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Inhibition effect on the evolution of twist grain boundary for Al/Ni bimetal interface under torsion

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Abstract: By using molecular dynamics method with EAM potential, we study the evolution phenomena of metals twist grain boundaries (GBs) in [100], [111] and [110] orientations, respectively, together with their bimetal interfaces under anticlockwise and clockwise torsion, respectively. Our results show that there are different evolution behaviors of the GB screw dislocations between single metals (Al and Ni) and their bimetal interfaces (Al/Ni) under torsion. Specifically, for single metals in [100] and [111] orientations, their GBs evolve toward lower or higher angle twist GBs depending on the twist directions. For Ni in [110] orientation, the dislocations spread not only in the GB region but also in the grain interior. However, for the bimetal interfaces, the propagation of dislocations are not only reduced dramatically but also limited in the interface regions, showing that there exists an inhibition effect. Therefore, such inhibition effect can enhance the stability of nanomaterials which is very useful to design nanodevices further.

Keywords: twist grain boundary, bimetal interface, dislocation

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1. Introduction

Nanomaterials have been extensively studied for the past two decades due to their interesting and unique optical, thermal, mechanical, electronic and magnetic properties. In the fabrication of nanodevices based on above properties, there will be all kinds of contacts of nanomaterials and inevitable exist GBs between them. In general, GBs, as the important structural features in nanomaterials, have been under extensively scientific investigation in recent years [1-4] due to their significant strengthening effect on nanomaterials. The types, directions, and volume fraction of GBs affect the mechanical[5-7], electrical[8,9], thermal[10,11], magnetic[12] and chemical[13] properties strongly.

For GBs under external loading, shear-coupled motion of tilt GBs has been studied theoretically by Karma et al. [14]. They proposed a fundamental relationship between GB shear-coupled motion and equilibrium fluctuations. A detailed theoretical mechanism of shear-coupled GB migration at low temperature has been developed by Rajabzadeh et al. [15-16] and they pointed that the general mechanism involving nucleation and motion of disconnections could be applied to numerous GBs including low-, high-angle, and asymmetrical GBs in various materials. And they also confirmed that GB dislocation stepper motion was associated with shear-coupled GBs migration experimentally. Homer et al. [17] studied the shear-coupled GB motion and they showed the generality of the shear coupling mechanism over numerous boundaries and boundary types.

Molecular dynamics simulation is an efficient tool to study the GB behaviors at the atomic scale and there are a lot of simulations carried out to investigate the GB motions and interactions. For tensile properties, Liu et al. [18] studied the twist GBs of thin Ni/Ni_3Al (001) under uniaxial

tension. Simulations were carried out by Chen et al. [19] to study the mechanical properties of Cu(001)/Ni(001) interface boundaries with different twist angles subjected to uniaxial loading. For GB motion, a comprehensive molecular dynamics study of low-angle GB mobility was made by Rahman et al. [20] in a pure aluminum system. Yan et al [21] performed simulations to characterize the atomic motions that govern GB migration in a series of twist boundaries. Farkas et al. [22] made simulations on GB migration during room temperature deformation of nanocrystal Ni. As for crack propagation of GB, Adlakha et al. [23] studied the role of GB structure and crystal orientation on crack growth asymmetry and Gao et al. [24] studied the effects of twist twin boundary and stacking fault on crack propagation of nanocrystal Al. In addition, the compression properties of twist GBs including [100], [110] and [111] orientated nanowires have also been investigated in detail [25], and so on.

Torsion effects are the very common phenomena in micromechanical application of nanodevices such as molecular motors, nano gears and nano bearings. In the fabrication and process of nanomechanical materials, the existence of GBs is a more universal phenomenon [26-28], and of course many of the dislocations can develop into low angle GBs. However, compared with the extensively studies of shear, tension, motion, crack propagation and compression response of GBs above mentioned, the torsion effects are relatively lack of studies both in experimentally and in theoretically. As far as we know, only Christopher et al. [29] reported the torsion of defect-free nanowires, where an interesting phenomenon was identified: dislocation networks localized at GBs in the [111] and [100] oriented nanowires, whereas coaxial dislocation nucleation existed in the [110] oriented nanowire. There are few papers about the structures response of such low-angle GBs in nanowires under torsion. As for Al/Ni interface

boundary under torsion, there are no studies presented yet. To meet this, we make a comprehensive study of the Al/Ni twist GB in a low angle of 8.8 degree under different torsion.

In this work, we carry out molecular dynamics simulations to investigate the evolution of twist GBs under anticlockwise and clockwise torsion for both simple metals and bimetal, respectively. For single metals twist GBs, we identify that the low angle twist GBs in both [100] and [111] orientations evolve toward lower angle twist GBs under clockwise torsion and to higher angle twist GBs under anticlockwise torsion. But for Al/Ni bimetal twist GB, it exhibits different behaviors from the simple metals. The phenomena reflect that the asymmetric evolution phenomenon of twist GBs under anticlockwise and clockwise torsion exists in both single metals and Al/Ni bimetal interfaces. And we have found inhibition effects on the evolution of twist GBs in bimetal interfaces, which affects the directions and speed of dislocation evolution.

