Full Length Article

Compositional effects on dislocation properties in NiCo and NiFe alloys using atomistic simulations

Sho Hayakawa, Juntan Li, Jaswanth Bommidi, Haixuan Xu *

Department of Materials Science and Engineering, The University of Tennessee, Knoxville, TN 37996, United States

ABSTRACT

The equiatomic face-centered cubic NiCoCrFeMn high entropy alloy has exhibited a rare but desired combination of the strength and ductility at cryogenic temperatures, and a similar phenomenon has been observed in equiatomic subsets of the alloy. To obtain a fundamental understanding of the underlying deformation processes, here we investigate the compositional effects on dislocation properties in the model NiCo and NiFe alloys using atomistic simulations. First, the fidelity of the employed interatomic potential is examined by comparing calculated material properties with available experimental data and first principles calculations. Then, we systematically examine the dislocation energy, core radius, core width, Peierls stress, and separation distance between the Shockley partial dislocations for edge and screw dislocations, as a function of the composition. The core energy of a screw dislocation is found to be lower than that of an edge dislocation, suggesting screw dislocations are more energetically stable in both alloys. It is found the compositional dependence of the core width is not relevant to that of the Peierls stress in the alloys, in contradiction with the classical Peierls–Nabarro model. The results suggest local atomistic environment plays a significant role in the Peierls stress. The separation distance increases with decreasing Ni concentration, except for a screw dislocation in the NiFe, which is attributed to the compositional dependence of the stacking fault energy and shear modulus. This study provides fundamental insights into the dislocation properties of these alloys, which can serve as a basis for understanding many dislocation features and underlying deformation mechanisms in compositionally complex alloys.

1. Introduction

Multi-component concentrated solid solution alloys (CSSAs) have garnered substantial attention in recent years [1–3]. Particularly, the single-phase face-centered cubic (fcc) NiCoCrFeMn alloy, also known as the Cantor alloy [4], has exhibited some exceptional mechanical properties, e.g., tensile strength >1 GPa [5–7], outstanding ductility (>60%) [5–7], and fracture toughness exceeding 200 MPa-m 1/2 [7]. These alloys have shown an unusual increase in yield strength, ultimate tensile strength, and ductility (elongation to fracture) as the temperature is lowered to cryogenic temperatures [6]. This is a rare phenomenon, since strength and ductility are generally mutually exclusive in conventional dilute alloys. Furthermore, it has been shown that some fcc equiatomic binary, ternary, and quaternary subsets of the NiCoCrFeMn alloy demonstrate similar strengthening with decreasing temperature as the quinary alloy [8]. Since many structural applications require high ductility and strength, it is essential to understand the fundamental deformation mechanisms that lead to this attractive simultaneous increase in these properties.

While it has been assumed that deformation twinning in these alloys could contribute to the enhanced ductility at cryogenic temperatures from experimental observations [6,7,9–12], the behavior of dislocations could also play a key role in their mechanical properties. A previous experimental study reported the twins formed under deformation improve the ductility by merely <3% of the total true strain [13]. This indicates the deformation twinning alone would not sufficiently describe the underlying cause of the enhanced ductility. In addition, a recent computational study demonstrated the interaction between dislocations and twin boundaries could contribute to the improvement of the ductility at lower temperatures [14]. Some experimental studies have indeed observed the physical interaction between gliding dislocations and twin boundaries at cryogenic temperatures [9,10]. Furthermore, it was reported that the interactions between dislocations and nanotwin–hexagonal close-packed (hcp) lamella, which is a characteristic microstructure observed in NiCoCr CSSAs [15–18], could also lead to the cryogenic ductility [19]. Therefore, a fundamental
understanding of the dislocation properties and behavior is essential to reveal the mechanism associated with the intriguing mechanical properties of these alloys.

