geometry of each boundary is shown in addition to its shear strength as a function of loading direction. Only atoms not in perfect fcc stacking are shown to highlight the geometry of the boundary plane [22]. θ defines the loading direction in the x–y plane.

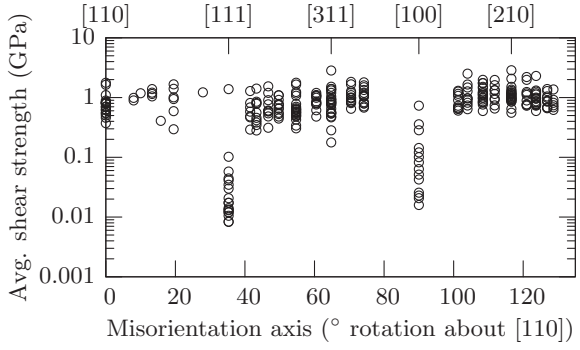

Figure 2. The effect of misorientation axis on average shear strength. The x axis indicates the misorientation axis, described as the total angle along the boundary of the standard stereographic triangle starting at the [1 1 0] direction. Each circle represents one of the boundary structures (72 directional simulations) in this survey.