Molecular dynamics investigation of the interaction of an edge dislocation with Frank loops in Fe–Ni₁₀–Cr₂₀ alloy

Jean-Baptiste Baudouin a, c, *, Akiyoshi Nomoto b, Michel Perez a, Ghiath Monnet c, Christophe Domain c

a Université de Lyon, INSA Lyon, MATEIS-UMR CNRS 5510, F69621 Villeurbanne, France
b Central Research Institute of Electric Power Industry, 2-11-1 Iwado Kita, Komae-shi, Tokyo 201-8511, Japan
c EDF-Laboratoire des Renardières, Département MMC, 77250 Moret sur Loing, France

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A B S T R A C T
The inhibition of dislocations motion by irradiation-induced defects, such as dislocation loops, is one of the main mechanisms of irradiation hardening of austenitic stainless steels. In this work, Molecular Dynamics (MD) simulations of interaction between an edge dislocation and Frank loops in Fe–Ni₁₀–Cr₂₀ ternary alloy mimicking austenitic stainless steels are carried out to investigate and model dislocation behavior. An empirical interatomic potential developed recently for a ternary FeNiCr system is used for the MD calculations. The interactions are calculated at different temperatures, loop orientations, loop size and solute atom configurations. The results show that the loop strength and the interaction processes depend on the solute atom configuration, the geometrical configurations between the dislocation and the loop and temperature. It is also demonstrated that a small Frank loop is not so weak an obstacle in the alloy. The interaction leads microstructural change such as loop shearing, loop unfaulting and loop absorption in the dislocation. In the former two cases, the loop remains after the interaction, however in some cases an absorption of the remaining loop by subsequent interactions with successive dislocations is observed.

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1. Introduction
The irradiation of reactor pressure vessel internals by neutrons during the operating time of nuclear power plants induces modifications of the microstructure resulting in the formation of black dots, Frank loops and voids/cavities [1]. These defects act as obstacles to the dislocation glide, and may lead to hardening and embrittlement [2], limiting thus the lifetime of the component and especially the 316L screws. In Pressure Water Reactor (PWR), the irradiation leads to Frank loops with 1/3⟨111⟩ Burgers vector and an average diameter of a few nms, which are observed only at a certain temperature and dose [3–5]. Moreover, the plastic deformation of irradiated materials leads to the emergence of channels or defect free areas [5]. These channels are softer and thus lead to plastic localization (until eventual failure) of irradiated stainless steels. The interaction of dislocations with Frank loops is certainly at the origin of the formation of these channels. However the mechanism leading to the formation of defect free zone still needs to be better understood, especially at the atomic scale.

The interaction mechanism between Frank loops and dislocations has already been investigated with Molecular Dynamics (MD) by Nogaret et al. [6] with a pure Cu “Embedded Atom Method” (EAM) potential and by Rodney et al. [7] with a pure Ni EAM potential. Terentyev’s potentials well reproduce Stacking Fault Energy (SFE) of austenitic stainless steels. However, more complex potentials are needed, (at least ternary) in order to account for Cr and Ni, which are known to strongly influence SFE and dislocation mobility [5]. These interaction mechanisms have been detailed at the atomic scale in Ref. [6] and reveal the formation, in the case of edge dislocation, of “superjogs” and, in the case of screw dislocation, of “helical turns”. In Refs. [6,8,9], both mechanisms are responsible for the complete removing of the Frank loops. The other types of interaction identified, conduct to shear the Frank loops or to unfault them. This last mechanism turns the interstitial loop into a perfect loop. The absorption mechanism is the one which needs
the most attention. In fact, the complete removing of the Frank loops conducts to form channels [5]. However, both Nogaret et al. [6] and Terentyev et al. [8,9] show that the formation of helical turn brings about a high unpinning stress which cannot be at the root of the channel formation.

In this paper, MD simulations are performed to study the precise interaction mechanism between an edge dislocation and a Frank loop in a ternary Fe–Ni–Cr model system. This contribution aims at shedding some light on the formation of these channels. This paper complements the study of Terentyev et al. [9] and Bakaev et al. [10], and focuses on edge dislocations. However, this article provides much broader and clearer descriptions of the reactions, describes the effect of the distributions of solute atoms and considers the Frank loops form 2 nm–10 nm size. The edge behavior indeed differs from screw dislocation by a possible formation of “superjog”, when entering into contact with the Frank loops [7]. In the first section of this paper, the simulation techniques are presented. Then, section two focuses on the interactions between an edge dislocation and a Frank loop through: (i) a description of resulting configurations of both the Frank loop and the dislocation and, (ii) the strength and the resistance of the obstacle associated to this interaction. Finally, in a third section, we discuss the correlation between the interaction type and the associated resistance or strength of the obstacle.

