Effect of Extrinsic Grain Boundary Dislocations on Mechanical Properties of Ultrafine-Grained Metals by Molecular Dynamics Simulations

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The effect of extrinsic grain boundary dislocations (EGBDs) in nonequilibrium grain boundaries on the mechanical properties of ultrafine-grained metals is investigated by molecular dynamics simulations. Aluminum bicrystall models containing cracks and EGBDs impinged from the crack tips are prepared. First, the dependence of the local grain boundary structure on the accommodation mechanism of EGBDs, and on its stress field is studied. Then, the shielding effect of EGBDs on the emissions of dislocations from crack tips is investigated, and the effect of nonequilibrium grain boundaries on the intragranular deformation is discussed. Finally, to investigate the relationship between EGBDs and intergranular deformations, shear loading is applied to the bicrystal models. It is found that extrinsic grain boundaries function as the intergranular deformation source, and the Burgers vector components of the EGBDs lead to anisotropic grain boundary sliding.


1. Introduction

Grain refinement is one of the techniques used to improve the mechanical properties of polycrystalline metals. Recently, severe plastic deformation (SPD) processes\textsuperscript{1} such as equal-channel angular pressing (ECAP),\textsuperscript{2,3} accumulative roll bonding (ARB),\textsuperscript{3,4} and high-pressure torsion (HPT)\textsuperscript{5,6} processes, have attracted the attention of researchers because grain sizes of several hundred nanometers can be obtained using these processes. Ultrafine-grained (UFG) metals produced by SPD processes show high strength consistent with the Hall-Petch relationship, and they also exhibit unusual mechanical properties compared to coarse-grained metals, for instance, a sudden decrease in uniform elongation,\textsuperscript{5,6,7} strain-rate sensitivity of flow stress,\textsuperscript{7,8} and improved low-temperature toughness.\textsuperscript{9} However, the detailed mechanisms of these unusual mechanical properties have not been fully understood yet.

In the case of coarse-grained metals, dislocation structures are formed in the grains, and a large number of interactions between the lattice dislocations take place. The mechanical properties of coarse-grained metals are governed mainly by these interactions. However, in the case of UFG metals, which have grain sizes below several hundred nanometers, dislocation structures in the grains do not form easily. Hence, obstacles in the grains to mobile dislocations decrease with the grain size. Comparatively, the proportion of grain boundary regions in UFG metals is larger than that in coarse-grained metals. Therefore, the interaction between lattice dislocations and grain boundaries is a very important phenomenon that has to be studied to elucidate the unusual mechanical properties.\textsuperscript{10}

It has also been reported that the grain boundaries of UFG metals produced by SPD processes consist of not only geometrically necessary defect structures, \textit{i.e.}, intrinsic grain boundary dislocations (IGBDs),\textsuperscript{11} but also many EGBDs,\textsuperscript{12-14} which do not contribute to the grain boundary misorientation angle. These grain boundaries containing EGBDs are called nonequilibrium grain boundaries, and they can transform into an equilibrium grain boundary after annealing. Interesting mechanical properties of hardening by annealing and softening by deformation in nanostructured metals have been reported.\textsuperscript{15} The result implies a long-range stress field of nonequilibrium grain boundaries due to the EGBDs than equilibrium grain boundaries and the Burgers vector components of the EGBDs in nonequilibrium grain boundaries could affect the mechanical properties of UFG metals.\textsuperscript{16} Therefore, to elucidate the unusual mechanical properties of UFG metals, it is important to investigate the mechanical behavior of nonequilibrium grain boundaries.