Atomic simulations are a powerful means to investigate the detailed properties and behavior of dislocations in fcc CSSAs. Osetsky et al. examined screw dislocation motion in fcc equiatomic NiFe alloys using molecular dynamics simulations [20]. They identified two modes of dislocation glide: (i) when the applied stress is low, the dislocation glides in a very rough manner, expressed as a jerky motion through a set of obstacles; (ii) in contrast, the dislocation motion is like lattice friction-controlled gliding in pure metals under high stresses. The behavior of edge dislocations in equiatomic NiFe alloys was studied by Zhao et al. [21]. They confirmed the threshold stress for the dislocation movement is much higher in the alloys than that in pure Ni. Additionally, it was found that the separation distance between the Shockley partial dislocations \(d_{\text{sep}}\) significantly varies in the alloys, which could be associated with the local fluctuation of stacking fault energy \(\gamma_{\text{SFE}}\) affecting the dislocation motion. Zeng et al. investigated the influence of the local \(\gamma_{\text{SFE}}\) variation on the strengthening of fcc CSSAs by constructing a dislocation dynamics model for the evolution of partial dislocations [22]. They reported the predicted yield stress increases with larger fluctuations of the \(\gamma_{\text{SFE}}\). Rao et al. performed molecular statics and dynamics simulations for the behavior of edge and screw dislocations in fcc CoFeNiTi [23]. It was shown that \(d_{\text{sep}}\) varies significantly, probably arising from the local fluctuations of concentrations. In addition, they revealed the critical stress to move the dislocation at 0 K is much higher than that in pure Ni. Pasiount et al. also performed atomistic simulations to elucidate the behavior and structure of edge and screw dislocations in fcc NiCoCrFeCu [24]. They reported the dislocation line is not straight but wavy and there are significant variations in the \(d_{\text{sep}}\) in the alloys. It was shown that these effects are more pronounced for edge dislocations, compared with screw dislocations. Furthermore, they found the Peierls stress calculated in the alloys is considerably higher than that in pure metals.

While these studies have provided critical insights into the dislocation behavior in fcc CSSAs, they have primarily focused on a specific alloy composition, the equiatomic composition. However, in general the material properties of alloys can vary considerably with composition. For instance, a recent study reported significant variations of the \(\gamma_{\text{SFE}}\) at different compositions in subsets of the NiCoCrFeMn alloys [25]. This could strongly affect the properties of dislocations, which dissociate into two Shockley partial dislocations with a stacking fault in-between. Moreover, the alloy compositions would affect the complexity of the local atomic environment of the alloys, which could further influence the dislocation behavior. Hence, it is crucial to elucidate the influence of the alloy compositions on the dislocation properties for a more complete understanding of the unusual mechanical behavior of the fcc CSSAs.

In this study, the compositional effects on fundamental dislocation properties of NiCo and NiFe alloys are systematically investigated by molecular statics simulations. As shown in a previous study [8], the NiCo and NiFe alloys also exhibit similar deformation behavior as the NiCoCrFeMn alloys, though they are compositionally simpler. Thus, the detailed investigation of the NiCo and NiFe alloys will provide a basis for an increased understanding of the NiCoCrFeMn alloys. The interatomic interactions in the alloys are modeled using an interatomic potential by Farkas et al. [26]. This potential was developed for random solid solution alloys, which is a good approximation for NiCo. In contrast, it is known that NiFe exhibits the Invar effect when the Ni concentration is 0.30–0.45 [27,28], further influencing the compositional dependence of the dislocation properties. We first conduct a fidelity analysis of the employed potential by comparing the shear modulus and Poisson’s ratio of the alloys with experimental data. Subsequently, we examine the compositional effects on the dislocation energy, dislocation core radius \(r_{\text{core}}\), core width of a partial dislocation \(w_{\text{core}}\), Peierls stress, and the separation distance between Shockley partial dislocations \(d_{\text{sep}}\).

