Molecular dynamical investigation on dislocation near twist-grain boundary of Ni under compression

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The dislocations and the strength of a nickel bicrystal are investigated in present study. There are three kinds of crystalline orientations of the nickel bicrystal, namely (100), (110), and (111). Misfit dislocations are presented on the interface between two nickel grains when a compression process is utilized on the bicrystal. The misfit dislocations on a Ni(100) interface form a square-latticed network and those on a Ni(111) form a triangle-latticed network. When a large twist angle is applied to the Ni bicrystal, the square- and triangle-latticed unit of the misfit dislocation networks will shrink or even disappear. Thus, a plane defects distribute over the interface. If the bicrystal is compressed further, dislocations within each grain are developed from the defects on the interface between grains. The configuration of the dislocations within grains is more regular when the applied twist angle is smaller. A Ni(111) bicrystal owns the largest amount of maximal stress no matter what the twist angle is. Those of a Ni(110) bicrystal is the second and of a Ni(100) bicrystal is the smallest. © 2011 American Institute of Physics. [doi:10.1063/1.3657948]

I. INTRODUCTION

Nanoscale materials have attracted great attention for recent years due to their outstanding mechanical properties, such as high hardness and good wear resistance,1 and their potential for applications.2,3 Additionally, the existence of grain boundaries.4,5 the existence of interfaces between grain boundaries play a significant role in determining the functional and mechanical properties of the metals as the grain size reduced to nanometer range. The Hall-Patch equation shows that the hardness and yield stress of materials are increased as reducing the grain size of the material. The improvement in mechanical properties of the material is associated with dislocation pile-ups at grain boundaries.4,5

There are some experimental investigations about the deformation behaviors of grain boundaries in polycrystalline materials.6–8 Wu9 used the high resolution electron microscopy (HREM) to observe deformation behaviors of nanocrystalline nickel. They found that the grain boundaries block slips of dislocations and make dislocations be piled up. The distribution of atoms for cracked and uncracked boundaries in polycrystalline nickel under low-cycle fatigue was studied by Lim.7 They found that boundaries with low-order coincident site lattices (CSL), which own no crack, are occurred during the deformation process.

Some numerical simulations focused on interface effects in materials.10–14 In these studies, molecular dynamics (MD) is a main technique of numerical simulations for presenting behaviors of atoms and molecules. Cao and Wei15 investigated the deformation of polycrystalline copper with twin boundary under tensile. They found that the existence of twin boundary is able to prevent dislocations from moving. Spearot et al.16 simulated the nucleation of dislocations around tilt bicrystal copper and aluminum interfaces during uniaxial tension. Their results illustrated that the interface structural unit of copper plays an important role and can have a significant effect on the dislocation nucleation. Ho et al.17 revealed the influence of grain boundaries of a bicrystal material during indentation. They indicated that, due to the interaction of dislocations with the grain boundary, the bicrystal has a greater ability to resist plastic deformation. Wang et al.18 studied

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<th>TABLE I. The rotating angles and the number of atoms of three different Ni surface, (100), (110), and (111).</th>
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different kinds of defects, such as point vacancies, line vacancies, and cracks, on interfaces of semi-coherent copper bicrystal under tensile and shear deformation. They revealed that the mechanical responses of the bicrystal interfaces are strongly affected by different kinds of the crystalline defects.

In the studies mentioned above, behaviors of misfit dislocation networks appear in a (100) plane of Face-Centered Cubic (FCC) copper have been investigated in different twist angles. However, behaviors of misfit dislocation networks in Cu(110) and Cu(111) planes are seldom mentioned. Additionally, nickel is applied broadly as an important raw material of superalloy,19,20 glassy metal,21 and alloys.22,23 Thus, nickel is important to industrial applications. In this study, two nickel grains are oriented such that the top surfaces are the (100), (110), and (111) planes, respectively. Those two grains are then contacted with a twist angle to form a Ni bicrystal and a interface is formed between the grains. A interface is said to be Ni(100) interface if it is the interface between two Ni(100) grains. Ni(110) and Ni(111) interfaces are defined in a similar way. The patterns of misfit dislocation networks and strength of the Ni bicrystal are affected by the amount of the twist angle. Our results show that the pattern of the misfit dislocation networks on Ni(100) interface is a square-latticed network and that of Ni(111) is a triangle-latticed one. However, there is no special pattern for the misfit dislocation network of Ni(110) interface. For each kind of Ni crystal place, the variation of yielding strength under various twist angles are different.