2. Methodology

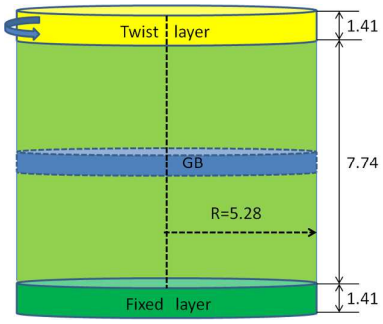


Fig. 1 Schematic of the simulation model (dimensional unit: nm).

Molecular dynamics (MD) simulations were carried out using the code LAMMPS program [30] with the EAM potentials [31-33]. The simulation model of the system consists of two equal cylindrical grains with the radius of 5.28nm and the length of 5.58nm, as shown in Fig. 1, totally including 70657, 70959 and 70604 atoms for Al/Ni interface boundary in [100], [110] and [111] orientations, respectively. The structures of GB were obtained by the following steps. Firstly, the

initial distance of two grains was set to larger than interlayer spacing of adjacent planes. Then perform an energy minimization of the system by conjugate gradient algorithm. In the beginning of the simulation, the relative anticlockwise torsion angle is set to 8.8 degree. Area of 1.41 nm length at the bottom and the top are fixed as the rigid layers, and a twist rate of $2\pi \times 10^{-3}$ rad/fs was applied to the top layer, which has been tested as a reasonable value for our MD torsion simulations. The canonical ensemble was applied throughout the whole MD simulations and the time step was chosen to be 1 fs. We also check the different time step which does not affect the results. In order to avoid the effect of temperature on the dislocation nucleation in the sliding process, the system is adjusted at a low temperature of 50K. The centro-symmetry (CS) parameter [34] for each atom in the model, except the rigid layers, is calculated to clearly visualize the various defects. For FCC metals, the CS parameter of dislocation core is about 1, here we make CS $\geq$ 1 which is enough to show all kinds of crystal defects. All the figures in this work are coloured based on atoms' CS values.

Generally speaking, there is an arbitrary angle between the direction of torsion and the area of GB. For simplicity, here we consider the plastic response of Al, Ni and Al/Ni bimetal along three axial directions ([100], [111] and [110]) with a low angle twist GB, perpendicular to the twist axis. Here we call them the GBs in [100], [111] and [110] orientations.

3. Results and discussions

Firstly, the evolution phenomena of Al twist GBs are investigated under anticlockwise and clockwise torsion. The results are present in Figs. 2(a), (b) and (c), respectively. Fig. 2(a_0) is the top view of the initial structure of Al twist GB in [100] orientation with uniformly distributed orthogonal dislocation lines forming dislocation network. Under anticlockwise torsion, the screw

dislocation lines move to the center of GB with the twist angle becoming larger, then the parallel dislocation lines close to each other leading to the shrink of dislocation network, as shown in Figs. $2(a_1)$ and (a_2), respectively. On the other hand, under clockwise torsion, the screw dislocation lines move to the border of GB with the twist angle becoming smaller, so the parallel dislocation lines are far away from each other, resulting in the expansion of the dislocation network. And GB begins to form inclined sliding plane at the border of GB expanding to the grain interior, as shown in Figs. $2(a_3)$ and (a_4), respectively. So we can find that the evolution phenomena of twist GB are asymmetric, and the dislocations are not limited in the GB region, which can also spread to the grain interior, under both anticlockwise and clockwise torsion.

Likewise, the evolution of twist GBs in [111] orientation shows a similar phenomenon. Anticlockwise torsion leads GB configuration to evolve toward a larger angle twist GB, whereas clockwise torsion results in a lower angle twist GB. The initial structure of twist GB in [111] orientation is shown in Fig. $2(b_0)$, dispersing uniformly with triangle-latticed misfit dislocations. When the torsion angle becomes larger, the individual triangle-latticed misfit dislocations shrink and almost maintain their pristine shapes. The density of dislocations is intensified with increasing covered GB region, as shown in Figs. $2(b_1)$ and (b_2), respectively. While the dislocation evolution process of clockwise torsion shows an opposite phenomenon. The individual triangle-latticed misfit dislocations expand making the density of dislocation reduce, and the dislocation lines move to the inner of the approximate triangle defects region making the crystal defect disappear finally, as shown in Figs. $2(b_3)$ and (b_4), respectively. Therefore, the asymmetric evolution of twist GB still exists in [111] orientation.

