Atomic-scale dynamics of edge dislocations in Ni and concentrated solid solution NiFe alloys

Shijun Zhao^{1,*}, Yuri Osetsky¹, Yanwen Zhang^{1,2}

¹ *Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*

² *Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN 37996, USA*

E-mail: zhaos@ornl.gov

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Abstract

Single-phase concentrated solid solution alloys (CSAs), including high entropy alloys, exhibit excellent mechanical properties compared to conventional dilute alloys. However, the origin of this observation is not clear yet because the dislocation properties in CSAs are poorly understood. In this work, the mobility of a $\frac{1}{2}\langle 110 \rangle \{111\}$ edge dislocation in pure Ni and equiatomic solid solution $\text{Ni}_{0.5}\text{Fe}_{0.5}$ (NiFe) is studied using molecular dynamics simulations with different empirical potentials. The threshold stress to initiate dislocation movement in NiFe is found to be much higher compared to pure Ni. The drag coefficient of the dislocation motion calculated from the linear regime of dislocation velocities versus applied stress suggests that the movement of dislocations in NiFe is strongly damped compared to that in Ni. The present results indicate that the mobility of edge dislocations in *fcc* CSAs are controlled by the fluctuations in local stacking fault energy caused by the local variation of alloy composition.

1. Introduction

Because of their unusual mechanical properties, concentrated solid-solution alloys (CSAs), including high entropy alloys (HEAs), have attracted great interest recently [1–3]. In contrast to conventional alloys, CSAs are comprised of two or more principal elements at or near equiatomic composition situated in a simple lattice. In dilute alloys, solid solution strengthening is usually regarded as the main mechanism contributing to the dislocation dynamics. Specifically, several alloying elements (solute) are added into a crystalline lattice (solvent) in order to induce local strain/stress field that makes the dislocation motion more difficult (e.g. [4–6]). However, for CSAs, the model of solid solution strengthening cannot be straightforwardly applied since there is no “solvent” or “solute” in the conventional sense. Consequently, the small localized obstacles for dislocation glide caused by the solute atoms in dilute alloys no longer exist in CSAs. Therefore, it is vital to understand the dynamic behavior of dislocations in CSAs in order to interpret their mechanical properties and develop corresponding plasticity models. In addition, static and dynamic properties of dislocations strongly affect the microstructure evolution in CSAs under radiation [7–9].

Among all the CSAs studied so far, the solid solutions within a simple face-centered cubic (*fcc*) lattice have received increasing attention. Because of the dissociation of perfect $\frac{1}{2}[110]$ dislocations in the *fcc* lattice, the behavior of dislocations is defined by the Shockley partial dislocations and a stacking fault ribbon between them. The separation distance between the two partials is mainly related to the value of stacking fault energy (SFE). For CSAs, it has been demonstrated that their SFEs are usually low [10], which implies that the separation between

partials is usually large (more than 2 nm) [11]. Therefore, the classical atomic scale modeling approach is particularly important to investigate the dislocation properties in CSAs because *ab initio* calculations are no longer feasible for such widely dissociated dislocations. Among atomistic simulation techniques, molecular dynamics (MD) provides the most direct and practical tool to investigate the dynamics properties of dislocations, which can be used further to establish a higher level theory of plasticity. Previous studies have shown that dislocation mobility can be studied using MD and the results can be used to compare with the elastic theory of dislocations [12,13].

In this work, the dynamic properties of a $\frac{1}{2}\langle 110 \rangle \{111\}$ edge dislocation in pure Ni and *fcc* equiatomic solid solution NiFe are studied over a wide range of stresses and temperatures using MD simulations with different empirical potentials. It is found that the threshold stress for the dislocation movement in NiFe is much higher than that in pure Ni. Besides, the dislocation motion in NiFe is greatly damped compared to pure Ni. The different behaviors are closely related to the fluctuation of SFEs in NiFe and Ni that are reproduced by the empirical potentials.