In this study, we investigate the effects of nonequilibrium grain boundaries containing EGBDs on the mechanical properties of UFG metals. For this, we use molecular dynamics simulations\textsuperscript{17} because they can directly express the interactions between defect structures with atomic resolution.\textsuperscript{18} Aluminum bicrystal models containing cracks are developed, and the following phenomena are studied by molecular dynamics simulations: the accommodation mechanism of impinged lattice dislocations at the grain boundaries, the shear-stress field of nonequilibrium grain boundaries and its shielding effect on the emissions of dislocations from the crack tip, and the effect of EGBDs on intergranular deformations. Finally, the effect of nonequilibrium grain boundaries on the mechanical properties of UFG metals is discussed on the basis of the obtained results.

2. Computational Setup

2.1 Analysis model

Figure 1 shows the schematic of the analysis model used in this study. The interatomic potential for aluminum can be
obtained by using the embedded-atom method proposed by Mishin et al.\(^{(19)}\) The analysis model consists of three periodic structural units: UA, UA, UB, UA, \(\ldots\). The Burgers vector \(\mathbf{b}_i = 1/2[110]\) of a lattice dislocation can be resolved into two components \(\mathbf{b}_{L}^i\) and \(\mathbf{b}_{S}^i\), which are normal and parallel to the grain boundary, respectively. \(\mathbf{b}_{L}^i = 1/10[152]\) and \(\mathbf{b}_{S}^i = 1/8[201]\).

The interface structure between grain I and II is set to be the \((112)\Sigma 5\) grain boundary. Therefore, \(\theta = 101.5^\circ\). A grain boundary consists of three periodic structural units: UA, UA, UB, UA, \(\ldots\). The Burgers vector \(\mathbf{b}_i = 1/2[110]\) of a lattice dislocation can be resolved into two components \(\mathbf{b}_{L}^i\) and \(\mathbf{b}_{S}^i\), which are normal and parallel to the grain boundary, respectively. \(\mathbf{b}_{L}^i = 1/10[152]\) and \(\mathbf{b}_{S}^i = 1/8[201]\).

2.2 Tensile loading-unloading simulations

To transform equilibrium grain boundaries into nonequilibrium grain boundaries, lattice dislocations are generated from the crack tip under tensile loading in the \(z\)-direction at 100 K, and the dislocations are impinged on the \((112)\Sigma 5\) grain boundaries at different sites by controlling the crack position. When the tensile strain \(\varepsilon_t\) reaches 0.02 or 0.025, one or two pairs of dislocations are formed from the crack tips, respectively. Then, unloading is carried out until \(\sigma_{zz}\) becomes zero. After unloading, using the Parrinello-Rahman algorithm, each model is relaxed for 10 ps at 100 K, maintaining \(\sigma_t\) and \(\sigma_z\) at zero. The strain rates of loading and unloading, \(\dot{\epsilon}_t\), are set to \(\pm 8 \times 10^3\) s\(^{-1}\). To investigate the dissociation of EGBDs, the model containing one pair of EGBDs at site 1 is annealed at 800 K for 500 ps.

2.3 Shear loading-unloading simulations

In order to examine the effect of EGBDs on the grain boundary motion, shear loading \(\sigma_{zz} = \pm 800\) MPa is applied for 90 ps at 100 K to the analysis models with equilibrium grain boundaries and nonequilibrium grain boundaries. Here, nonequilibrium grain boundaries contain one or two pairs of EGBDs. When the loading time reaches 90 ps, unloading is carried out and the models are relaxed for 20 ps at 100 K. To investigate the change in the grain boundary structure after the grain boundary sliding, the model containing one pair of EGBDs at site 1 is annealed at 800 K for 200 ps.