2. Simulation techniques

2.1. Interatomic potential

In the present study, we use a ternary Fe–Ni–Cr potential, based on the embedded atom method (EAM), and developed by Bonny et al. [11] to model austenitic stainless steels. For the Fe–Ni10–Cr20 target composition, the potential functions were fitted to get correct elastic constants and reasonable SFE as a function of composition. This potential predicts a stacking fault energy of about 20 mJ m$^{-2}$, which is in the range of common stainless steels [5,12]. This potential has also been used to study the interactions of screw dislocation with the Frank loops [9]. See Ref. [11] for more details on this potential.

2.2. Simulation box

The simulation cell is sketched in Fig. 1 including a Thompson tetrahedron to denote the Frank loop orientation gathered in Fig. 2. The FCC crystal is oriented along $\mathbf{X} = [\overline{T}00]$, $\mathbf{Y} = [\overline{1}T1]$ and $\mathbf{Z} = [T12]$. The perfect edge dislocation is introduced in the cell, thanks to the method developed in Refs. [13], with a Burgers vector $a/2[\overline{T}T0]$ parallel to the $\mathbf{X}$ axis and a dislocation line $\mathbf{Z}$ parallel to the $\mathbf{Z}$ axis. The edge dislocation glides along the $\mathbf{X}$ axis in a positive (M+) or negative (M–) direction of gliding. Periodic Boundary Conditions (PBC) are applied in the $\mathbf{X}$ and $\mathbf{Z}$ directions whereas fixed boundary conditions are applied on three upper and lower (1T1) atomic layers in the $\mathbf{Y}$ direction. The thickness of the grips is slightly higher than the cut-off radius of the ternary interatomic potential. The cell size in the $\mathbf{X}$ direction ensures that the dislocation distance (~10 nm) becomes independent of this dimension box size.

The Frank loop considered here has initially a circular shape, with diameters of 2 and 10 nm, and is an interstitial type. The Frank loop is introduced at the beginning of the simulations following the building of the edge dislocation in the simulation box, its center lying within the dislocation glide plane. The atoms constituting the extra disc are introduced to minimize the energy regarding their neighboring atoms in the upper and lower planes. Once the system is relaxed, the 2 nm Frank loop adopts a hexagonal shape with edges in the $\langle 110 \rangle$ directions whereas the 10 nm loop exhibits a rather circular shape. Due to PBC, the inter-loop distance in the $\mathbf{Z}$ direction corresponds to the box size. It has been set to about 20 nm for the Frank loop size of 2 nm. The axis dimension following the gliding direction fixed at 45 nm and the height of the cell at 32 nm. For a Frank loop diameter of 10 nm, the box size of free atoms in the $\mathbf{Z}$ direction (inter-loop distance) is 40 nm and the total height of the box is 43 nm to avoid inherent surface effect. Thus, the dislocation densities are for the 2 nm and 10 nm Frank loop size respectively $7.10^{14}$ m$^{-2}$ and $5.10^{14}$ m$^{-2}$.

A constant strain rate is applied to the simulation box using the method of Osetsky et al. [13]. The reactions occur over a time scale of a few tens of ps and for strain rate levels of $10^{2}$ s$^{-1}$, which yields a dislocation velocity of almost 55 m s$^{-1}$.

The time step is $10^{-15}$ s for all the simulations. The energy of the system is firstly minimized with a quench algorithm during 50 time steps. The quenched configuration is then relaxed for $2 \times 10^{-2}$ ns in the NVT ensemble for thermalization (with a Nose-Hoover Thermostat). The temperature attributed to the system is 300, 600 or 900 K. After this procedure, the shearing of the simulation box starts by displacing the upper and lower grips. Depending on the thermal expansion, the crystal is scaled up with the appropriate lattice parameter for minimizing the internal pressure.

For the 2 nm and 10 nm size, the simulation cell contains respectively about 2.6 million mobile atoms and ~7 million mobile atoms. The simulations were conducted with a classical MD code developed in the Central Research Institute of Electric Power Industry (CRIEPI). The simulations have been run in parallel on EDF R&D supercomputer with 576 and 729 processors respectively for simulation boxes used for the interactions with the 2 nm and 10 nm Frank loops. Each interaction is carried out for 3 random alloying initial configurations.

The loop is set beyond the critical distance from the nearest partial dislocation, called the capture distance of the dislocation. The loop is separated by a distance of 15 nm from the center of the dislocation core and relaxes during the minimization energy to form the expected loop without any direct interactions with the nearest Shockley partial. Below a critical distance, called capture distance [14], the loop is unstable and glides towards the edge dislocation. This phenomenon is supposed to increase with temperature and loop size. But in this study, this kind of absorption has not been observed, whatever the temperature and the loop size. Thus, we supposed the capture distance should be situated around 3 nm, based on the work done by Rodney et al. [14] and should not
vary much with the temperature and loop size.