II. METHODOLOGY

The schematic diagram of a Ni bicrystal is shown in Fig. 1. The bicrystal contains of two grains labeled as Ni A and Ni B, respectively. Three different kinds of substrates, namely (100), (110), and (111) planes, are modeled as a cylinder with radius 68 Å and height 113 Å. A misorientation angle (or a twist angle) for the bicrystal is obtained by fixing the bottom grain, Ni B, and rotating the upper grain. Table I shows the twist angles and the total number of atoms for those three cases. The temperature is kept at 300 K for 100 ps to relax the interface in the equilibrium process. After relaxation, the bicrystal is squeezed by two sp3 structural carbon slabs with a constant velocity of 0.14 m/s and an equilibrium time after squeezing 100 ps. In order to emphasize behaviors of the Ni bicrystal, the slabs are not shown in Fig. 1. During the compression process, the temperature of

![Fig. 1](image1.png)

**Fig. 1.** (Color online) The schematic diagram for MD simulations with a twist angle.

![Fig. 2](image2.png)

**Fig. 2.** (Color online) The top view of the misfit dislocation of Ni(100) grains with twist angles 5°, 15°, 25°, and 45°.

![Fig. 3](image3.png)

**Fig. 3.** (Color online) The stress-strain curves of Ni(100) grains with twist angles 5°, 15°, 25°, and 45° under compression.
Ni bicrystal is kept at 300 K and the rescaling method is used for temperature corrections. But the temperature of carbon slabs is kept at 0 K and simply used for applying pressure on the Ni bicrystal.

Two kinds of atomic interactions are considered, namely interactions between the nickel atoms and interactions between the nickel and carbon atoms. The many-body tight-binding potential is employed to present the interactions between Ni atoms. The main advantage of this potential is that the interactions between one atom to another and to its local environment are considered together. It is verified that material characteristics of some transient metals predicted by the many-body tight-binding potential are more accurate than those predicted by the embedded atom model (EAM). Moreover, the computational algorithm of the many-body tight-binding potential is simpler than that of the

FIG. 4. (Color online) The morphologies of Ni(100) grains with twist angles 5°, 15°, 25°, and 45° under compression. Only the value of slip vector greater than 0.3 is shown.
This potential commences to sum the band energy, which is characterized by the second moment of the \( d \)-band density of state, and a pairwise potential energy of the Born-Mayer type. Thus, the inter-atomic energy of atom \( i \) is expressed as follows:

\[
E_i = -\left\{ \sum_j \zeta^2 \exp \left[ -2q \left( \frac{r_{ij}}{r_0} - 1 \right) \right] \right\}^{1/2} + \sum_j A \exp \left[ -p \left( \frac{r_{ij}}{r_0} - 1 \right) \right],
\]

where \( \zeta \) is an effective hopping integral, \( r_{ij} \) is the distance between atom \( i \) and \( j \), and \( r_0 \) is the first-neighbor distance. The parameters \( A, p, q, \) and \( \zeta \) are determined by the experimental data concerning cohesive energy, lattice parameter, bulk modulus, and shear elastic constants \( C_{44} \) and \( C' = 1/2(C_{11} - C_{12}) \), respectively. Furthermore, the interaction force on atom \( i \) is given by

\[
F_i = \sum_{j \neq i} \frac{\partial E_i}{\partial r_{ij}} + \frac{\partial E_j}{\partial r_{ij}}.
\]

Table II lists the parameters of the tight-binding potential for nickel.\(^{19}\) Besides, the Lenard-Jones potential utilized for the interactions between the nickel atom \( i \) and the carbon atom \( j \) is expressed by

\[
U_{ij} = 4\varepsilon \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} + \left( \frac{\sigma}{r_{ij}} \right)^{6} \right].
\]

The values of parameters \( \sigma \) and \( \varepsilon \) in Eq. (3) are 3.3425 Å and 4.3025 \( \times \) 10\(^{-12} \) eV, respectively.

In order to identify the nucleation of the misfit dislocation on the interface between two Ni grains, the technique of the coordination number is applied in this study.\(^{21}\) The coordinate number for a perfect FCC structure is defined as 12. In the results which will be shown in Sec. III, we make atoms with coordination number 12 invisible to illustrate defects on the interface clearly.

Although the coordination number can specify the defects in the Ni bicrystal, it cannot offer the information about migrations of dislocations. Therefore, a slip vector is used to show obviously how the defects move under compression. The slip vector was first developed by Zimmerman et al.\(^{22}\) and can be used to detect the deformation and the evolution of dislocations in materials under compression. The slip vector at atom \( i \) is defined as follows:

\[
S_i = \frac{1}{n_i} \sum^n_{j \neq i} \left( r_{ij}^{\prime} - r_{ij} \right),
\]

where superscript \( j \) indicates neighbor atoms of the atom \( i \), \( n \) is the number of nearest neighbors to the atom \( i \), and \( n_s \) is the number of slipped neighbors. Here, \( r_{ij}^{\prime} \) and \( r_{ij} \) are the vector differences of atom \( i \) and \( j \) current and the reference positions, respectively. The arrangement of atomic positions, which is associated with the zero mechanical stress, is set to be the reference configuration of the Ni bicrystal.

