Effects of stacking fault energies on the interaction between an edge dislocation and an 8.0-nm-diameter Frank loop of self-interstitial atoms

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\textbf{A B S T R A C T}

Molecular dynamics simulations were conducted to investigate the effects of stacking fault energy (SFE) as a single variable parameter on the interaction between an edge dislocation and a Frank loop of self-interstitial atoms with a diameter of 8.0 nm. The physical contact between the edge dislocation and the loop causes constriction of the edge dislocation, followed by the formation of a D-Shockley partial dislocation. The latter process is associated with either the formation of a screw component and its cross-slip, or the direct core reaction between the dislocation and the loop. These processes induce either the absorption of the loop into the dislocation or the transformation of the loop into a perfect loop. The SFE influences the interaction morphologies by determining the separation distance of the two partial dislocations and consequently the rate of constriction. The dependence of the interaction morphology on the SFE varies with the habit plane of the loop. A higher SFE increases the probability of the absorption or transformation interaction; however, only loop shearing is observed at the lower limit of the SFE range of austenitic stainless steels.

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1. Introduction

In austenitic stainless steels, which are used as in-core structural materials of light water reactors (LWRs), we observe two significant changes in their mechanical properties due to neutron irradiation. The first is an increase in yield stress, which is mainly caused by irradiation-induced defects impeding the glide motion of dislocations. The other is the localization of the plastic deformation in shear bands, above a certain irradiation dose. This is caused by the removal of irradiation-induced defects by dislocations that exist on or near the glide planes of the dislocation. The removal of these defects makes subsequent dislocations move more easily in these narrow regions [1]. The dominant irradiation-induced microstructures are self-interstitial atom (SIA)-type Frank loops occurring within the temperature range of LWRs [2–4]; thus, it is important to evaluate the interaction with a dislocation to investigate the micro-mechanisms responsible for the aforementioned changes.

Molecular dynamics (MD) simulations for pure face-centered-cubic (FCC) metals have shown that there are three types of interaction morphologies between an edge dislocation and an SIA-type Frank loop: loop drag, transformation, and loop shearing [5,6]. The loop drag and transformation interactions require the conversion of an SIA-type Frank loop into a perfect loop. This process is initiated by local constriction of the two partials into a dislocation, and it is completed with sweeping the stacking fault of the loop either by a single D-Shockley partial or by two Shockley partials [6]. Since the separation distance between the two partials is inversely proportional to stacking fault energy (SFE) [7], the SFE influences the probability of constriction and the resultant interaction morphology [8,9].

The SFE of austenitic stainless steels ranges from 16–25 mJ/m\(^2\) at room temperature to 31–34 mJ/m\(^2\) at approximately 330 °C [10], which is lower than that of other pure FCC metals such as Ni or Al. Although the SFE of Cu is as low as the upper limit of the SFE of austenitic stainless steels, the SFE of austenitic stainless steels is still lower, particularly at room temperature. Therefore, it is
necessary to evaluate the effect of the SFE on the interaction to utilize the data obtained with the Cu potential.

In this study, we conducted MD simulations by using recently developed embedded atom method (EAM)-type interatomic potentials to investigate the effect of the SFE on the interaction of an SIA-type Frank loop with a diameter of 8.0 nm with an edge dislocation. We performed a detailed analysis of the change in the interaction morphologies associated with the core reaction between the dislocation and the 8.0-nm-diameter loop.

2. Simulation methods

We used the EAM-type potentials developed by V. Borovikov et al. [11]. The SFE ranges from 14.6 mJ/m² to 186.5 mJ/m², while other material properties were kept almost identical. Four interatomic potentials with SFEs of 14.6, 24.8, 44.1, and 186.5 mJ/m² were used in this study. The SFEs of the three lower potentials are within the range for typical austenitic stainless steels, and the potential with the highest SFE was chosen to clarify the characteristic behavior in low-SFE metals. By using these potentials, we evaluated the effects of the SFE as a single variable parameter on the interaction between an edge dislocation and an SIA-type Frank loop.

