Atomic simulations of twist grain boundary structures and deformation behaviors in aluminum

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The structures and behaviors of grain boundaries (GBs) have profound effects on the mechanical properties of polycrystalline materials. In this paper, twist GBs in aluminum were investigated with molecular dynamic simulations to reveal their atomic structures, energy and interactions with dislocations. One hundred twenty-six twist GBs were studied, and the energy of all these twist GBs were calculated. The result indicates that \( <001> \) and \( <111> \) twist GBs have lower energy than \( <101> \) twist GBs because of their higher interplanar spacing. In addition, 12 types of \( <001> \) twist GBs in aluminum were chosen to explore the deformation behaviors. Low angle twist GBs with high density of network structures can resist greater tension because mutually hindering behaviors between partial dislocations increase the twist GB strength. © 2017 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/).

I. INTRODUCTION

Grain Boundaries are common in polycrystalline materials and strongly influence the deformation responses and mechanical properties of materials. A fundamental understanding of structures and deformation behaviors of grain boundaries is necessary to develop materials design principles to improve the mechanical properties of polycrystalline materials. Over the past 40 years, numerous experiments and computational simulations have been performed to study basic properties of grain boundary, including GB energy, mobility and diffusivity.\(^\text{1}\) At present, atomistic simulation methods are regarded as an effective way to understand structures and properties of materials. GB structures and its interactions with other defects, such as edge dislocation-GB interactions,\(^\text{2,3}\) have been simulated at the atomic level.

Grain boundaries are important to the deformation mechanism of polycrystalline materials,\(^\text{4}\) including GB migration,\(^\text{5}\) GB diffusion, dislocation nucleation around grain boundaries,\(^\text{6-8}\) and interaction of lattice dislocations and grain boundaries.\(^\text{9-12}\) Before studying these GB behaviors, the basic properties of GBs should be investigated. In early 1989, Wolf\(^\text{13}\) used computational simulation to calculate tilt GB energy. At that time, only certain tilt GBs with a specific coincidence site lattice had been investigated. At present, much research related to grain boundary has been conducted by using molecular dynamics (MD) simulation; for example, dislocation nucleation from GBs in aluminum by Spearot \textit{et al.},\(^\text{14}\) behaviors about tilt GBs under tensile force by Tschopp \textit{et al.},\(^\text{15-19}\) and twist GB energy analysis by Zhang.\(^\text{20}\) However, there is a lack of the systematic research on structures and deformation behaviors of twist GBs in aluminum, and how twist GBs affect the nucleation and the growth of dislocations. In this paper, the structure and deformation behavior of twist GBs was systematically investigated with MD methods. The results show that interplanar spacing in \( (001), (101) \) and \( (111) \) twist GBs plays an important role in twist GBs Energy. For low angle twist GBs (<15\(^\circ\)), a theory of network structures can explain the stress-strain curve.

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II. COMPUTATIONAL MODELS AND METHODS

A large-scale atomic molecular massively parallel simulator (LAMMPS)\textsuperscript{21} developed by Sandia National Labs and Temple University was used to simulate the symmetric twist GBs. The forces between atoms were calculated by the embedded atom (EAM) potential for aluminum, as described in detail elsewhere by Mishin et al.\textsuperscript{22} This potential has been used to investigate the tension behavior for the nanowire with a tilt GB and accurately described Young’s modulus of aluminum. All the models were visualized by AtomEye visualization software\textsuperscript{23} in this work.