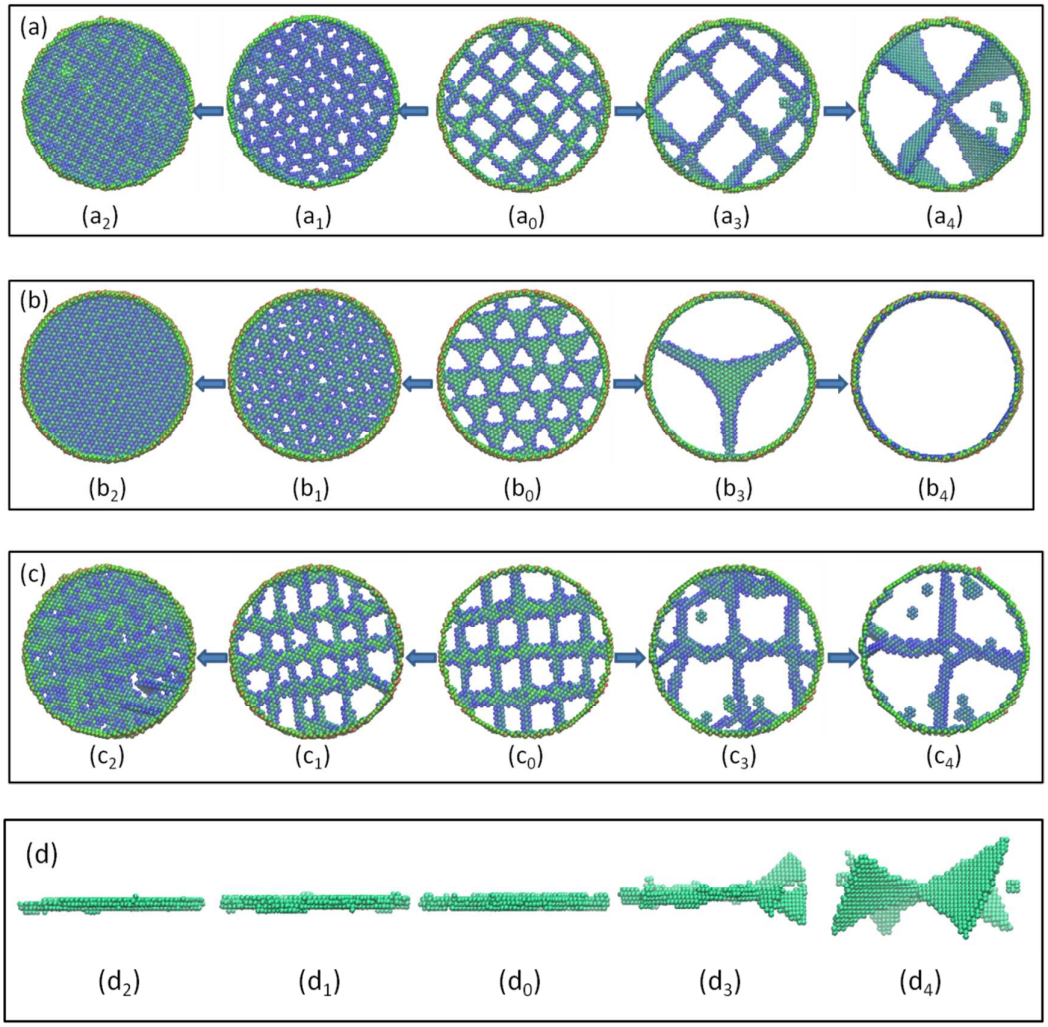


Fig. 2 (a_0), (b_0) and (c_0) are the initial configurations of twist GB for Al in [100], [111] and [110] orientations in the simulation model, respectively. $(a_1),(a_2)$ and $(a_3),(a_4)$ are anticlockwise and clockwise twist GBs' configurations of Fig. $2(a_0)$ after 20 ps and 40 ps, respectively. $(b_1),(b_2)$ and $(b_3),(b_4)$ are twist GBs' configurations of Fig. $2(b_0)$ after 20 ps and 40 ps, respectively. Likewise, $(c_1),(c_2)$ and $(c_3),(c_4)$ are anticlockwise and clockwise twist GBs' configurations of Fig. $2(c_0)$ after 20 ps and 40 ps, respectively. Fig. 2(d) shows the lateral views of Al in [100] orientation corresponding to Fig. 2(a) for reference.

As for the evolution result of twist GBs in [110] orientation, it is similar to the case in [100] orientation. The initial configuration of twist GB in [110] orientation is shown in Fig. $2(c_0)$, forming a dislocation network which consists of relatively wide parallel horizontal dislocation

lines and relatively narrow parallel vertical dislocation lines. The parallel dislocation lines close to each other under anticlockwise torsion leading to the shrink of dislocation network, as shown in Figs. 2(c_1) and (c_2) respectively. As for the clockwise torsion, the parallel dislocation lines are far away from each other resulting in the expansion of dislocation network, as shown in Figs. 2(c_3) and (c_4), respectively. Likewise, the evolution outcome in [110] orientation follows the asymmetric phenomenon, too.