The large-scale atomic/molecular massive parallel simulator (LAMMPS), which was developed by Sandia National Laboratories and designed for parallel computers [12], was used in this study. Fig. 1 shows a schematic diagram of the simulation cell. The x, y, and z axes were taken as the [1 0 −1], [1 −2 1], and [1 1 1] directions, respectively. Periodic boundary conditions were used in the x and y directions, whereas a free boundary condition was applied in the z direction. The cell lengths were set at 74.1, 22.3, and 22.1 nm for the x, y, and z directions, respectively. An edge dislocation was placed in the cell with the Burgers vector of \( \mathbf{b} = a_0/2[101] \) parallel to the x-axis and a line parallel to the y-axis [13]. A hexagonal SIA-type Frank loop with the (121) directions on their edges was also inserted on the \( \alpha \), \( \gamma \), and \( \delta \)-planes (Fig. 1). The center of the loop was on the glide plane of the dislocation. The initial distance between the core of the dislocation and the loop was approximately 37 nm.

Prior to the application of shear strain, the cell was maintained at 100 K for approximately 70 ps with a pressure almost zero. The microcanonical ensemble without temperature control was chosen for the simulations. Shear stress \( \sigma_{xy} \) was applied to the cell by exerting forces to the upper and lower layer of the z planes at a constant strain rate of \( 4.0 \times 10^6 \) s⁻¹. Time integration was performed by using the Verlet algorithm at a constant time step of \( 1.0 \times 10^{-14} \) s. Although the time step set in this study is slightly longer than that in previous studies [5,6], we confirmed that the energy is conserved within 0.01 eV at each time step.

The common neighbor analysis (CNA) was employed for visualization [14]. In a color version, the blue regions indicate a hexagonal-closed-pack (HCP) structure, which is synonymous with a stacking fault in an FCC structure. The red regions indicate neither an FCC nor HCP structure, which describes the core of the dislocation or the loop in most cases. For the Burgers vector analysis, the dislocation extraction algorithm (DXA) was employed [15,16].

Different distributions of the initial atomic velocity sometimes resulted in different interaction morphologies [17]. Hence, we repeated the calculations at least twice for each condition by changing the random seed of the initial velocity distribution. If a significant difference in the interaction morphology was obtained (the cases of the \( \alpha \)-plane at an SFE of 24.8 mJ/m² and those of the \( \gamma \)-plane at an SFE of 186.5 mJ/m²), we conducted up to five repeated calculations, and all the obtained interaction morphologies and their reaction probabilities are presented in the results section.

3. Results

Table 1 summarizes the interaction morphologies for each habit plane. The probability of loop shearing increases with decreasing SFE. In the following subsections, we will show the effect of the SFE on the detailed interaction morphologies in each habit plane.

3.1. Interaction of the loop on the \( \alpha \)-plane

Fig. 2 shows snapshots of the interaction on the \( \alpha \)-plane at an SFE of 44.1 mJ/m². When the dislocation starts to move and approaches the loop because of the applied shear strain, the leading partial bends owing to the repulsive interaction (Fig. 2(a)). Then, the dislocation physically touches the loop, which locally constricts the dislocation at its top, where the screw component is formed (Fig. 2(b)). The dislocation starts to cross-slip on the plane along the loop edge, which is different from the original slip plane.
Through this process, a D-Shockley partial is created on the loop edge by the following reaction (Fig. 2(c)):

\[ a_0/2[10\bar{1}] + a_0/3[\bar{1}1\bar{1}] \rightarrow a_0/6[1\bar{2}\bar{1}]. \]

(1)

The screw component again changes the slip plane to the next loop edge, where it progressively creates another D-Shockley partial as it continues to cross-slip (Fig. 2(d)). These D-Shockley partials eliminate the stacking fault of the loop toward the bottom (Fig. 2(e)) until this half part of the loop becomes completely unfaulted (right half of Fig. 2(f)). The right half of the loop is absorbed by the dislocation. As the shear strain increases, the dislocation detaches from the remaining half of the loop, and a double superjog forms on the dislocation (Fig. 2(g)). The interaction morphology for the case with the highest SFE of 186.5 mJ/m² is fundamentally the same. Note that this type of interaction was previously observed by Nogaret et al. in Cu with an SFE of 44.4 mJ/m², despite the difference in loop size and temperature [5].