3. Results

3.1 Dissociation of impinged lattice dislocations in grain boundaries

The accommodation mechanism of the core structures of the lattice dislocations impinged at a grain boundary could be affected by the local grain boundary structure where the dislocations are impinged.\(^{(22)}\) Hence, the energy per unit length of a lattice dislocation could change when it enters a grain boundary because the impinged dislocation dissociates depending on the local grain boundary structure. To investigate the effect of the local grain boundary structures on the energy change in the impinged dislocations, tensile loading-unloading simulations are carried out. In the simulations, one dislocation is formed from each crack tip, and the dislocations are impinged at the grain boundaries at different sites.
Figure 2 shows the shear stress distributions $\tau_{x'z'}$ and structural changes around the impinged dislocations at three different sites. Here, $x'$ and $z'$ correspond to the directions parallel and normal to the direction of the slip plane of the impinged dislocations, respectively. It can be confirmed that the lattice dislocations are trapped when they enter the equilibrium (112)Σ5 grain boundary at any site and thus do not disappear. We can also confirm that the shear stress fields far from the trapping sites precisely correspond to those at isolated lattice edge dislocations. Therefore, when it is
difficult for the impinged dislocations to transform into IGBDs in the case of low temperature, the shear stress fields due to EGBDs may affect the intragranular deformation.\(^{30}\)

We compare the energy of a lattice dislocation, \(E^L\), and the energy of the impinged lattice dislocation in a grain boundary, \(E^{GB}\). First, \(E^L\) is calculated using a single-crystal model with one edge dislocation dipole under the periodic boundary condition. The dislocation density in the single-crystal model is the same as that in the \((112)\Sigma 5\) grain boundary models containing one EGBD at each grain boundary. \(E^L\) is found to be equal to 1.41 nJ/m. Using the linear dislocation theory,\(^{24}\) the energy of a lattice edge dislocation not including the core contribution can be estimated at 1.14 nJ/m.\(^{25}\) This energy is of the same order as the energy obtained using the atomic model. Then, \(E^{GB}\) is estimated from the energy change in the grain boundary model before and after the tensile loading-unloading simulations. Therefore, \(E^{GB}\) can be calculated by the following equation.

\[
E^{GB} = \frac{E^{NEG} - E^{EGB}}{2L_y}
\]

(Equation 1)

Here, \(E^{EGB}\) is the energy of the model with equilibrium grain boundaries before loading, \(E^{NEG}\) is the energy of the model with nonequilibrium grain boundaries after loading, and \(L_y\) is the dimension of the model in the dislocation line direction. Table 1 shows \(E^{GB}\) for each grain boundary site. Even though the dislocations exist at different sites, such as a crystal lattice or a grain boundary, the differences between \(E^L\) and \(E^{GB}\) are not large. However, it can be confirmed that \(E^{GB}\) shows different values for different sites. In particular, at site 2, \(E^{GB}\) is higher than \(E^L\). The energy difference could be due to the difference in the accommodation mechanism of impinged dislocations.

Tables 2(b), 2(d), and 2(f) shows the local structural change around the trapping sites. At sites 1 and 3, a step in the vicinity of the trapping sites at the interface can be observed. The steps are formed by the 1/5[201] DSC dislocation\(^{26}\) indicated by the broken arrows in Fig. 1, which corresponds to the component \(b_1\) of the impinged lattice dislocation with \(b_n = 1/2[110]\), as shown in Fig. 1. Therefore, the impinged dislocations at site 1, \(b_1\), should decompose into at least two grain boundary dislocations, \(b_{1i}^{gb}\) and \(b_{1s}^{gb}\), as shown by the blue dislocations. Generally, \(E^L\) of the dislocation is proportional to the square of the magnitude of the Burgers vector. Hence, at sites 1 and 3, \(E^{GB}\) is lower than \(E^L\). It should be noted that the decrease in the energy of the dislocations is also caused by the difference in the shear moduli of the grain boundary region and the crystal structure. On the other hand, at site 2, double steps due to the grain boundary dislocations, \(b_{2i}^{gb}\) and \(b_{2s}^{gb}\) indicated in blue, can be observed. Moreover, a grain boundary dislocation dipole, \(b_{2i}^{gb}\) and \(b_{2s}^{gb}\) indicated in red, is generated. Hence, at site 2, \(E^{GB}\) becomes higher than \(E^L\) probably due to the extra components of the grain boundary dislocations generated in the dipole. However, even though the dissociation of the impinged dislocations occurs at different sites, the long-range shear stress field at each site is not strongly affected by the accommodation mechanism, which is also shown in the next section, because of the short range of the dissociation area.