Figure 1(a) shows a schematic of a twist GB model. This computational cell was also used to investigate tilt GB.\textsuperscript{24} The system consists of the upper simulation cell, Grain 1, and lower simulation cell, Grain 2. A twist GB with a specific misorientation or a specific CSL $\Sigma$ value can be built by twisting upper and lower cells. Table I lists 12 examples of twist GBs that is obtained by rotating Grain 1 by $+\theta/2$ and rotating Grain 2 by $-\theta/2$ along rotation axis $<001>$. $<hkl>_1/<hkl>_2$ represents $X$ direction of Grain 1 and Grain 2 after rotation, respectively. Sigma value denotes that if two crystal lattices are allowed to overlap, $1/\Sigma$ percent points are coincident. The sigma value is coupled with a specific misorientation angle $\theta$ about a specific rotation axis. Since atoms near the twist GB are too close to each other and disturb the whole system, these atoms are deleted by defining a critical distance.\textsuperscript{25} To allow the crystal lattices to translate during energy minimization, 3D periodic boundaries are set in the simulation. Therefore, two twist GBs are formed: one periodic twist GB (TGB$^1$) at the upper and lower boundaries of the cell; and the other twist GB (TGB$^2$) in the middle of the cell. The normal direction of the boundary plane is represented by $n$, which is the rotation axis. Figure 1(b) shows a twist GB cell that is visualized by AtomEye. In this paper, 57 twist GBs along $<001>$ rotation axis, 40 twist GBs along $<101>$ rotation axis, and 29 twist GBs along $<111>$ rotation axis were studied.

Since two twist GBs in the system might interact with each other, the size of the system must be large enough to minimize the interaction. According to convergence studies, the distance between the twist GBs (lattice constant $a_0 = 4.05$ Angstroms) is set to be over 8nm, while the minimum distance in the X and Y directions is larger than 7nm. The periodic distances along X-, Y- and Z-axes are related to the rotation axis and misorientation angle by

$$\frac{L}{2} = n a_0 \sqrt{h^2 + k^2 + l^2} \geq 8\text{nm}, \text{ and}$$

$$B, W = m a_0 \sqrt{h^2 + k^2 + l^2} \geq 7\text{nm}$$

where L, B and W are box sizes of Z, Y and X directions, as shown in Figure 1(a), h, k and l are the orientation indices of grain orientation, and n and m are integers to satisfy the size requirement. The energy related to the grain boundary was calculated by the following equation:\textsuperscript{26}

$$E^{GTB} = \frac{E^{GTB}_{CSL} + N \cdot E^{FCC}_{Perfect}}{2A}$$  \hspace{1cm} (1)

FIG. 1. (a) Schematic of a 3D periodic computational cell, and (b) Twist GB model visualized by AtomEye.
TABLE I. Parameters used in the simulation for 12 $<001>$ twist GBs.

| Twist Angle (°) | X-direction $\langle hkl \rangle_1/\langle chkl \rangle_2$ | Sigma Value | Twist Angle (°) | X-direction $\langle hkl \rangle_1/\langle chkl \rangle_2$ | Sigma Value |
|----------------|-----------------------------------------------|-------------|----------------|-----------------------------------------------|-------------|
| 10.3°          | $<11 \bar{1} 0>/\langle11 \bar{1} 0>$         | $\Sigma 61$ | 28.0°          | $<4 1 0>/\langle4 \bar{1} 0>$                   | $\Sigma 17$ |
| 12.6°          | $<9 \bar{1} 0>/\langle9 \bar{1} 0>$           | $\Sigma 41$ | 31.8°          | $<7 2 0>/\langle7 \bar{2} 0>$                   | $\Sigma 53$ |
| 14.2°          | $<8 1 0>/\langle8 \bar{1} 0>$                 | $\Sigma 65$ | 36.8°          | $<3 1 0>/\langle3 \bar{1} 0>$                   | $\Sigma 5$  |
| 16.2°          | $<7 1 0>/\langle7 \bar{1} 0>$                 | $\Sigma 25$ | 41.1°          | $<8 3 0>/\langle8 \bar{3} 0>$                   | $\Sigma 73$ |
| 18.9°          | $<6 1 0>/\langle6 \bar{1} 0>$                 | $\Sigma 37$ | 42.0°          | $<15 \bar{3} 0>/\langle15 3 \bar{0} 0>$        | $\Sigma 97$ |
| 22.6°          | $<5 1 0>/\langle5 \bar{1} 0>$                 | $\Sigma 13$ | 43.6°          | $<5 2 0>/\langle5 \bar{2} 0>$                   | $\Sigma 29$ |

where $E_{GTB}^{GB}$ is the twist GB energy, $E_{GTB}^{CSL}$ represents the energy of the computational cell including N atoms, $E_{FCC}$$_{Perfect}$ refers to the potential energy of the perfect crystal lattice (-3.36 eV per atom), and A is the area of twist GB (B*W).