2. Methods

All the simulations herein are performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software [29]. For constructing the simulation cells of the NiCo and NiFe alloys, the constituent elements are randomly distributed while the number of atoms of each element is determined in accordance with the composition of interest. Based on convergence tests, molecular statics simulations are performed using 40 atomic configurations with different random elemental distributions, unless mentioned otherwise. The presented dislocation properties are the average values obtained from these samples of random elemental configurations. Note, the effects of the short-range ordering [30–32] of the constituent elements are not explicitly considered because, in binary alloys, the short-range ordering is not considered to be significant, compared to ternary, quaternary, and quinary alloys.

For the calculations of the screw dislocation properties, the simulation cell is oriented along the \(x\) [1\(\overline{1}\)2], \(y\) [\(\overline{1}\)\(\overline{1}\)0], and \(z\) [1\(\overline{1}\)0] directions, for which the cell dimensions are \(\sim 450\) Å, \(\sim 450\) Å, and \(\sim 70\) Å, respectively (Fig. 1 (a)). The cell contains \(\sim 1,385,000\) atoms in total. A periodic boundary condition (PBC) is applied along the \(x\)-direction to generate an infinitely long dislocation, while a free boundary condition (FBC) is used in the \(y\)-direction. In the \(x\)-direction, a PBC is employed while applying the shifted boundary condition (SBC), described in [33,34]. To generate a perfect screw dislocation with the Burgers vector of \(\alpha[0\overline{2}1\overline{1}]\), the atoms are displaced based on the elasticity theory [35] (\(\alpha_0\) lattice constant). Then, the system energy is minimized, resulting in the dissociation of the perfect dislocation into two Shockley partial dislocations with a stacking fault in-between. For the construction of an edge dislocation, the simulation cell is oriented along the \(x\) [1\(\overline{1}\)0], \(y\) [\(\overline{1}\)\(\overline{1}\)0], and \(z\) [1\(\overline{1}\)2] directions with dimensions \(\sim 430\) Å, \(\sim 430\) Å, and \(\sim 70\) Å, respectively (Fig. 1 (b)). The cell contains \(\sim 1,146,000\) atoms in total. PBCs are applied along the dislocation line (\(z\)) direction and the Burgers vector (\(x\)) direction, while a FBC is applied along the \(y\)-direction. We create an edge dislocation following a method developed by Osetsky et al. [36]: the simulation cell is divided into the upper and lower crystals along the \(y\)-direction, and two adjacent (110) atomic layers are removed in the upper crystal. The system energy minimization is then performed after changing the system size by \(b_{\text{perfect}}/2\) along the boundary of the \(x\)-direction, which creates a relaxed structure of two Shockley partial dislocations with a stacking fault in-between. Note, the \(b_{\text{perfect}}\) denotes the magnitude of the Burgers vector of a perfect dislocation.

The strain energy in the system due to the existence of a dislocation \(E_{\text{strain}}\) can be divided into two parts [35]:

\[
E_{\text{strain}} = E_{\text{core}} + E_{\text{elastic}},
\]