2. Methods

Molecular dynamics (MD) simulations were performed using the large-scale atomic/molecular massively parallel simulator (LAMMPS) [14]. Two sets of embedded atom method (EAM) interatomic potentials developed by Bonny et al. [15,16], denoted by Bonny2013 [15] and Bonny2011 [16] respectively, were employed. The simulation cell was oriented along [110],

$[\bar{1}11]$ and $[1\bar{1}2]$ directions, as illustrated in Figure 1. A perfect $\frac{1}{2}\langle 110 \rangle$ edge dislocation was introduced between the two central $[\bar{1}11]$ planes in the cell, with the dislocation line along $Z=[1\bar{1}2]$ axis and the Burgers vector, $\mathbf{b}$, along the $X=[110]$ axis. Periodic boundary conditions (PBC) were applied in both the X and Z directions as adopted in previous studies [17–19]. Fixed boundary conditions were used in the Y direction. Along this direction, the volume was divided into three regions, in which the central region contained usual MD mobile atoms while the upper and lower regions of several atomic layers were fixed. The periodic boundary conditions applied in the X and Z directions resulted in an array of dislocations separated at a distance L_x . Such a simulation setup led to certain stress due to the image dislocations in periodic cells and therefore necessitating that a large enough dimension be chosen in this direction. Here the simulated cell had dimensions of about $30 \times 24 \times 22 \text{ nm}^3$ and contained around 1.5 million atoms. The solid solution NiFe alloy was simulated by randomly distributing Ni and Fe atoms in the lattice before the dislocation was introduced.

Figure 1 Relaxed $\frac{1}{2}\langle 110 \rangle \{111\}$ edge dislocation in pure Ni. The atoms in non-*fcc* structures as determined by common neighbor analysis are shown: hcp (red), bcc (blue) and others (white).

Atomic relaxation using the NPT ensemble was first carried out to ensure that the stresses in X and Z directions were minimized to zero. Then the stress-controlled loading was applied by adding external forces to the atoms in the upper and lower regions [12,18]. The magnitude of force was $F_x = \pm \sigma A / N_{\pm}$, where A was the area of the x-z plane, $N_{\pm}$ was the number of atoms in the upper or lower region and σ was the stress applied to the dislocation. The positive and negative sign denoted the opposite force exerted in the upper and lower regions, respectively. The following simulations were performed in the NVE ensemble with the temperature controlled by a Berendsen thermostat [20]. A time step of 1 fs was used. Dislocation was analyzed using the common neighbor analysis and dislocation extraction algorithm (DXA) [21] as implemented in the OVITO software [22].

3. Results

3.1 Dislocation core structure

During relaxation, the perfect $\frac{1}{2}\langle 110 \rangle \{111\}$ edge dislocation dissociates into two Shockley partial dislocations in its glide plane, bounding an area of stacking fault following the reaction: $\frac{1}{2}[110] \rightarrow \frac{1}{6}[211] + \frac{1}{6}[12\bar{1}]$. The separation between partials in pure Ni (L_D) is around 2 nm for both Bonny2013 and Bonny2011 potentials. The separation is related to the similar SFEs reproduced by these two potentials, which are equal to 130 and 113 mJ/m² for Bonny2013 and Bonny2011, respectively. According to linear elasticity, the dissociation distance is inversely

proportional to SFE (E_{SF}) via $d=Gb^2(2+\nu)/8\pi(1-\nu)E_{SF}$ [23]. Here G is the shear modulus of the material and ν is the Poisson's Ratio. In fact, the spacing between partial dislocations can be used to deduce the stacking fault energy, which is a standard experimental method to estimate SFE [23].