After initial construction, atom deletion and energy minimization are executed by iteratively adjusting atom coordinates to reach the equilibrium states. In order to avoid thermal phenomena, a 10 K temperature is built via NPT ensemble. Nose-Hoover thermostats are applied to keep the constant temperature of 10 K. The next setup is the loading condition. The Z dimension of the box is changed at a constant engineering strain rate 1.0e9/s, which is regularly used in MD tension simulation, by 200000 time steps until the strain reaches 20%. A time step of 0.001 ps is used in all the simulations.

III. RESULTS AND DISCUSSION

A. Twist GB structure and energy

For perfect crystal structure, the twist GB plane in FCC crystal has square (AB Stacking Sequence), rectangular (AB Stacking Sequence) and hexagonal (ABC Stacking Sequence) structures along $<001>$, $<101>$ and $<111>$ rotation axes, respectively (Figure 2). Thus, the twist angle cycles of twist GBs along $<001>$, $<101>$ and $<111>$ rotation axes are 90°, 180° and 120°, and symmetry axis of each cycle is 45°, 90° and 60°, respectively. Figure 3 shows the relationship between twist GB energy and the twist angle. The energy is zero at 90° (Figure 3(a)) because it is a perfect crystal without grain boundary. $\Sigma 5$ twist GB with 36.8° and 53.1° twist angles have local minimum energy. In Figure 3(c), $\Sigma 3$ twist GB has local minimum energy. Also, $<001>$ and $<111>$ twist GBs have lower energy than $<101>$ twist GBs on average, which might be related to interplanar spacing. The relationship between the interplanar spacing of (101), (001) and (111) planes corresponding to rotation axes $<101>$, $<001>$ and $<111>$ is 0.354$a_0$/0.50$a_0$/0.577$a_0$, respectively. Because of larger interplanar spacing, $<001>$ and $<111>$ twist GB structures can accommodate greater deviation of atoms, with lower energy and more stable structures.27

FIG. 2. Stacking sequence of FCC crystal along three rotation axes: (a) $<001>$, (b) $<101>$, and (c) $<111>$. 
FIG. 3. Comparison of twist GB energy: (a) twist GBs along <001> rotation axis, (b) twist GBs along <101> rotation, and (c) twist GBs along <111> rotation axis.

B. Twist GB deformation behaviors

According to the results for $0^\circ \sim 90^\circ$ twist GBs, shown in Figure 3(a), the curve is symmetric with $45^\circ$ axis. Therefore, 12 <001> twist GBs (twist angle less than $45^\circ$) are chosen to have tension simulation, and the stress-strain curves are shown in Figure 4. It was calculated that the Young’s modulus for all the <001> twist GBs is approximately 60.05 GPa (69 GPa for single crystal Al). For all FCC materials, the modulus is dependent on the orientation.28
The results also indicate that $\Sigma 5$ (36.8°) twist GB has the highest tensile strength (9.21 GPa) but narrow yield area. Compared with $\Sigma 5$ (36.8°) twist GB, all other twist GBs have smaller tensile stress but clear yield area. The relationship between tensile strength and twist angle is presented in Figure 5. As can be seen from the Figure 5, the twist GB with $\Sigma 5$ (36.8°) has the highest tensile strength, while for low angle twist GB (<15°), the tensile strength keeps near constant with the reduction of twist angles.