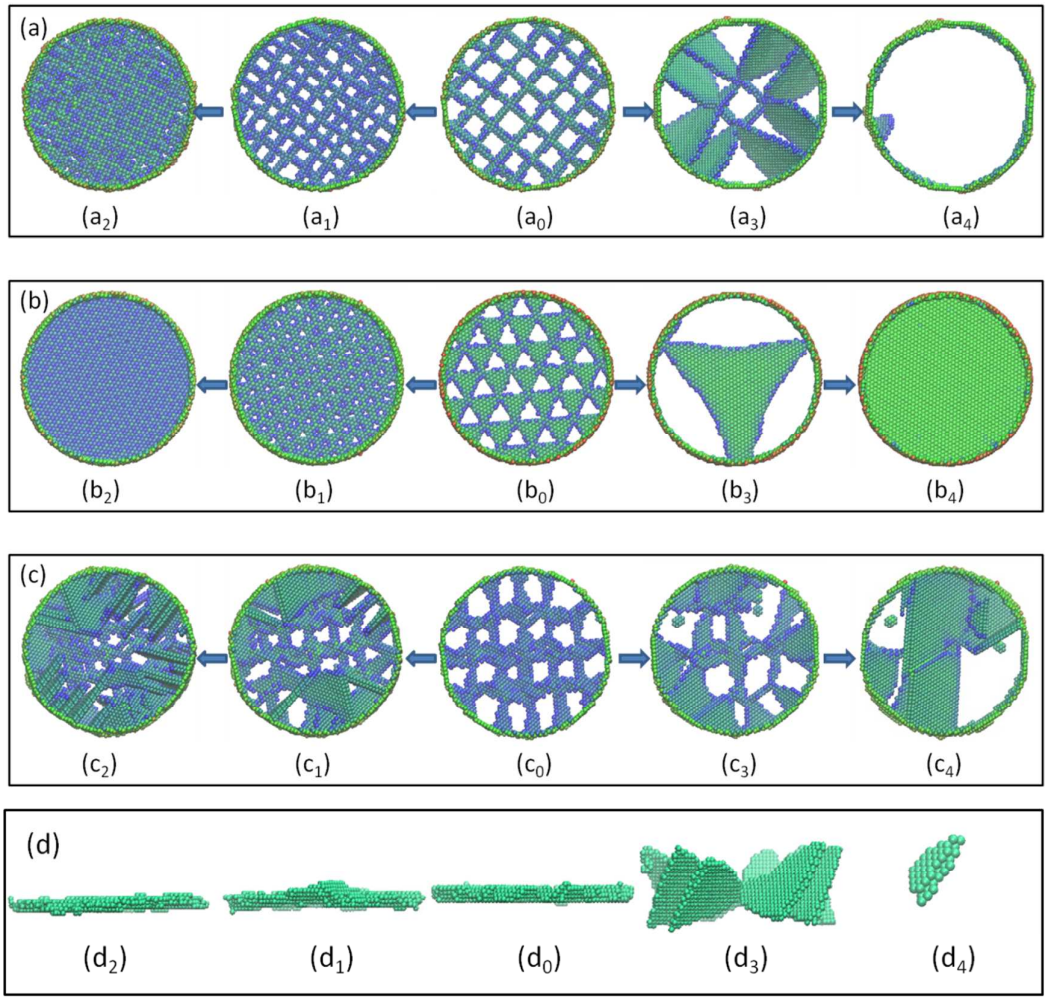


Fig. 3 (a_0), (b_0) and (c_0) are the initial configurations of Ni twist GB in [100], [111] and [110] orientations in the simulation model, respectively. (a_1),(a_2) and (a_3),(a_4) are anticlockwise and clockwise twist GBs' configurations of Fig. 3(a_0) after 20 ps and 40 ps, respectively. (b_1),(b_2) and (b_3),(b_4) are twist GBs'

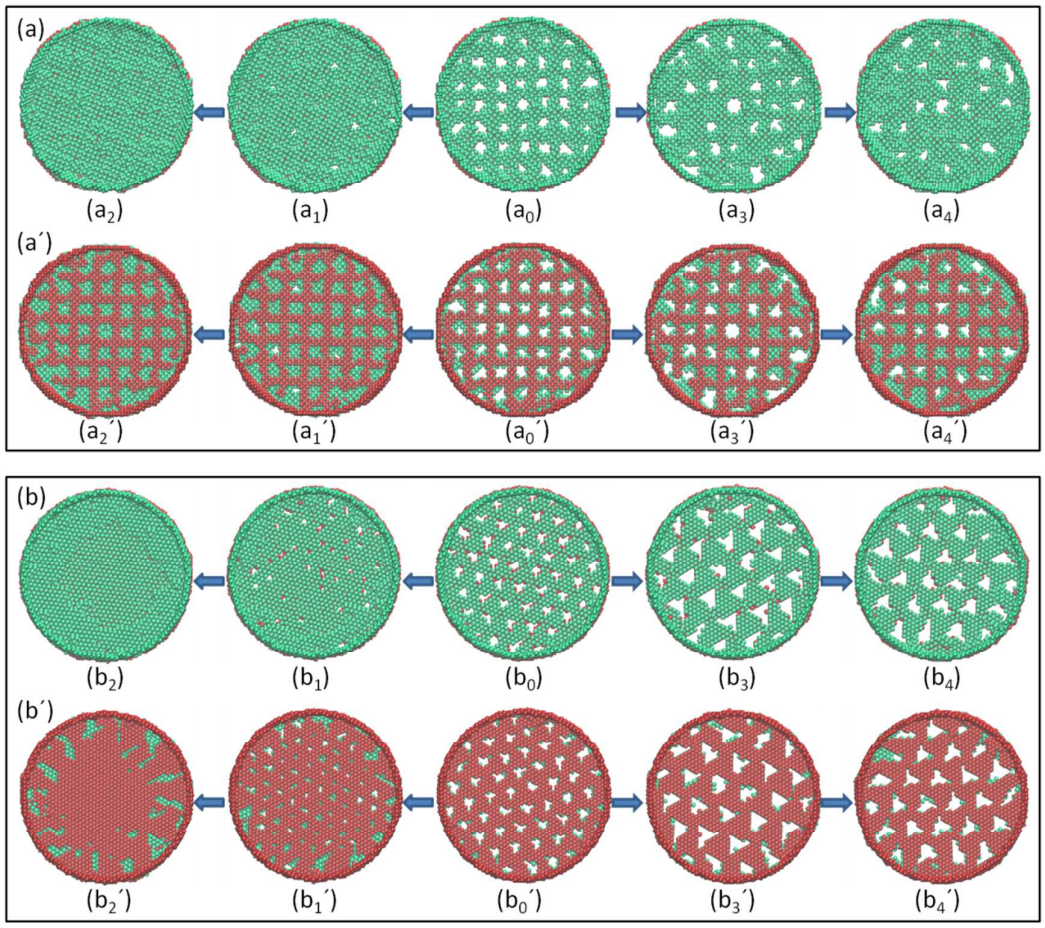
configurations of Fig. 3(b_0) after 20 ps and 40 ps, respectively. Likewise, (c_1),(c_2) and (c_3),(c_4) are anticlockwise and clockwise twist GBs' configurations of Fig. 3(c_0) after 20 ps and 40 ps, respectively. Fig. 3(d) shows the lateral views of Ni in [100] orientation corresponding to Fig. 3(a) for reference.