For the NiFe alloy, the dissociation distance is much larger than that in pure Ni. For our simulation setup, L_D is about 6.0 and 4.5 nm obtained with Bonny2013 and Bonny2011 potentials, respectively. The larger separation between the two partials can be traced back to the lower SFE in NiFe. In the random NiFe alloy, the specific SFE value strongly depends on the local stacking fault structure. To illustrate this, the distributions of SFE in NiFe calculated using the two potentials are presented in Figure 2, which includes the statistic of 3000 different stacking fault structures with an area around 1.0 nm^2 . It can be seen that the distribution obtained with Bonny2013 shifts towards lower energies compared to that with Bonny2011, which implies a higher probability to observe a wide dissociation using Bonny2013 compared to Bonny2011. The relatively lower SFE from Bonny2013 is consistent with the larger L_D presented above. The distribution of SFE is rather wide for both potentials, which suggests that the dissociation distance can vary substantially depending on the local atomic environment. In particular, a considerable fraction of SFE values in NiFe are in the negative region, which indicates that the *fcc* structure can be locally unstable. These localized fluctuations in the composition, structure and stability should have a significant impact on the dislocation motion.

Figure 2 The distribution of SFEs in NiFe calculated from 3000 different stacking fault structures with an area around 1 nm² using Bonny2011 and Bonny2013 potentials.

3.2 Dislocation mobility

The glide of a dislocation is initiated here by applying a constant shear stress. As an example, Figure 3 presents the dislocation positions as a function of time obtained with Bonny2013 potential at 300 K at different applied stresses. The dislocation positions are averaged from the positions of the two partial dislocations at each timestep. The time dependent positions of each partial dislocation are displayed in the insets. It can be seen that the dislocation dissociation distance is larger in NiFe compared to Ni. In addition, the distance is constant in Ni, whereas it

fluctuates along with time in NiFe. For both Ni and NiFe, the dislocation moves smoothly when the applied shear stress exceeds some critical values. This threshold stress corresponds to the onset stress for plastic deformation. A larger threshold stress is required to initiate the motion of edge dislocations in NiFe than in Ni. The dislocation velocity is then calculated as the slope of the glide distance with respect to time. It is worth pointing out that in the calculations, the dislocation glide distance is more than 10 times larger than the cell size in the X direction (along the [110] glide direction). This implies more than $10b$ plastic displacement of the upper half of the simulated cell (above the dislocation slip plane) with respect to the lower half.

Figure 3 Positions of dislocation at 300K under different applied stress obtained with Bonny2013 potential.

In order to illustrate different dislocation behaviors in NiFe and Ni under the applied stress, the dislocation velocities (V_D) obtained at 300 K with different interatomic potentials are presented in Figure 4 as a function of the applied stress. It is seen that the dislocation velocity is lower in NiFe compared to that in pure Ni at the same stress. In pure Ni, a linear increase of dislocation velocity with applied stress is observed at $\sigma < 200$ MPa. The linear relation also suggests that the Peierls stress is very small for Ni, as expected for *fcc* metals [24]. The linearity can be understood by the scaling rule predicted by phonon damping theories [25]. Higher stress leads to the saturation of the velocity, which is the sound speed of shear waves around 2.2 km/s (“forbidden velocity”). These results are in agreement with previous MD simulations [26,27], though different interatomic potentials are used. In NiFe, a much higher stress threshold required to initiate the movement of dislocations is observed using both potentials. When the applied shear stress increases above the threshold stress, a linear increase of the dislocation velocity versus applied stress is also revealed and finally the velocity saturates at the “forbidden velocity”.

Figure 4 Velocity of edge dislocation in pure Ni and NiFe at 300K calculated using Bonny2013 and Bonny2011 potentials.

The dislocation velocities predicted by Bonny2013 and Bonny2011 at the same applied stress are different in Ni and NiFe. In pure Ni, the dislocation moves faster using the Bonny2013 potential than Bonny2011. However, the opposite trend is observed in the NiFe alloy: Bonny2013 potential predicts a slower dislocation than Bonny2011. Nevertheless, for both potentials, the edge dislocation moves slower in the NiFe alloy than in pure Ni. Besides, the increase of velocity versus applied stress in NiFe is much slower from Bonny2013, which also yields a higher value of threshold stress. These observations can be correlated with the different dislocation core structures predicted by these two sets of potentials. In pure Ni, Bonny2011 predict a lower SFE value than Bonny2013. However, Bonny2013 reproduces lower SFEs and larger separations of partial dislocations in the NiFe alloy (Figure 2). For NiFe, the fluctuations in the local SFE indicate variations of the local structural stability as well as the dislocation energy along the dislocation line. These fluctuations have significant influence on the dislocation motion.