Fig. 3 shows the difference in the interaction at the lowest SFE of 14.6 mJ/m². D-Shockley partials are created on the two loop edges according to the reaction in Eq. (1), which is same for the case with an SFE of 44.1 mJ/m² in Fig. 2(d). They temporarily eliminate the stacking fault of the loop (Fig. 3(a)). However, the separation distance between the two partials is so large that the dipole segments of the leading partial join and close before the D-Shockley partials complete unfaulting the loop (Fig. 3(b)). The temporarily unfaulted part of the loop returns to the original Frank loop when the trailing partial detaches (right half in Fig. 3(c)). This results in the loop shearing interaction. This type of interaction was previously observed by Terentyev et al. in Fe-20Cr-10Ni with an SFE of approximately 20 mJ/m² [6].

For the interaction at an SFE of 24.8 mJ/m², repeated calculations provided different results in the interaction morphologies, i.e., either loop drag (1/5) or loop shearing (4/5), depending on the initial velocity distribution of the atoms. These results indicate that the critical SFE at which the interaction morphology changes from loop shearing to loop drag is near 24.8 mJ/m² for an 8.0-nm-diameter loop. Note that the critical SFE exists within the SFE range of austenitic stainless steels—at least for an 8.0-nm-diameter loop—which indicates that even if we use the Cu potential, which
has been used as a prototype low-SFE metal, it is difficult to reveal the lowest SFE behaviors on this habit plane.

3.2. Interaction of the loop on the $\gamma$-plane

Fig. 4 shows snapshots of the interaction on the $\gamma$-plane at an SFE of 186.5 mJ/m$^2$. When the dislocation starts to move and approaches the loop because of the applied shear strain, the leading partial bends owing to the attractive interaction (Fig. 4(a)). Then, the two partials are constricted at both of the intersection points (Fig. 4(b)). The constricted dislocation detaches from the bottom and continues to glide inside the stacking fault of the loop. During this process, the dislocation reacts with the loop, creating a D-Shockley partial by the following reaction (Fig. 4(c)):

$$a_0/2[101] + a_0/3[111] \rightarrow a_0/6[121].$$

(2)

The D-Shockley partial eliminates the stacking fault of the entire half of the loop, which results in creating a perfect component (right half in Fig. 4(d)):

$$a_0/6[121] + a_0/3[111] \rightarrow a_0/2[101].$$

(3)

The same process progressively occurs on the other half of the loop (left half in Fig. 4(e)). Then, the entire loop converts to a perfect loop with the Burgers vector of $a_0/2[101]$, which is parallel to that of the dislocation. The loop edge is cut at the top, and each end is separately connected to the dislocation (Fig. 4(f)). When the dislocation glides because of the further application of shear strain, the loop may (2/5) or may not (3/5) be absorbed, depending on the initial velocity distribution. If it is absorbed, the connected shape of the loop is retained through the glide motion of the dislocation (Fig. 4(g-1)), whereas if it is not absorbed, the perfect loop remains after the dislocation detaches (Fig. 4(g-2)).

Fig. 5 shows snapshots of the interaction at the lower SFE of 44.1 mJ/m$^2$. Constriction of the two partials seldom occurs at the loop edges (Fig. 5(a)) because the separation distance between the two partials is larger than that at the higher SFE. Consequently, the reaction described in Eq. (2) is not induced. Instead, the leading partial detaches (Fig. 5(b)), followed by the trailing partial (Fig. 5(c)). This results in the loop shearing interaction. The interactions at the lowest two SFEs are fundamentally the same.

The interaction on this plane is categorized into two groups: the high SFE of 186.5 mJ/m$^2$, and low SFEs of 44.1 mJ/m$^2$ or lower. Both Cu and austenitic stainless steels for all possible range of SFEs belong to the low SFE group. Therefore, the atomistic interaction for the austenitic stainless steels can be simulated by using Cu potentials on this habit plane.