Next, we studied the GB evolution behaviors of Ni under torsion. We find that it has similar GB evolution behaviors with Al in [100] and [111] orientations, as shown in Figs. 3(a) and (b), respectively. Figs. 3(a_0) and (b_0) show the initial twist GB structures of Ni in [100] and [111] orientations, respectively. For twist GB in [100] orientation, the evolution outcome is similar to Al under anticlockwise torsion, while the dislocations form double-deck inclined sliding planes which propagate to the grain interior and almost disappeared finally under clockwise torsion, as shown in Figs. 3(a_3) and (a_4), respectively. As for the GB in [111] orientation, the triangle-latticed misfit dislocations expand with their pristine shapes under clockwise torsion, until fill the whole GB region finally, as shown in Figs. 3(b_3) and (b_4), respectively. Then we can learn that the dislocations are not limited to the GB region and the asymmetric evolution behaviors are still applicable to metal Ni.

But the evolution results in [110] orientation are different from the case of Al. It exhibits an intriguing behavior under torsion. Fig. 3(c_0) is the initial twist GB structure of Ni in [110] orientation, consisting of zigzag dislocation bands. The dislocation sliding planes which are perpendicular to GB generate in the grain interior under anticlockwise torsion propagating to the grain center, and the dislocation region in twist GB expands tending to occupy the whole GB, as shown in Figs. 3(c_1) and (c_2), respectively. While the inclined sliding planes generate at the border of GB under clockwise torsion, and form a huge sliding plane finally, as shown in Figs. 3(c_3) and (c_4), respectively. Then we learn that the dislocations for Ni tend to spread to the

grain interior in [110] orientation.

Compare the evolution phenomena between Al and Ni, we find that the GB evolution phenomena of Al and Ni are similar in [100] and [111] orientations, but obviously different in [110] orientation. In [100] and [111] orientations, the dislocation structures shrink under anticlockwise torsion, but expand under clockwise torsion. The dislocations are limited in the GB under anticlockwise torsion, but propagate to the grain interior under clockwise torsion in [100] orientation. As for [110] orientation, the dislocations of Al are limited in the GB, while the dislocations of Ni tend to spread to the grain interior. So we can draw a conclusion that the dislocations can spread both in the GB and in the grain interior for FCC single metals. And they all present the asymmetric evolution phenomena.