Finally, in order to visualize defect atoms, the Centro-Symmetric Deviation (CSD) parameter [15] is computed for each atom $i$. For that purpose, pairs of neighbors of atom $i$ are formed and summed. $N_i$ is the number of neighbors of atoms $i$, the CSD parameter $P_i$ is defined as the minimum sum of all $N_i(N_i-1)/2$ possible neighbor pairs that can contribute to the sum:

$$P_i = \text{MIN} \left( \sum_{j \in (1 \ldots N_i)} \left( \overline{r_{ij}} + \overline{r_{ik}} \right)^2 \right)$$  \hspace{1cm} (1)

where $j$ and $k$ are neighbors of atom $i$. Generally, atoms of a perfect FCC crystal have a zero CSD parameter, whereas atoms with CSD parameter ranging between 0.01 and 0.03 nm$^2$ correspond to the core of the partial dislocations and a CSD parameter larger than 0.03 nm$^2$ is associated to the stacking fault area between the two Shockley partials. The main advantages of this visualization method are that (i) the noise induced by thermal displacements is minimized and, (ii) CSD parameter does not depend on the interatomic potential functions, unlike the energy filtering method.

2.3. Configurations

All possible configurations between edge dislocation and the Frank loop have been investigated. Fig. 2 details the orientation of the Frank Loop based on the Thompson tetrahedron notation seen from the side of $\overline{Y}$ coordinates. This is the same Tetrahedron used in Fig. 1. The edge dislocation has a CD Burgers vector and lying in the $(1\overline{1}1)$ habit plane. The Frank loop is extended in a $(111)$ plane and can adopt one of the four planes proposed by the tetrahedron (noted $V_1$ to $V_4$ here), including the habit plane of the edge dislocation. The dislocation can approach the Frank loop from two sides depending on the shearing conditions with an $M+$ or $M-$ motion direction. The habit plane of the edge dislocation and the Frank loop is identical for $\overline{V}_1$ orientation (Burgers vector of $1/3\langle 11\overline{1} \rangle$).

A configuration is thus characterized by 2 main variables: the motion direction ($M-$ or $M+$) and the orientation of the Frank loop ($V_2$, $V_3$, $V_1$ and $V_4$). The combination generates 8 possible interactions as detailed in Table 1. Moreover, as the simulations are carried out in a random alloying environment, three different seed for alloy generation are chosen for the random number generators and applied to each combination of the 2 main variables. This gives a total of 24 configurations for each temperature.

3. Results

3.1. Interaction with a 2 nm Frank loop

Depending on the initial configurations between the edge dislocation and the Frank loop, three main resulting configurations are observed which is in agreement with the previous studies in FCC crystals [6,8,9]. The different reactions are presented here depending on the new configuration adopted by the Frank loop. First a structural analysis is developed based on the shape of the dislocation and the character of the loop. Second, a critical stress, necessary to unpin the dislocation from the Frank loop, is reported. MD simulations are performed at three temperatures (300 K, 600 K and 900 K). The configurations adopted by the Frank loops after the interaction with the edge dislocation core can be classified into three main categories:

1. /Shearing/the dislocation shears the Frank loops creating a step at its surface. This reaction mechanism is detailed in Fig. 3;
2. /Unfaulting/the Frank fault is transformed into a perfect dislocation loop. Different types of unfaulting have been identified, i.e. the Frank loop can be unfaulted with the formation of a bridge segment (see Fig. 4), after the unpinning, into a new habit plane, and after being dragged along short distance;
3. /Absorption/a part or the whole Frank loop is integrated to the dislocation core. Different types of absorption have been identified. The Frank loop can be absorbed on a Shockley partial, with the formation of a “Superjog” (see Fig. 5).