### III. RESULTS AND DISCUSSIONS

#### A. Ni(100)

Figures 2(a)–2(d) show top views of Ni(100) interfaces with twist angles of 5°, 15°, 25°, and 45°, respectively. Only the atoms with coordination number not equal to 12 are plotted in these figures. One can find that misfit dislocations are accumulated on the interface and form a square-latticed network. There are two directions in the misfit dislocation network: one is [011] and the other is 011. We know that a Burgers vector \( \mathbf{b} \) of a dislocation relates to energy \( E \) of the dislocation. \( E \) is proportional to the square of the norm of \( \mathbf{b} \), i.e., \( E \propto |\mathbf{b}|^2 \). On a (100) plane of nickel, the shortest lattice
vector is \( \frac{1}{2}(001) \). Therefore, Burger vectors of the misfit dislocations on the Ni(100) interface are \( \frac{1}{2}(011) \) and \( \frac{1}{2}(011) \). The size of the square-latticed unit of the network shrinks as increasing the twist angle. Consequently, if the twist angle is greater than \( 20^\circ \), the misfit dislocation network disappears and plane defects are form due to the large twist angle. The results are in agreement with those of Liu et al. In their study, misfit dislocation networks are obvious when twist angles are less than \( 14^\circ \). The similar results are also observed in the experiment.

Figures 3 and 4 represent the stress-strain curve and the morphologies for Ni(100) bicrystal with different twist angles under compression, respectively. In Fig. 4, atoms are plotted only if the norms of their slip vectors are larger than 0.3 \( \text{Å} \). As it can be seen in Fig. 3, the stress of the Ni bicrystal with twist angle \( 5^\circ \) is lower than that with other larger twist angles. On the initial stage of compression process (see Figs. 4(a)–4(d)), the deformation of the Ni grains accumulates on the interface. The larger the applied twist angle is, the more deformation concentrates near the interface. We can say that the misfit dislocations on the interface become a barrier for the dislocation migration, that is, the dislocations in each grain are difficult to cross the interface. According to Figure 3, when the strain reaches to 6.5\(\%\) (corresponding the stress values of 5Gpa), the dislocations pile up within two grains. Figures 4(e)–4(l) show morphologies of the further stage of the compression process. In the Ni bicrystal, the dislocations pile up and cross the interface between two grains.

FIG. 7. (Color online) The morphologies of Ni(110) grains with twist angles \( 5^\circ , 15^\circ , 25^\circ , \) and \( 90^\circ \) under compression. Only the value of slip vector greater than 0.3 is shown.
During the compression process, the dislocations move through a crystalline lattice until encountering the grain boundary. The atomic mismatch between the two grains creates a repulsive stress field to oppose the continued dislocation motion. As more dislocations transit to this boundary, dislocation pile up occurs as a cluster of dislocations. In this state, the dislocations are still blocked by the boundary. As continue to increase the strain, the dislocation and the repulsive forces are accumulated at the boundary. The accumulated repulsive forces act as a driving force to reduce the energetic barrier for diffusion across the boundary, such that additional pile up causes dislocation diffusion across the grain boundary, allowing further deformation in the bicrystal. One can see that in Figure 4(b), the dislocations transit through the interface at the strain 6.5% in the case of the twist angle 5°. However, in the cases of the twist angle 15°, 25°, and 45°, the dislocations are not easy to propagate across the interface. We point out that as a large difference in the orientation of the two adjacent grains, the dislocation may not move from one grain to the other. Instead, it creates a new source of dislocation in the adjacent grain. Figures 4(i)–4(l) show the structure of the Ni bicrystal when the compression strain is 31.426%. One can find that most of the deformations occur in the [011] direction. However, the configuration of the deformation in the case of low twist angle is more regular than the other cases.

B. Ni(110)

Figures 5(a)–5(d) show the top views of Ni(110) interfaces with four different twist angles of 5°, 15°, 25°, and 90°, respectively. When the twist angle is 5°, the misfit dislocations on the interface are irregular and sparse. When the twist angle is increased, plane defects are formed on the interface. Stress-strain curves for Ni(110) bicrystal with different twist angles under compression are shown in Fig. 6. The maximal stress of each case is larger than the corresponding case of the Ni(100) bicrystal. And when the twist angle is larger, the maximal stress values at corresponding yield point [the strain is about 6.175%] become larger significantly. Figures 7(a)–7(d) show the structures of the Ni(110) bicrystal with different twist angles at strain 6.175%. Major defects are located near the interface except for the case of twist angle 5°. If the compression process continues to strain 11.115%, the dislocations within each grain develope from the interface and move to the upper and bottom grains, as one can see in Figs. 7(e)–7(h). Nevertheless, the larger the twist angle is, the less defects and dislocations within each grain are.