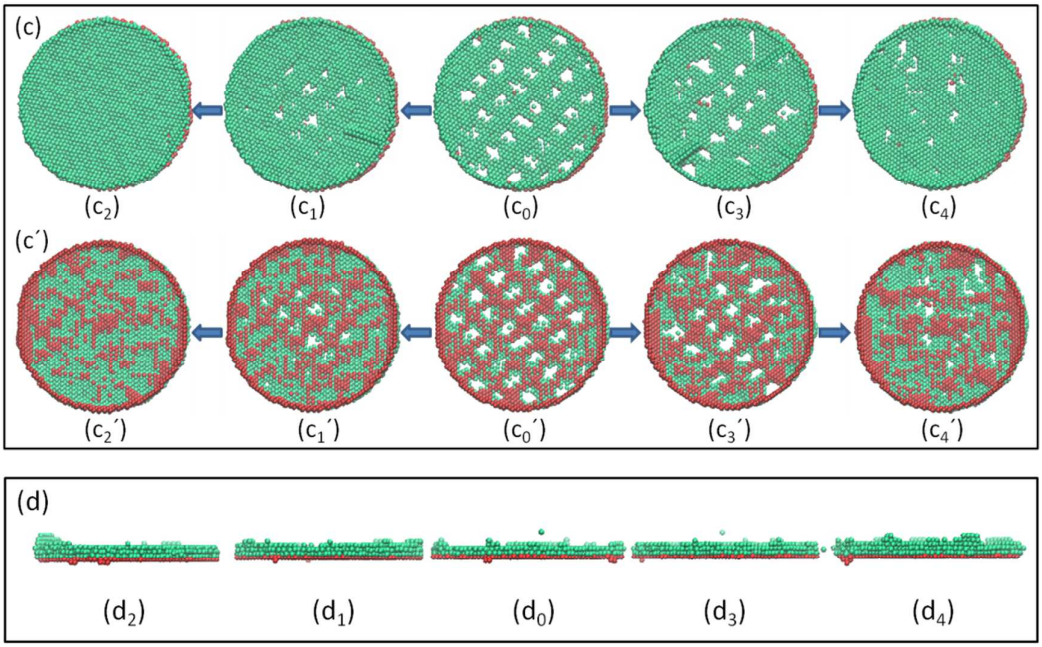


Fig. 4 (a), (b) and (c) are the GB evolution behaviors of Al/Ni bimetal viewing from the side of Al in [100], [111] and [110] orientations, respectively. At the same time, (a′), (b′) and (c′) are the GB evolution behaviors viewing from the side of Ni in the three orientations, respectively. Green atom represents Al while red atom represents Ni. (a_0), (b_0) and (c_0) are the initial GB configurations in the three orientations. (a_1),(a_2) and (a_3),(a_4) are anticlockwise and clockwise twist GBs' configurations of Fig. 4(a_0) after 20 ps and 40 ps, respectively. (b_1),(b_2) and (b_3),(b_4) are anticlockwise and clockwise twist GBs' configurations of Fig. 4(b_0) after 20 ps and 40 ps, respectively. Likewise, (c_1),(c_2) and (c_3),(c_4) are anticlockwise and clockwise twist GBs' configurations of Fig. 4(c_0) after 20 ps and 40 ps, respectively. Fig. 4(d) shows the lateral views of Al/Ni in [100] orientation corresponding to Fig. 4(a) for reference.

Then we turn to study the case of twist GB for Al/Ni bimetal interface under torsion. The initial GB structures of Al/Ni bimetal interface in [100] orientation are shown in Figs. 4(a_0) and (a_0'), forming dislocation network by parallel dislocation lines like single metals Al and Ni. Fig. 4(a) presents the evolution behaviors of twist GB on the side of Al. The same as Al and Ni, the units of dislocation network gradually reduce and eventually disappear under anticlockwise torsion, as

shown in Figs. 4(a_1) and (a_2), respectively. But it presents a different phenomenon with Al and Ni under clockwise torsion, the units of dislocation networks do not expand but reduce randomly, as shown in Figs. 4(a_3) and (a_4), respectively. Fig. 4(a') shows the evolution phenomena of twist GB on the side of Ni. The GB configuration maintains its pristine structure all the way under both anticlockwise and clockwise torsion. Different from the Al and Ni, the dislocations of bimetal are always localized in the GB plane in [100] orientation. The similar phenomenon has been observed in other simulation work by Gao et al. [35-36].

Figs. 4(b_0) and (b_0') are initial structures of twist GB for Al/Ni bimetal interface in [111] orientation, presenting similar phenomena to single metals Al and Ni, dispersing with approximate triangle-latticed misfit dislocations. On the side of Al, the approximate triangle-latticed misfit dislocations shrink under anticlockwise torsion and disappear finally, as shown in Figs. 4(b_1) and (b_2), respectively. While they expand to a fixed size and then stop expanding under clockwise torsion, as shown in Figs. 4(b_3) and (b_4), respectively. On the side of Ni, the dislocations under anticlockwise torsion present a similar phenomenon to the case on the side of Al, but the irregular misfit dislocations generate at the GB's border, as shown in Figs. 4(b_1') and (b_2'), respectively. It has the same evolution phenomenon to Al in Al/Ni bimetal interface under clockwise torsion, as shown in Figs. 4(b_3') and (b_4'), respectively. Compared with the GB evolutions of Al and Ni, the dislocation spread speed of bimetal interface reduces evidently. Then we can conclude that Al/Ni bimetal interface has an inhibition effect on the spread of twist GB in [111] orientation, especially under clockwise torsion.

Different from the evolution phenomena in [100] and [111] orientations, the twist GB in [110] orientation does not show any obvious patterns under torsion. Figs. 4(c_0) and (c_0') are initial

structures of twist GB for Al/Ni bimetal interface in [110] orientation. For the twist GB on side of Al, the initial structure is a network with orthogonal misfit dislocation bands. Whether the anticlockwise torsion or the clockwise torsion, the misfit dislocation region expands to occupy the whole GB finally, as shown in Fig. 4(c). For the twist GB on the side of Ni, dispersing with fuzzy orthogonal dislocation lines as shown in Fig. 4(c′). The dislocation lines disappear gradually under anticlockwise torsion, but still remain some dislocation regions, as shown in Figs. 4(c_1') and (c_2'), respectively. The evolution behaviors under clockwise torsion are similar to the case under anticlockwise torsion, as shown in Figs. 4(c_3') and (c_4'), respectively. But the evolution phenomena under anticlockwise and clockwise torsion are still asymmetric. The evolution phenomena of the twist GB for Al and Ni in [110] orientation present extremely intriguing behaviors propagating to the grain interior; but that of Al/Ni bimetal interface is relative normal staying in the GB. So we can conclude that Al/Ni bimetal interface has an inhibition effect on the evolution directions of twist GB in [110] orientation.