To investigate the effect of temperature on the dissociation of an impinged dislocation, nonequilibrium grain boundaries each containing one EGBD at site 1 are annealed at 800 K for 500 ps. Figures 3(a) and 3(b) shows the stress distributions of the first invariant of stress \(I_1 = \sigma_x + \sigma_y\) of the nonequilibrium grain boundaries before and after annealing, respectively. When the dissociation of an impinged dislocation occurs, it is not easy to identify their slip plane. Therefore, \(I_1\), which does not depend on the selection of rectangular coordinate systems, is adopted instead for \(\tau_{xx}\). From the stress distribution shown in Fig. 3(a), it can be assumed that the impinged dislocations do not decompose into some dislocations. Contrary to this assumption, the impinged dislocations dissociate into at least two grain boundary dislocations in the narrow region, as shown in Fig. 2(b). A different stress distribution is observed after annealing, as shown in Fig. 3(b). From the stress field \(I_1\), it is observed that the grain boundary dislocation with \(b_{1i}\) parallel to the grain boundary gets separated from the grain boundary dislocation with \(b_{1s}\) perpendicular to the grain boundary. The grain boundary dislocations with \(b_{1i}\) slide along the grain boundary during annealing. Therefore, we call these grain boundary dislocations \(b_{1i}\) and \(b_{1s}\) as glissile and sessile grain boundary dislocations, respectively. In order to dissociate the sessile grain boundary dislocations along the grain boundary, the climb process is required, but it is difficult to simulate the dissociation phenomenon within the treatable time scale in molecular dynamics simulations.

We have also considered a case of asymmetrical grain boundaries produced by rotating grain II around the \((112)\) axis; in this cases, \(\theta\) is equal to 78.5°. Figure 3(c) shows \(I_1\) obtained after annealing the asymmetrical grain boundaries at 800 K. Even though the asymmetrical grain boundaries containing one impinged dislocation are subjected to annealing, no remarkable dissociation similar to that in the symmetrical grain boundaries is observed. This absence could be due to the high resistance to the sliding of glissile grain boundary dislocations in such asymmetrical structures. Consequently, it can be confirmed that the symmetry of a grain boundary structure could also affects the dissociation of the impinged dislocation into glissile and sessile grain boundary dislocations. The population of symmetrical grain boundaries could be one of the important factors controlling the mechanical properties of UFG metals.

### 3.2 Shielding effect of impinged dislocations on dislocation emissions from cracks

As discussed in previous sections, nonequilibrium grain boundaries show longer-range stress fields than equilibrium grain boundaries due to EGBDs, though the stress field becomes smaller when EGBDs transform into IGBDs. Hence, these stress fields may affect the motion of mobile lattice dislocations at the vicinity of grain boundaries. Furthermore, the impinged dislocations generated from a
dislocation source may exhibit a shielding effect on the source due to their back stress. To investigate the effect of EGBDs on the stress fields around the crack tips in our analysis models, the average shear stresses \( \sigma_{\text{eff}} \) in regions within 5 nm from the crack tips \( S_1 \) and \( S_2 \) around the left and right crack tips (Fig. 4) are calculated. Table 2 shows each value of \( \sigma_{\text{eff}} \). Figure 4 shows the shear stress distributions around the cracks. In the case of equilibrium grain boundaries, \( \sigma_{\text{eff}} \) is equal to 26 MPa under no applied loading. Under tensile loading, \( \sigma_{\text{eff}} \) becomes equal to \(-878\) MPa just before the formation of the first dislocation from the crack tip. In the case of nonequilibrium grain boundaries, each contains one impinged dislocation at different sites, \( \sigma_{\text{eff}} \) is approximately 140 MPa in the relaxed state. Therefore, it can be confirmed that the EGBDs produce a shielding effect on the crack tip. It should be noted that the dependence of the grain boundary structures where the dislocations are impinged, shown in Figs. 2(b), 2(d), and 2(f), on the value of \( \sigma_{\text{eff}} \) is small in this simulation. In the case of nonequilibrium grain boundaries, each containing two EGBDs at site 1, \( \sigma_{\text{eff}} \) is equal to 249 MPa, the dislocation shielding effect is stronger than in the previous case.