where the \(E_{\text{core}}\) is the core energy and the \(E_{\text{elastic}}\) is the elastic energy, which is the energy stored outside the dislocation core region. While the \(E_{\text{elastic}}\) would be well described by the elasticity theory, the evaluation of \(E_{\text{core}}\) requires atomistic simulations due to the complex atomic structure of the dislocation core, and the inelastic effects introduced therein. The detailed procedure of evaluating the \(E_{\text{strain}}\) and \(E_{\text{core}}\) is: the \(E_{\text{strain}}\) is defined as the potential energy difference between the relaxed dislocation structure and relaxed perfect crystal structure. Previous studies have evaluated the \(E_{\text{strain}}\) within a cylindrical region centered at the dislocation core and along the dislocation line direction as a function of cylinder radius, \(R_{\text{cylinder}}\) [37,38], as shown in Fig. 2 (a). We follow this procedure: first, we prepare a perfect crystal of a random alloy with a concentration of interest, followed by an energy minimization. Next, we construct a dislocation and minimize the system energy, as described above. Then, we evaluate the change in the energy of each atom before and after the dislocation construction. The energy changes are then summed up for the atoms in the cylindrical region, and the sum is defined as the \(E_{\text{strain}}\) after it is divided by the dislocation line length. We employ this procedure to minimize the influence of the change in the
The local atomic environment before and after the dislocation construction can be described in terms of the averaged value of $E_{\text{strain}}$. The dislocation core region can be defined as the one where $E_{\text{strain}}$ deviates from the logarithmic dependence on the $R_{\text{cylinder}}$ [37]. Based on this, we first calculate $E_{\text{strain}}$ as a function of $R_{\text{cylinder}}$, as described above, and evaluate the differential of $E_{\text{strain}}$ with respect to $\ln R_{\text{cylinder}}$. For instance, the differential varies at a smaller $\ln R_{\text{cylinder}}$ while it becomes constant when the $\ln R_{\text{cylinder}}$ is larger due to the logarithmic dependence of $E_{\text{strain}}$ on $R_{\text{cylinder}}$. We take the value of $R_{\text{cylinder}}$ as the $r_{\text{core}}$ when the differential converges to a certain value, and the $E_{\text{core}}$ is defined as $E_{\text{strain}}$ at $r_{\text{core}}$. Note that the $r_{\text{core}}$ denotes the core radius of a full dislocation, including the two Shockley partial dislocations. The convergence criterion is set to 0.04 eV/Å in this study.

We evaluate the separation distance between the Shockley partial dislocations, $d_{\text{sep}}$, by the dislocation extraction algorithm (DXA) [39], which is implemented in the OVITO software [40]. The core width, $w_{\text{core}}$, is analyzed based on the disregistry of atomic coordination across the slip plane, defined as the distance over which the $\Delta u$ is greater than half of its maximum value. The more detailed explanation is given elsewhere [35].

For the calculation of the Peierls stress, we incrementally apply a shear strain of $4.5 \times 10^{-6}$ to the simulation cell by displacing the atoms...
in the upper $xz$ surface along the Burgers vector direction while fixing the lower $xz$ surface. The system energy is minimized after every strain application, and the shear stress is recorded. The Peierls stress is calculated by averaging the peak values of the stress recorded during the strain applications, which are observed when the dislocation glide occurs. We employ up to 150 samples for obtaining the averaged stress values due to the significant fluctuation of each peak stress. In addition, the $z$ direction of the simulation cell is lengthened to ~150 Å in both edge and screw dislocation cases. Note, we focus on the NiCo for the Peierls stress calculations because of the computational cost to obtain a large number of samples.

3. Results and discussion

The dissociation into two Shockley partial dislocations is essential for the dislocation properties in fcc metals. The $d_{\text{dis}}$ can be written in the isotropic elasticity theory [35], as follows:

$$d_{\text{dis}} = \frac{G b_{\text{partial}}}{8\pi(1-\nu)\gamma_{\text{SFE}}} \quad \text{(edge)}$$

$$d_{\text{dis}} = \frac{G b_{\text{partial}}^2}{8\pi(1-\nu)\gamma_{\text{SFE}}} \quad \text{(screw)}$$

where the $G$, $b_{\text{partial}}$, and $\nu$ denote the shear modulus, magnitude of the Burgers vector of a partial dislocation, and Poisson’s ratio, respectively. Based on Eq. (2) and (3), we consider $a_0$, $G$, and $\gamma_{\text{SFE}}$ to benchmark the fidelity of the employed potential. A previous study [25] calculated the $a_0$ and $\gamma_{\text{SFE}}$ of NiCo and NiFe alloys over a wide range of the Ni concentration using the potential employed in this study [26]. They compared the calculated values with those from density functional theory calculations and experiments, showing the potential exhibits reasonable values in terms of the numerical accuracy and compositional influences. Therefore, we here focus on the benchmarking of $G$ and $\nu$.