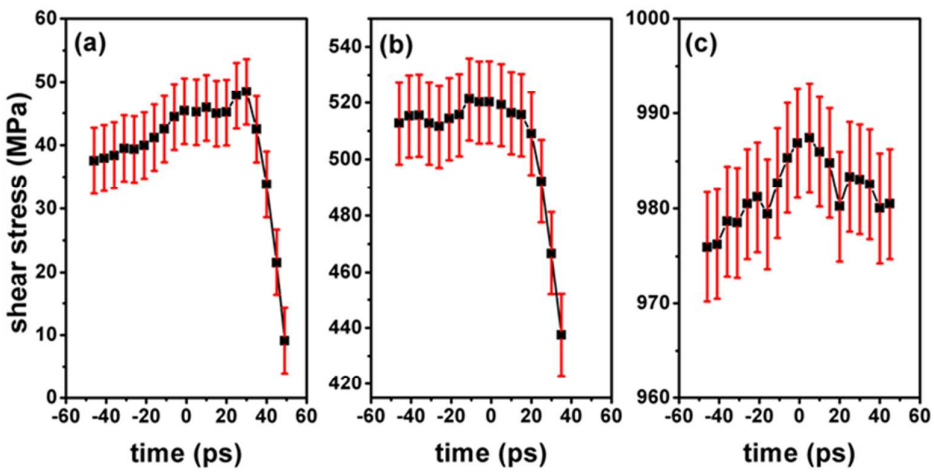


Fig. 5 (a), (b) and (c) are shear stress curves of GBs of Al, Ni and Al/Ni at the top of specimens in [100] orientation, respectively. The parts on the left of zero point represent the shear stresses under anticlockwise torsion, while the parts on the right represent the shear stresses under clockwise torsion.

Fig. 5(a) shows the shear stress decreases slightly under anticlockwise torsion, while it decreases evidently under clockwise torsion. This is because dislocations increase and tend to equilibrium under anticlockwise torsion, but decrease and form inclined slip planes under clockwise torsion. Fig. 5(b) shows a similar phenomenon to Fig. 5(a). This is because dislocations increase and tend to equilibrium under anticlockwise torsion, but form inclined slip planes and then decrease obviously under clockwise torsion. Fig. 5(c) shows that the shear stress is relative big at the beginning of torsion, but decreases gradually under torsion. This is because dislocations change evidently at first, but form stable structure eventually. Compare Figs. 5(a) and (b) to Fig. 5(c), we can learn that the shear stress is relative little in single metal GB, but becomes very large in bimetal interface. That is to say, bimetal interface is more stable than single metal GB. That may be the reason for inhibition effect in Al/Ni bimetal interfaces.

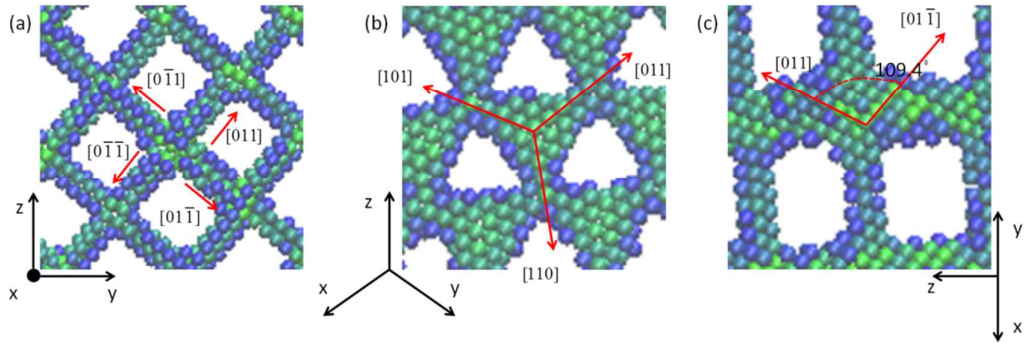


Fig. 6 (a), (b) and (c) are the local structures of Figs. 1(a_0), (b_0) and (c_0), respectively. The red arrows represent the slip directions of FCC metals when plastic deformation is present.

Nucleation and interactions of dislocations have been described clearly by other scholars [37-40] before. Now, we present an understanding of GB structures which have been studied above. As we all know, <110> crystal orientation family are the slip directions of FCC metals when plastic deformation occurs. They are the directions of maximum atoms density where Burgers vector **b** takes the minimum value. Atoms tend to move along these directions to form the stable structure,

which results in the dislocations. So dislocation structure has a relationship with the slip directions of the crystal. The GB structure in $[100]$ orientation is shown in Fig. 6(a), crystal orientations, i.e. $[011]$, $[01\bar{1}]$, $[0\bar{1}\bar{1}]$ and $[0\bar{1}1]$, are marked with red arrows, using to describe the slip directions of the Al. They are parallel to the dislocation lines, and forming an orthogonal structure which are consistent with the dislocation structure. Then we can infer that the initial GB structure depends on the slip directions of crystal. Under anticlockwise torsion, the propagation directions of dislocation lines are perpendicular to the dislocation lines and point to the center of GB. The dislocation lines close to each other leading to the shrink of dislocation network. Under clockwise torsion, the propagation directions of dislocation lines point to the GB's border leading to the expansion of dislocation network.