The dislocation velocities as a function of applied stress obtained at different temperatures are presented in Figure 5 for both Ni and NiFe. The most visible difference between Ni and NiFe is that V_D in Ni decreases with increasing temperature at the same applied stress whereas it increases with increasing temperature in NiFe. In pure Ni, both potentials predict the same trend, although the velocities calculated with Bonny2011 are slightly lower. Nevertheless, a remarkable difference is found in NiFe from these two potentials. The velocity from Bonny2011 is almost

independent of temperature, while Bonny2013 predicts a significant increase of V_D with increasing temperature.

Existing dislocation theory suggests that in the region where V_D is well below the elastic wave speed (speed of sound), V_D is related to the applied shear stress σ as $V_D = b\sigma/B(T)$ [17,26]. Here $B(T)$ is the drag coefficient that is dominated by the scattering of lattice vibrations (phonons). The phonon drag mechanism predicts that the velocity of dislocation is linear with the applied stress and inversely proportional to temperature, since the scattering is reduced at low temperature and thereby B decreases [26]. The present results for pure Ni are consistent with this mechanism and the obtained V_D is in agreement with that found in previous simulations [26,27]. However, the results for NiFe do not follow this mechanism, though a linear regime and the saturation of dislocation velocity at high applied stress are also observed.

Figure 5 Dislocation velocity in pure Ni and NiFe at different temperatures calculated with Bonny2013 and Bonny2011 potentials.

In the linear region of V_D versus σ , the dislocation velocity can be fitted to get the drag coefficient $B(T)$ [26]. The results are provided in Figure 6. For all the temperatures considered, NiFe exhibits larger $B(T)$ compared to Ni for both potentials. The difference is more pronounced at low temperatures. For example, $B(T)$ in NiFe from Bonny2013 is more than 8 times larger than that in pure Ni. The large drag coefficient indicates that the dislocation velocities in NiFe are much smaller than those in pure Ni as shown above. In addition, Figure 6 reveals a linear relationship between $B(T)$ and T . The obtained coefficients $B(T)/T$ are given in the vicinity of

the corresponding curves. For pure Ni, the value from Bonny2013 is 3.90×10^{-8} Pa·s/K, lower than 5.24×10^{-8} Pa·s/K from Bonny2011. Note that a similar value of 5.0×10^{-8} Pa·s/K is reported by a previous MD simulation [26]. For NiFe, $B(T)/T$ becomes very small with Bonny2011, which predicts 0.13×10^{-8} Pa·s/K, contrary to a large negative value of -5.14×10^{-8} Pa·s/K obtained with Bonny2013.

Figure 6 Temperature dependent drag coefficients of Ni and NiFe.

The results presented so far are obtained by applying opposite forces so that the dislocation moves along one specific direction (the $[110]$ direction in Figure 1). In general, however, the dislocation mobility depends on the glide direction, the dislocation line, and the Burgers vector. The two partial dislocations formed after the full dislocation dissociation have different Burgers vectors, e.g. $\frac{1}{6}[211]$ and $\frac{1}{6}[12\bar{1}]$, for the geometry presented in Figure 1 and the V_D results presented above are obtained for one glide direction. To study the dependence of V_D on the glide direction, the dislocation is forced to move in the opposite direction by applying reversed shear stress. The steady state dislocation velocities under the reversed stress are calculated in the same