When the distance between the crack tips and the grain boundaries becomes larger, \( \sigma_{\text{eff}} \) dramatically decreases to 60 MPa, as shown in Fig. 4(c). The dependence of the EGBD shielding effect on the distance between the crack tips and the grain boundaries can be confirmed from Fig. 5, which shows the stress-strain curves of the bicrystal models with \( L_4 = 45 \) and 73 nm under tensile loading at \( \dot{\varepsilon}_t = 1 \times 10^8 \text{s}^{-1} \) at 100 K. The circles and triangles indicate the formation of lattice dislocations from \( S_1 \) and \( S_2 \), respectively. It is clearly observed that after the formation of the first dislocation, the rate of increase in the tensile stress in the model with \( L_4 = 45 \) nm is higher than that in the model with \( L_4 = 73 \) nm. Therefore, the absolute back stress value of EGBDs around the crack tips, which depend on the distance between the crack tips and the grain boundaries, prevents the formation of successive lattice dislocations at the same tensile stress at which the previous dislocation has been generated.

Figure 4(d) shows the shear stress distribution of the nonequilibrium grain boundaries each containing one EGBD after annealing at 800 K for 500 ps. As shown in Fig. 3(b), the impinged dislocation dissociates into two grain boundary dislocations after the annealing; hence, \( \sigma_{\text{eff}} \) reduces after annealing. Consequently, the EGBD shielding effect on the crack tips is strongly affected by the temperature and the applied loading that controls the dissociation of the EGBDs.

More detailed discussions about the EGBD shielding effect can be found elsewhere.

### 3.3 Effect of impinged dislocations on grain boundary sliding

It is essential to study the intergranular deformation in order to determine the mechanical properties of UFG metals, especially nanocrystalline metals that contain a large number of grain boundaries. To investigate the effect of EGBDs on the intergranular deformation, a shear stress \( \tau_{\text{ss}} = \pm 800 \text{MPa} \) is applied to bicrystal models containing 0, 1, and 2 EGBDs in each grain boundary at 100 K. At this temperature, it is not easy for atoms forming a grain boundary to diffuse in the interface by a thermal activation process. Therefore, interface sliding is expected to take place by the motion of the glissile dislocations at the grain boundaries. Figure 6 shows the change in equivalent strain distributions at an interval of 5 ps in the upper nonequilibrium grain boundaries each containing one EGBD under the applied shear stress of 800 MPa. The dashed line indicates the position where the lattice dislocation was impinged under tensile loading. It can be observed that atoms with large equivalent strains are generated from the site of the impinged dislocation, and the distributions can be divided into two parts on the basis of the direction of the grain boundary sliding under shear loading. Figure 7 shows detailed atomic arrangement in the white boxes A and B shown in Fig. 6. The atomic arrangement before shear

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**Table 2 Average shear stress around crack tip.**

<table>
<thead>
<tr>
<th></th>
<th>0, EGBD</th>
<th>1, EGBD</th>
<th>2, EGBDs</th>
</tr>
</thead>
<tbody>
<tr>
<td>( L_4/\text{nm} )</td>
<td>45</td>
<td>45</td>
<td>73</td>
</tr>
<tr>
<td>Slip plane</td>
<td>site 1</td>
<td>site 2</td>
<td>site 3</td>
</tr>
<tr>
<td>( \sigma_{\text{eff}}/\text{MPa} )</td>
<td>26 (–878)*</td>
<td>138 (124)**</td>
<td>140 138 60 249</td>
</tr>
</tbody>
</table>