Fig. 6(b) is the local GB structure in $[111]$ orientation, crystal orientations, i.e. $[011]$, $[110]$ and $[101]$, are noted with red arrows, using to represent the crystal slip direction. The driving forces of the three directions are equal in size because the angles between the three crystal orientations are the same. So the dislocation is presented as a triangular structure. During the anticlockwise twist, dislocation sliding orientations direct to the center of GB resulting in the shrink of triangle dislocations area. Conversely, during the clockwise twist, dislocation sliding orientations direct to the border of GB leading to the triangle dislocation area expand.

The local GB structure in $[110]$ orientation is shown in Fig. 6(c), the red arrows represent the crystal slip directions which are parallel to the atoms arrangement directions in the dislocation area. And the angle between the two atoms arrangement directions is 109.4° which is in agreement with the theoretical value. Evidently, the dislocations are related to the crystal slip directions. Under anticlockwise torsion, the propagation directions of crystal slip directions are perpendicular

to crystal slip directions and point to the internal area of angle leading to the dislocation bands become wider. Under clockwise torsion, they point to the external area of angle leading to the dislocation bands become narrower. Therefore, we can infer that the crystal slip directions have an influence on the dislocation structure which may explain the initial structure of GB. And the initial dislocation structure of Ni presents the same mechanism, too.

4. Conclusions

In conclusion, MD simulations have shown clearly evolutions of twist GBs for single metals (Al and Ni) and bimetal interface (Al/Ni) in three orientations, i.e. [100], [111] and [110], under anticlockwise and clockwise torsion. For [100] orientation, the dislocations of single metals tend to evolve in the GB plane under anticlockwise torsion and propagate to the grain interior under clockwise torsion. But the dislocations of bimetal interface boundary tend to change only in the twist GB plane. For [111] orientation, the GB structures of single metals change faster than bimetal, and their changes are notable. For [110] orientation, the dislocations of twist GB for single metals spread both in the GB plane and in the grain interior, but dislocations only propagate in the GB plane for bimetal. To compare the evolutions of twist GBs between single metals and bimetal, we can conclude that bimetal interface has an inhibition effect on the evolution of twist GB under torsion both in evolution direction and in evolution speed, and the evolution behaviors of twist GB are asymmetric under torsion. We have found that the initial structure of twist GB has a relationship with the crystal slip directions, which may explain the twist GB structure. As for the bimetal interface, the driving forces along the crystal slip directions in the different metals are unequal, which may affect the movement of atoms. This is likely to be the reason for the inhibition effect of GB evolution. Simulations in a large torsion angle also have been performed, and show

that the inhibition effect still exists. Our findings are meaningful to enhance the stability of metal and alloy materials which can use for developing nanodevices.

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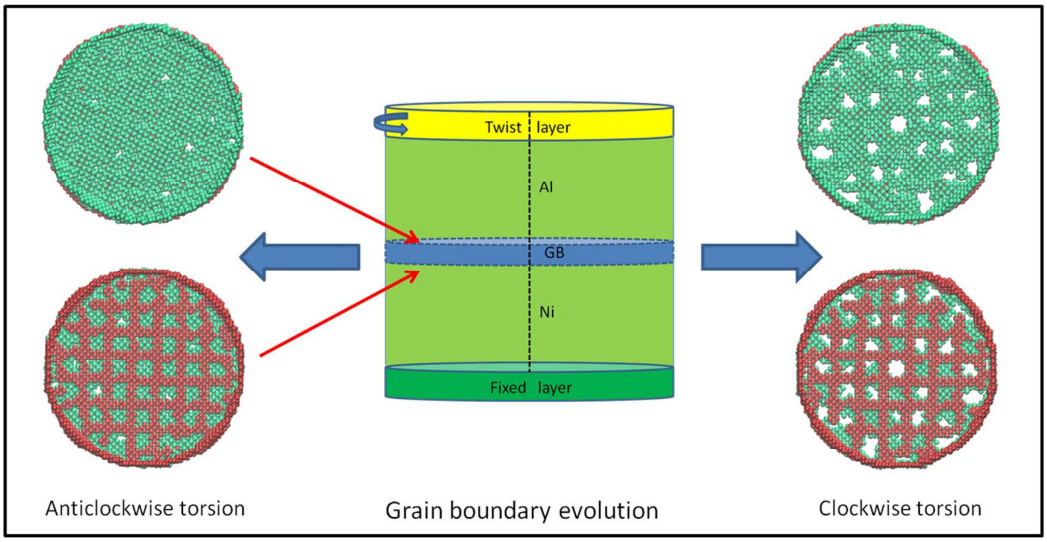

we study the evolution phenomena of metals twist grain boundaries (GBs) in [100], [111] and [110] orientations, respectively; together with their bimetal interface under anticlockwise and clockwise torsion.