To study twist GB structures and deformation behaviors, AtomEye was used to visualize the tensile process of atomic models, as shown in Figure 6. The defects within the system are located and colored based on the centrosymmetry parameter $c$. The central symmetry parameter can be controlled in a threshold (0.005~6.86). Gradation in color happens only for atoms whose $c$ value is within the threshold. Atoms whose $c$ value is outside the threshold will be invisible. Each GB includes different density of dislocation sources that emit dislocations with diverse behaviors. The configurations of three twist GBs before fracture are shown in Figure 6. In $\Sigma 5$ twist GB (Figure 6(b)), partial dislocation loops are generated at the beginning, then some of the dislocation loops are absorbed by the twist GB, while some of the dislocation loops migrate from the boundary to the lattice. Nucleation of dislocation loops, and interaction between dislocation loops and GB interface are very important to the strength of materials. The mechanical strength could be enhanced, to some extent, by increasing the density of dislocations and the mutual interference between the dislocations. For instance, the density and the movement of the dislocations in $\Sigma 5$ twist GB are more active than $\Sigma 37$ twist GBs (Figure 6(a) and (b)), and the movements of dislocation loops in $\Sigma 5$ twist GB occur in a wider range of strain from 10% to 17% (Figure 4), which is a stress enhancement factor because the deformation process.
can be accommodated by its neighbors. In Figure 6(c), this enhancement mechanism isn’t shown in $\Sigma 29$ twist GB that has relatively higher energy than $\Sigma 5$ twist GBs.

Figure 7 shows the Atomic structures of $<001>$ twist GBs before deformation for different twist angles. In Figure 7(a), $\Sigma 61$ (10.3$^\circ$) twist GB has a clearly net structure in the GB plane before deformation, and partial dislocations (Figure 8), marked with red lines, nucleate on each unit of networks during deformation. The mutual hindering behaviors between partial dislocations increase the twist GB strength. On the other hand, high angle twist grain boundaries have facial structure (Figure 7(b) and (c)) defects, which have relatively higher energy because there are more atoms deviating from the perfect coordination number. Also, there are less slip systems, and faster dislocation

![Figure 6](image1.png)

**FIG. 6.** Schematic of three twist GBs before fracture: (a) $\Sigma 37-18.9^\circ$ at $\varepsilon = 14\%$, (b) $\Sigma 5-36.8^\circ$ $\varepsilon = 16\%$ and (c) $\Sigma 29-43.6^\circ$ $\varepsilon = 14\%$ (The centrosymmetry parameter is used as scale).

![Figure 7](image2.png)

**FIG. 7.** Atomic structures of $<001>$ twist GBs before deformation: (a) $\Sigma 61-10.3^\circ$, (b) $\Sigma 5-36.8^\circ$ and (c) $\Sigma 85-64.9^\circ$ (The centrosymmetry parameter is used as scale).

![Figure 8](image3.png)

**FIG. 8.** Partial dislocations on $\Sigma 61-10.3^\circ$ twist GB at $\varepsilon = 12\%$ (The centrosymmetry parameter is used as scale).
behaviors have a great influence on materials’ strength. It has been identified that dislocation loops and GB interface was observed in some high angle twist GBs. These deformation network structures can resist greater tension. Nucleation of dislocation loops, and interaction between higher interplanar spacing. The simulation results show that low angle twist GBs with high density of <.011> Al were studied by using LAMMPS. GB structures and deformation behaviors have been studied in detail. Generally, <001> and <111> twist GBs have lower energy than <101> twist GBs because of higher interplanar spacing. The simulation results show that low angle twist GBs with high density of network structures can resist greater tension. Nucleation of dislocation loops, and interaction between dislocation loops and GB interface was observed in some high angle twist GBs. These deformation behaviors have a great influence on materials’ strength. It has been identified that $\Sigma$ twist GBs with relatively low energy has the highest tensile strength among all the twist GBs.

IV. CONCLUSION

The energies and microstructures of twist GBs along $<001>$, $<101>$ and $<111>$ rotation axes in Al were studied by using LAMMPS. GB structures and deformation behaviors have been studied in detail. Generally, $<001>$ and $<111>$ twist GBs have lower energy than $<101>$ twist GBs because of higher interplanar spacing. The simulation results show that low angle twist GBs with high density of network structures can resist greater tension. Nucleation of dislocation loops, and interaction between dislocation loops and GB interface was observed in some high angle twist GBs. These deformation behaviors have a great influence on materials’ strength. It has been identified that $\Sigma$ twist GBs with relatively low energy has the highest tensile strength among all the twist GBs.

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