C. Ni(111)

Figures 8(a)–8(d) show the top views of Ni(111) interfaces with four different twist angles 5°, 15°, 25°, and 30°, respectively. At the twist angle of 5°, we cannot find any mismatch on the interface. As the twist angle increases to 15°, the misfit dislocations are observed as a triangle-latticed network on the interface. The dislocation lines are parallel to the directions [011], [101], and [110] as shown in Fig. 8(b). In any {111} slip plane, the most favorable way to slip is the dislocations passes as two partial dislocations, 1/6 (112), one immediately after the other. Therefore, the Burgers vectors of these dislocations are 2/6 [112], 2/6 [211], and 2/6 [121], as the green arrows shown in Fig. 8(b). Because the region A and B, shown in Fig. 8(b), correspond to the atomic shift of 2/6 [112], the region B may be the hexagonal closed packed (HCP). For the other twist angles, 25° and 30°, because the twist angles are large enough to form plane defects, the type of the misfit dislocations on the interface are irregular. Stress-strain curves for Ni(111) bicrystals with different twist angles under compression is shown in Fig. 9. The stress strain responses are almost the same before the stress reaches its maximal value. Meanwhile, the maximal stress ca. 22

![Figure 8](image-url)

**FIG. 8.** (Color online) The top view of the misfit dislocation of Ni(111) grains with twist angles 5°, 15°, 25°, and 30°.

![Figure 9](image-url)

**FIG. 9.** (Color online) The stress-strain curves of Ni(111) grains with twist angles 5°, 15°, 25°, and 30° under compression.
Gpa of each case are higher than those of Ni(100) and Ni(110) bicrystals. Figures 10(a)–10(d) show the structures of Ni(111) bicrystals with different twist angles at the strain of 10.005%. Most of the deformation of the Ni(111) bicrystals are accumulated at the interface at the beginning of the compression process except for the case of twist angle 5°. It is reasonable since the Ni(111) bicrystal with such small twist boundary cannot form misfit dislocation or plane defect in the interface as presented in Fig. 8(a). At strain of 12.229%, the dislocations glide into two grains. The dislocations glide from the surface and then move into the interface in the case of Ni(111) with twist angle 5°, as shown in Fig. 10(e). However, for Ni(111) bicrystals with other twist boundaries, the interface is the origin of the dislocations within each grain. The dislocations glide from the interface and move into the grains, as shown in Figs. 10(f)–10(h).

IV. CONCLUSION

The dislocations and the strength of a nickel bicrystal are investigated in present study. There are three kinds of crystal-line orientations of the nickel bicrystal, namely (100), (110),
The nickel bicrystal is combined by two grains with a twist angle. Misfit dislocations are presented on the interface between two nickel grains when a compression process is utilized on the bicrystal. The misfit dislocations on a Ni(100) interface form a square-latticed network, and the dislocation lines are parallel in [110] and [110] directions. The misfit dislocations on a Ni(100) interface are irregular and sparse. In Ni(100) and Ni(110) case, when stress reaches to yield point, the dislocations pile up from or cross interface to two grains. Consequently, the misfit dislocations on a Ni(111) form a triangle-latticed network and the dislocation lines are parallel in [101], [011], and [110] directions. An exception is that no misfit dislocations occur on the Ni(111) interface and no dislocations are piped across the interface when reaching the yield point ca. strain 10% at the twist angle 5°. At a strain of 12.229%, the dislocations glide into two grains. In the case of Ni(111) with a twist angle of 5°, the dislocations glide from the surface and then move into the interface. When a large twist angle is applied to the Ni bicrystal, the square- and triangle-latticed unit of the misfit dislocation networks will shrink or even disappear. Thus, a plane defects distribute over the interface. If the bicrystal is compressed further, dislocations within each grains are developed from the defects on the interface between grains. The configuration of the dislocations within grains is more regular when the applied twist angle is smaller. A Ni(111) bicrystal owns the largest amount of maximal stress no matter what the twist angle is. Those of a Ni(110) bicrystal is the second and of a Ni(100) bicrystal is the smallest. In this work, the Ni bicrystal nano-cylinders have been investigated. It is noted that the phenomena of the dislocation pile-up in the bicrystal nano-cylinders is meaningful to compare with that in bulk and bulk polycrystalline. The comparison would be helpful for understanding the difference between the nanograins in bulk and nanostructure on the dislocation mechanisms.