Fig. 3 (a) and (b) show the comparison of the calculated $G$ values with experimental data for the NiCo and NiFe, respectively. Note, we plot the value of the Hill empirical average for each composition, described in Ref. [41]. For the NiCo, the calculated $G$ agrees very well with the experimental values [42] over the whole compositional range considered here. For the NiFe, the calculated $G$ also exhibits good agreement with experiments in the Ni concentration range from 0.6 to 1.0, especially for the values by Shirakawa et al. [43] and Bower et al. [44]. However, a relatively large discrepancy between the calculated $G$ and the experimental value is found at the Ni concentration below 0.6. This might be due to the Invar effect, arising from the magnetism [27,28], which cannot be completely incorporated in the interatomic potential. Nevertheless, the interatomic potential shows qualitative agreement with the trend of the experimental values, where $G$ exhibits a peak in the high Ni concentration region. Overall, the obtained results capture the general trend of the influences of the alloy composition on the $G$ in the NiCo and NiFe alloys within the concentration range considered here.

Fig. 4 (a) and (b) show the comparison of the calculated $\nu$ and experimental values for the NiCo and NiFe, respectively. For NiCo, the calculated values are in good agreement with experiments [42] across the whole concentration range considered here. For NiFe, the obtained results are consistent with the experimental values [44,47], except for the Ni concentration of 0.5. Nonetheless, the difference at the Ni concentration of 0.5 is only ~6%, demonstrating the sufficient fidelity of the potential. We conclude that the employed interatomic potential is reliable enough for investigated compositional effects on the $\nu$ in NiCo and NiFe within the concentration range considered here.

Fig. 5 (a) and (b) show the $E_{\text{strain}}$ as a function of the $R_{\text{cylinder}}$ for an edge dislocation in the NiCo and NiFe, respectively. The $E_{\text{strain}}$ for a screw dislocation is depicted in Fig. 5 (c) and (d) for the NiCo and NiFe, respectively. For all the cases, the $E_{\text{strain}}$ has a linear relationship with the logarithm of the $R_{\text{cylinder}}$ except for the dislocation core region. The linear relationship between the $E_{\text{strain}}$ and logarithm of the $R_{\text{cylinder}}$ was also reported in previous computational studies for pure fcc metals [37,38]. In contrast, the $E_{\text{strain}}$ in the dislocation core region deviates from the linear relationship, which is associated with the dissociation into Shockley partial dislocations [37,38]. For the NiCo, the $E_{\text{strain}}$ becomes lower with decreasing Ni concentration at the core region for both dislocation types while the slope of a fitted line of $E_{\text{strain}}$ at the linear region is not significantly influenced by the concentration, as shown in Fig. 6 (a). This indicates the compositional dependence of $E_{\text{strain}}$ for NiCo is mainly determined in the core region. This would lead to similar compositional dependences of $E_{\text{strain}}$ and $E_{\text{core}}$ (the details of the dependence of $E_{\text{core}}$ will be given in Fig. 7). Meanwhile, for both dislocation types in NiFe, the compositional dependence of $E_{\text{strain}}$ is influenced by $R_{\text{cylinder}}$. This is because the slope of the fitted line of $E_{\text{strain}}$ depends on the concentration, as shown in Fig. 6 (b). The slope peaks at a concentration of 0.7–0.8, leading to crossovers of some fitted lines between different concentrations (see the insets of Fig. 5 (b) and (d)). According to the elasticity theory [35], the strain energy per unit length of dislocation is linearly dependent on the $G$, as follows:

$$E_{\text{strain}} = \frac{G b_{\text{partial}}^2}{4\pi(1-\nu)} \ln \left( \frac{R_{\text{cylinder}}}{R_{\text{core}}} \right)$$
\[ E_{\text{strain}} = \frac{G b^2 \rho_{\text{perox}}}{4 \pi} \ln \left( \frac{R_{\text{cylinder}}}{r_{\text{core}}} \right) \]  \text{(screw)}

As shown in Fig. 3 (b), the \( G \) exhibits the maximum value at a concentration of 0.7–0.8 for the NiFe, which results in the nonmonotonic dependence of the slope of the fitted line.