3.3. Interaction of the loop on the $\delta$-plane

Fig. 6 shows snapshots of the interaction on the $\delta$-plane at an SFE of 186.5 mJ/m$^2$. In this case, the normal vector of the habit plane is perpendicular to the Burgers vector of the dislocation. When the dislocation enters the stacking fault of the loop because of the applied shear strain, neither the shape of the loop nor that of the dislocation changes strongly (Fig. 6(a)). The dislocation detaches from the loop with the formation of a step on the loop edge (Fig. 6(b)). This interaction is observed for all the SFEs, so it is likely a common feature of FCC metals.

4. Discussion

We confirmed the existence of three types of interaction morphologies that occur between an edge dislocation and an SIA-type Frank loop: loop drag, transformation, and loop shearing. One mechanism for the loop drag, which occurs on the $\alpha$-plane, is the local constriction of the dislocation, followed by the screw component cross-slip. Unfaulting of the loop is accomplished by a single D-Shockley partial shearing the loop—a mechanism that was previously observed by Nogaret et al [5]. In this study, a different mechanism for the loop drag is observed on the $\gamma$-plane. The reaction between the dislocation and the loop directly creates a D-Shockley partial inside the loop, which by itself completes the unfaulting of the entire loop. Although this type of interaction is observed only at the highest SFE and not for the SFE ranges of austenitic stainless steels, we found that the unfaulting of an SIA-type Frank loop occurs without formation of screw components or its cross-slip. Since these mechanisms start from constriction of the dislocation, followed by the formation of a D-Shockley partial, the SFE is a crucial parameter for determining the interaction morphologies by controlling the probability of constriction.

The critical SFE, which changes the interaction morphologies from loop shearing to loop drag, depends on the habit plane. The critical SFE for the $\alpha$-plane in particular lies within the SFE range of austenitic stainless steels. A previous study showed that loop shearing is the dominant interaction with an edge dislocation, while loop drag is observed only on the $\alpha$-plane in Cu with an SFE of 44.4 mJ/m$^2$ [5]. However, even on the $\alpha$-plane, we found that the loop drag may not occur for austenitic stainless steels with a lower range of SFEs.

In this study, the temperature was set to just above the zero kelvin at 100 K. However, higher temperatures, including the operating temperature of nuclear reactors, may change the critical SFE, which will be evaluated in a future study.
5. Conclusions

We conducted MD simulations at 100 K to investigate the effects of the SFE on the interaction between an edge dislocation and an 8.0-nm-diameter SIA-type Frank loop with the (121) directions on their edges, by using the recently developed EAM potentials for FCC metals. The interaction morphologies and their dependency on the SFE differ among the habit planes of the loop.

For interactions on the \(\alpha\)-plane, higher SFEs induce the loop drag interaction through the constriction of two partial dislocations, formation of the screw component and its cross-slip, followed by the formation of a D-Shockley partial. The loop shearing interaction is observed at lower SFEs. The critical SFE, which changes the interaction morphologies, is near 24.8 mJ/m\(^2\). For interactions on the \(\gamma\)-plane, higher SFEs induce the loop drag or transformation interaction through the constriction of two partial dislocations at the loop edges, followed by the formation of a D-Shockley partial. This reaction is not induced for the SFEs of 44.1 mJ/m\(^2\) or lower, resulting in the loop shearing interaction instead. For interactions on the \(\delta\)-plane, no significant change in the shape of the dislocation or in the shape of the loop is observed through the physical contact. The loop shearing interaction occurs, which is independent of the SFE.

For austenitic stainless steels, the interaction on the \(\gamma\)- and \(\delta\)-planes is loop shearing, whereas on the \(\alpha\)-plane, it is either loop drag or loop shearing depending on the SFE within their range.
**Fig. 5.** The CNA visualizations of the interaction on the $\gamma$-plane at an SFE of 44.1 mJ/m$^2$. Two snapshots from a different angle are shown in the left- and right-hand side figures in (a).

**Fig. 6.** The CNA visualizations of the interaction on the $\delta$-plane at an SFE of 186.5 mJ/m$^2$.

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