way and the velocity ratio V_{Dright}/V_{Dleft} is presented as a function of applied stress in Figure 7, for both Ni and NiFe at different temperatures. Here only the results obtained with the Bonny2013 potential are shown, since this potential predicts stronger temperature effect (Figure 5). It can be seen that in general the ratio of the two velocities is very close to unity, which means that the difference in the glide direction and the Burgers vectors of two partial dislocations do not induce recognizable differences in the dislocation velocities, especially at high stress. Certain deviations of V_{Dright}/V_{Dleft} from unity can be observed at low applied stress and different behaviors are found in pure Ni and NiFe. In pure Ni, the deviation at low stress is rather stochastic with respect to the temperature. The exact reason for this is not clear and more precise modeling of slow dislocations is necessary to clarify the effect. In the NiFe alloys, the deviation tends to be less than unity, indicating a systematic effect which we attribute mainly to the different local environment when the dislocation moves in different directions.

Figure 7 Ratio of dislocation velocity at opposite directions calculated with Bonny2013 potentials.

4. Discussion

In *fcc* structures, the $\frac{1}{2}\langle 110 \rangle \{111\}$ dislocation dissociates into two Shockely partials with a separation distance. Because of the dissociation, the motion of an edge dislocation involves the motion of both partial dislocations and the fault area between them. In this process, the leading partial continuously creates a new stacking fault while the trailing partial removes it. When dislocation glides in pure Ni where SFE is constant over the whole material, the interaction

between partial dislocations is constant, and therefore the separation between them varies only slightly during the gliding owing to thermal fluctuations. Figure 8a shows that the whole dislocation, as well as partial dislocation lines, remain practically straight in pure Ni during its glide at 300 K under 200 MPa applied stress. On the other hand, a variable separation between partial dislocations in NiFe can be clearly seen in Figure 8b. In the instant configuration, the distance between partial dislocations varies along the dislocation line and the whole dislocation line changes its shape when the dislocation glides through the crystal at 300 K under 500 MPa applied stress. There are at least two possible reasons responsible for the variation in the dissociation distance along the dislocation line of a moving dislocation. One reason is that the SFE in NiFe exhibits a wide distribution of local values (see Figure 2), which causes variations in the local separation between the two partials when the dislocation passes through the alloy with locally variable composition. Another reason is related to the interaction between partial dislocations with local chemical/structural features in the random alloy. This can be seen in Figure 8b where both leading and trailing partial dislocation lines are bent due to the localized resistance against their motion towards the right direction. Similar configurations are often observed during dislocation glide through an alloy and qualitatively they are similar to those found in the interaction process between a dislocation and a localized obstacle such as void, interstitial cluster or stacking faulty tetrahedron (e.g. [13]). A combination of these two mechanisms can lead to fluctuations in the dislocation energy, which also depends on local fluctuations in the alloy composition. These fluctuations make the dislocation line strongly non-uniform and further affect the dislocation motion. In particular, the energy dissipation is enhanced significantly when the dislocation moves through such a non-uniform environment, which helps to increase the phonon drag coefficient and reduce the dislocation velocity.

Figure 8 Core structures of dislocations in Ni and NiFe during the glide process at 300 K: (a) Ni under 200 MPa and (b) NiFe under 500 MPa observed with the Bonny2013 potential. The direction of motion is toward the right. The atom color code is the same as in Figure 1.

5. Conclusion

The velocity of edge dislocations in Ni and random equiatomic NiFe alloys is investigated as a function of applied stress and temperature using MD simulation with different EAM potentials. The edge dislocation in both Ni and NiFe dissociates into two partial dislocations surrounding a stacking fault ribbon, which is determined by the SFE. It is shown that there is a stress threshold to initiate the dislocation movement in both Ni and NiFe, and this stress is much higher in NiFe. At the same applied stress, the dislocation moves much slower in NiFe compared to Ni. The drag

coefficient extracted from the linear regime of the dislocation velocity versus applied stress shows that it increases linearly with temperature in Ni while it decreases or remains nearly constant in NiFe, depending on empirical potentials. The dislocation behaviors in concentrated random alloys are found to be strongly influenced by the local variation in the alloy composition and SFEs.

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