![Fig. 3] Stress distributions of first invariant of stress \( I_1 \) of nonequilibrium grain boundaries each containing one EGBD at site 1. (a) Before and (b) after annealing at 800 K. Dissociation of EGBD is observed after annealing. (c) Asymmetrical grain boundaries with the same structures where the dislocations are impinged, shown in Figs. 2(b), 2(d), and 2(f), on the value of \( \sigma_{\text{eff}} \)}
loading is shown in Fig. 2(b). The origin of grain boundary sliding from the impinged dislocation can be observed in Fig. 7(a), and it propagates in the D2 direction, as shown in Fig. 7(b). The atomic arrangements after grain boundary sliding shows us that the components of grain boundary sliding correspond to the DSC lattice, as shown by the arrows inside the ellipses in Fig. 1, and grain boundary migration accompanies grain boundary sliding. Hence, a coupling motion takes place in the grain boundary under shear loading. In case of nonequilibrium grain boundaries each containing two EGBDs, the intergranular deformation also occurs from the site of the impinged dislocations. On the other hand, in the case of equilibrium grain boundaries containing no impinged dislocation, atoms with large equivalent strain are generated from the different sites from the nonequilibrium grain boundaries. Figure 8 shows the generation of the coupling motion under shear loading of 800 MPa at 100 K. At 16.5 ps, two parts corresponding to the coupling motion are generated, and each edge propagates in the opposite direction, as shown in Fig. 8(b). The coupling motion of the equilibrium grain boundary cannot be observed under low shear loading. However, the intergranular deformation can be confirmed in nonequilibrium grain boundaries under shear loading of up to 600 MPa. Comparing the atomic arrangements in Figs. 7(b) and 8(b), it is found that the coupling motions in the nonequilibrium and equilibrium grain boundaries are the same. Therefore, the EGBDs function as the source of intergranular deformation, and reduce the energy barrier for the intergranular deformation. This is the same tendency reported by Kurtz et al.30

Fig. 4 Stress distributions of $\sigma_{xy}$ after tensile deformation at site 1, which shows shielding effect of EGBDs on the crack tip. (a), (b), and (d) $L_I = 45$ nm and (c) $L_I = 73$ nm.
Although the coupling motion is the same in both equilibrium and nonequilibrium grain boundaries, it is found that the propagation velocities are different. Table 3 shows the propagation velocities of the intergranular deformation in each grain boundary. The symbol of ‘’—’’ indicates the absence of intergranular deformation in the

![Stress-strain curves of bicrystal models with different L_I values under tensile loading. The circles and triangles indicate the tensile strains when dislocations are generated from the left and right crack tips, respectively. The red and blue plots show the cases of L_I = 45 and 73 nm, respectively.](image)

![Change in equivalent strain distributions of nonequilibrium grain boundaries, each containing one EGBD under shear loading τ_s = 800 MPa at 100 K. The directions of grain boundary motions are defined in the lower right panel.](image)

![Grain boundary coupling motion in the D2 direction in the upper nonequilibrium grain boundaries each containing one EGBD under shear loading τ_s = 800 MPa in white broken boxes A and B shown in Fig. 6. (a) 5 ps and (b) 20 ps. The atomic arrangement before shear loading is shown in Fig. 2(b).](image)