Fig. 7 (a) and (b) show the \( E_{\text{core}} \) as a function of the Ni concentration for the NiCo and NiFe, respectively. It is found that, in both alloys, the \( E_{\text{core}} \) of a screw dislocation is lower than that of an edge dislocation across the entire concentration range. This indicates screw dislocations possess higher core stabilities and would be more energetically favorable than edge dislocations in these alloys. The higher stability of screw dislocations has also been suggested in experimental studies. Experimental data by Echigoya et al. [48] showed that for Fe–31 wt% Ni, Fe–35 wt% Ni, and Fe–45 wt% Ni alloys, the dislocation population at the initial stage of deformation are primarily screw dislocations. For
Fe–82 wt% Ni nano crystalline alloy [49], the dislocations are found to be of mixed character but close to screw type. As shown in Fig. 7 (a), the $E_{\text{core}}$ increases linearly with Ni concentration for both dislocation types in the NiCo. Comparatively, for the NiFe, $E_{\text{core}}$ becomes higher with an increase in concentration for both dislocation types when the concentration is below 0.6–0.7. However, when the concentration exceeds 0.7, $E_{\text{core}}$ starts to decrease as the concentration becomes larger.

Fig. 8 (a) and (b) show $r_{\text{core}}$ as a function of Ni atomic concentration for the NiCo and NiFe systems, respectively. Note, $r_{\text{core}}$ denotes the core radius of a full dislocation, including the two partial dislocations, as mentioned previously. For an edge dislocation, $r_{\text{core}}$ increases linearly with decreasing Ni concentration in NiFe while it increases drastically once the concentration becomes lower than 0.6 in NiCo. Since the core region here includes both partial dislocations, the value of $r_{\text{core}}$ is considered to be closely related to their separation distance, $d_{\text{sep}}$. Indeed, we confirm similar compositional dependences for $d_{\text{sep}}$ of an edge dislocation, as will be discussed in Fig. 11. In contrast, we do not observe clear dependences for a screw dislocation in both alloys. This might be because, as will be
The compositional dependence of $d_{sep}$ of a screw dislocation is not significant, rendering the dependence of $r_{core}$ unclear. Fig. 9 (a) and (b) show the values of $w_{core}$ as a function of Ni concentration for NiCo and NiFe, respectively. Note, $w_{core}$ here denotes the core width of a partial dislocation, as mentioned previously. It is shown that $w_{core}$ increases with decreasing Ni concentration for both edge and screw dislocations in NiCo while little compositional dependence is observed in NiFe. According to the Peierls–Nabarro model, $w_{core}$ is a key parameter for the Peierls stress, where the stress exponentially increases with decreasing $w_{core}$ [35]. Additionally, a previous study discussed the relationship between the $w_{core}$ and Peierls stress in Ni-based CSSAs to describe the temperature dependence of the yield stress [8]. To investigate the relationship of these two values, we calculate the Peierls stress as a function of the Ni concentration in NiCo, as shown in Fig. 10. It is seen that the stress peaks at a concentration of 0.7–0.8, which is not consistent with the compositional dependence of $w_{core}$ (Fig. 9 (a)). This indicates $w_{core}$ is not a controlling factor for the Peierls stress in the alloys. Considering the stress is the highest at an intermediate concentration, it could be rather affected by the local atomistic environment and the degree of the chemical disorder. Indeed, a previous study [25] has reported that the complexity of the atomic configurations could have reported that the complexity of the atomic configurations could render the dislocation line wavy [20, 21, 23, 24], the averaged values of $d_{sep}$ can be described by the elasticity theory with the averaged material properties of the alloys, regardless of the concentration.

Fig. 10. Values of the Peierls stress as a function of Ni atomic concentration in NiCo. The error bars denote the standard deviation of the average.

4. Summary

We perform atomistic simulations for investigating the fundamental properties of edge and screw dislocations in NiCo and NiFe alloys as a function of the composition. The interatomic interactions are described by an embedding atom method potential developed by Farkas et al. [26], which is demonstrated to capture the qualitative compositional effect on some of the material properties with reasonable accuracy. Using the potential, we examine the compositional effects on the $E_{strain}$, $w_{core}$, $r_{core}$, $w_{core}$, Peierls stress, and $d_{sep}$. Several important observations are summarized below:

- The $E_{strain}$ exhibits a logarithmic dependence on $R_{cylinder}$ in the elasticity region for both dislocation types in NiCo and NiFe. Additionally, the slope of the $E_{strain}$ v.s. $R_{cylinder}$ curve is not influenced by the Ni concentration in NiCo, which would lead to the similar compositional dependence between the $E_{strain}$ and $E_{core}$. In NiFe, the slope is steeper at an Ni concentration of 0.7–0.8, arising from a larger $G$ at this concentration range.
- The $E_{core}$ of a screw dislocation is lower than that of an edge dislocation across the entire concentration range, which suggests screw dislocations have higher core stability and are more energetically
favorable than edge dislocations, which are consistent with experimental observations. It is found that, for both dislocation types, $f_{\text{core}}$ increases linearly with Ni concentrations in NiCo. For NiFe, $f_{\text{core}}$ exhibits a peak at a concentration range of 0.6–0.7 for both dislocations.

- The $f_{\text{core}}$ of an edge dislocation increases with decreasing Ni concentration as an overall trend, though that of a screw dislocation exhibits little dependence. These dependences could be associated with the compositional variation of $d_{\text{sep}}$.
- The $w_{\text{core}}$ increases with decreasing Ni concentration for both dislocation types in NiCo while we observe little compositional dependence in NiFe. Additionally, the dependence of the Peierls stress is not consistent with that of $w_{\text{core}}$ in NiCo. These dependences suggest that the $w_{\text{core}}$ is not the only controlling factor of the Peierls stress in these alloys, which could be rather influenced by local atomistic environment and the degree of the chemical disorder.
- For NiCo, $d_{\text{sep}}$ increases with decreasing Ni concentration for both dislocation types, which arises from a decreasing $\gamma_{\text{SFE}}$. For NiFe, the increase in the $d_{\text{sep}}$ of an edge dislocation is less pronounced than that for NiCo, and little compositional dependence is observed for a screw dislocation. These phenomena are due to the competing contributions of $\gamma_{\text{SFE}}$ and $G$.

This study provides fundamental insights into dislocation properties in the NiCo and NiFe alloys, which can serve as a basis for understanding dislocation plasticity in compositionally more complex CSSAs, such as the Cantor alloy. Finally, this investigation of dislocation properties expands the understanding of interactions between dislocations and other microstructures, e.g., twin boundaries, which is essential for uncovering the underlying mechanisms that result in the excellent mechanical properties observed in these alloys.

Data availability

The processed data required to reproduce these findings are available upon request.

CRediT authorship contribution statement

Sho Hayakawa: Methodology, Investigation, Data curation, Formal analysis, Writing – original draft, Visualization. Juntan Li: Methodology, Investigation, Data curation, Formal analysis, Visualization. Jaswanth Bommidi: Methodology, Investigation, Data curation, Formal analysis, Visualization. Haixuan Xu: Conceptualization, Methodology, Formal analysis, Writing – review & editing, Funding acquisition, Supervision, Project administration.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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