![Generation of intergranular deformation in upper equilibrium grain boundaries containing no EGBD under shear loading τ_s = 800 MPa at 100 K. (a) 16.5 ps and (b) 17 ps at the same position.](image)
simulations. The propagation directions are defined in the lower right panel in Fig. 6. The propagation velocities in equilibrium grain boundaries do not show strong dependence on the direction. However, in the case of \( \tau_{xx} = 800 \text{ MPa} \), the propagation velocities in the D2 and D3 directions are higher than those in the D1 and D4 directions, respectively, and vice versa in the case of \( \tau_{xx} = -800 \text{ MPa} \), except for D3 and D4 for two EGBDs. High propagation velocities can be observed in the direction of the Peach-Koehler force acting on the glissile grain boundary dislocations with \( \mathbf{b} \) decomposed from the impinged dislocations with \( \mathbf{b} \) under shear loading. This behavior is more pronounced when the number of EGBDs is larger. As a result, the intergranular deformation depends strongly on the Burgers vector component of the impinged dislocations, and the mobility is remarkably anisotropic with respect to the loading direction. Grain boundary sliding related to the glissile grain boundary dislocations could take place under high shear loading even at low temperature, although no remarkable difference in atomic arrangement after the coupling motion is observed.

Figure 9(a) shows the distributions of the first invariant of stress \( I_1 \) of nonequilibrium grain boundaries each containing one EGBD after shear loading. After annealing, the grain boundaries far away from the impinged dislocations show shorter-range stress fields shown in Fig. 9(b) than that of nonequilibrium grain boundaries after shear loading shown in Fig. 9(a); therefore, the grain boundaries regain their equilibrium states, as shown in Fig. 9(b). On the other hand, regions where lattice dislocations are impinged show longer-range stress fields than equilibrium grain boundaries, which correspond to the vertical component of the impinged lattice dislocation; the component of \( \mathbf{b} \) exists even after the shear loading and annealing processes within the limitation of treatable time scale in the molecular dynamics simulations.

### 4. Conclusions

To investigate the effects of nonequilibrium grain boundaries containing EGBDs on the mechanical properties of UFG metals, aluminum bicrystal models with the \( \{112\} \Sigma 5 \) grain boundaries are used in molecular dynamics simulations. The following results were obtained.

1. The stress field of the EGBD in the nonequilibrium grain boundary remains because the Burgers vector of the impinged dislocation does not immediately disappear in the grain boundary at low temperature. Moreover, it was found that the stress field of the EGBD does not strongly depend on the local grain boundary structure, although the accommodation mechanism of the dislocation core structure depends on the local grain boundary structure.
The stress field of the EGBDs can affect the formation of dislocations from the crack tip. The shielding effect is affected by the distance between the crack tip and the grain boundary and by the number of EGBDs. Moreover, the EGBD shielding effect on the crack tips is strongly affected by the temperature and the applied loading that controls the dissociation of the EGBDs.

(3) The EGBDs can function as the intergranular deformation sources under shear loading even at low temperature by decomposing the Burgers vector into two components $\mathbf{b}_1$ and $\mathbf{b}_2$, which are normal and parallel to the grain boundary, respectively. Therefore, the intergranular deformation strongly depends on the Burgers vector component of the impinged dislocations, and the mobility is remarkably anisotropic with respect to the loading direction.

It was found that the EGBDs in nonequilibrium grain boundaries play important roles for both intragranular and intergranular deformations, and the EGBDs can be transformed into other structures at the grain boundaries easily compared to the lattice dislocations in a crystal structure. As the grain size decreases to several hundred nanometers, the proportion of grain boundaries increases dramatically. Therefore, the dependence of nonequilibrium grain boundaries on temperature and strain rate could be one of causes of unusual mechanical properties of UFG metals.

Acknowledgments

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REFERENCES

23) Stress distributions at 0.1 K are shown in all cases in this paper in order to eliminate the influence of thermal vibration.
25) The energy of a lattice dislocation is estimated using $\mu b^2 / [4\pi(1-\nu)]\ln(R/n_0)$. Here, $\mu = 30$ GPa, $b = 2.86$ Å, $\nu = 0.33$, $R = 50$ nm, and $n_0 = 1$ nm. $R$ is determined to obtain the dislocation density, which is the same as density obtained from the atomic model.