Table 1

<table>
<thead>
<tr>
<th>Shockley partial</th>
<th>$\overline{b}_1$ – $1/6\langle 11\overline{2}\rangle (M+)$</th>
<th>$\overline{b}_2$ – $1/6\langle 11\overline{2}\rangle (M-)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frank loop</td>
<td>$V_1$ – $1/3\langle 11\overline{1}\rangle$</td>
<td>$1/6\langle 01\overline{1}\rangle$</td>
</tr>
<tr>
<td></td>
<td>$V_1$ – $1/3\langle 1\overline{1}1\rangle$</td>
<td>$1/6\langle 1\overline{1}\rangle$</td>
</tr>
<tr>
<td></td>
<td>$V_3$ – $1/3\langle 1\overline{1}0\rangle$</td>
<td>$1/6\langle 1\overline{0}1\rangle$</td>
</tr>
<tr>
<td></td>
<td>$V_4$ – $1/3\langle 10\overline{1}\rangle$</td>
<td>$1/6\langle 10\overline{1}\rangle$</td>
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<tr>
<td></td>
<td>$V_1$ – $1/3\langle 1\overline{1}1\rangle$</td>
<td>$1/6\langle 1\overline{1}\rangle$</td>
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<td></td>
<td>$V_3$ – $1/3\langle 1\overline{1}0\rangle$</td>
<td>$1/6\langle 1\overline{0}1\rangle$</td>
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<tr>
<td></td>
<td>$V_4$ – $1/3\langle 10\overline{1}\rangle$</td>
<td>$1/6\langle 10\overline{1}\rangle$</td>
</tr>
</tbody>
</table>
Table 2 gathers the reaction outcome depending on temperature, orientation of the Frank loop and alloying random generator for a positive shearing $M_\text{+}$ of the crystal. We can see that unfaulting is the main interaction mechanism. Absorption can be subcategorized into two configurations where the Frank loop can be completely or partially absorbed, on one or two partials, or completely as a double “superjog” [16] by the dislocation core. The absorption mechanism is the second main resulting configuration obtained after the first passage of the edge dislocation on the Frank loop. Only four occurrences of shearing are observed. Regarding the low SFE value for our material, i.e. $18 \text{ mJ/m}^2$, this observation is in contradiction with the result obtained by Terentyev et al. [8], where
a decrease of SFE enhanced formation of shearing to the expense of unfaulnting for high SFE material, which is true here. Those three mechanisms have also been identified by Nogaret et al. [6] with a pure copper potential with associated SFE similar to the one of austenitic stainless steel. The absorption can be done into a glissile “superjog” [17] on straight edge dislocation. The unfaulnting mechanism is mainly controlled by a cross-slip process. Contrary to previous studies, the unfaulnting mechanism occurs only after being into contact with the loop, maybe because a low SFE value reduced the probability to initiate partials segments inside the Frank loop. Two Shockley partial dislocation segments are supposed to be initiated and propagate at the loop surface. The propagation of those partials removes the fault to turn the Frank loop into a perfect loop of Burgers vector $\vec{b} = 1/2\langle110\rangle$.

Table 3 gathers the new configurations of the Frank loop after the first interaction with the two partials in a negative shearing $M-$ of the crystal. At 300 K, Contrary to the positive motion $M+$, the predominant reaction between the Frank loop and the edge dislocation is the shearing mechanism except for $V_1$ orientation where unfaulnting is the predominant mechanism. The outcome of the interactions gathered in Table 3 is in accordance with the result obtained by Terentyev et al. [8] where absorption of the loop is a process thermally activated with an alternative unfaulnting mechanism at 600 K. For both shearing directions ($M+$ and $M-$), the random number generator for solute distribution seems to affect strongly the reaction mechanism. There are for example two cases where the three mechanisms are observed for one orientation and one temperature. This can point out that considering the size of the loop (2 nm), the mechanism of interaction depends strongly on the local alloying content around the Frank loop.

3.2. Description of interaction mechanisms

3.2.1. Shearing (Fig. 3)
Shearing produces steps that can emerge on one side of the loop or within the faulted loop depending on its orientation towards the edge dislocation. However, the life-time of this step is usually lower than 5 ps, the time window used here. For the first passage of the edge dislocation in the case of an $M+$ dislocation motion, shearing is observed for $V_1$ at 300 K, $V_2$ at 600 K and $V_3$ orientation at 300 K and 600 K. Fig. 3 represents the shearing reaction between the $V_1$ Frank loop and edge dislocation at 300 K. The maximum stress associated to this interaction is 273 MPa (see Fig. 3, snapshot (b)). Pinning occurs on the leading partial, whereas the trailing partial bows out for the other cases. During the second and the third passage of the dislocation due to the PBC, the shearing is observed only on two cases which have already been sheared. In all cases the step created after the passage of the two partials is recombined and the Frank loop recovers its planar surface almost immediately. At the beginning of the interaction and for $V_1$ and $V_2$ orientations, the leading partial is repelled by the defect and first contacts are made between the small segment of the leading partial and the $(110)$ edges of the Frank loop. In the case of an $M+$ motion, for all the shearing cases, no permanent damage is observed and the Frank loop does not unfaulnt at 300 K. However, the position of the Frank loop is slightly translated of 1–2 $b$ after the passage of the two partials.

When a negative strain is applied, the shearing mechanism becomes the majority at low temperature. A step is generated on the side of the loop in the case of $V_1$, $V_2$ and $V_3$ orientation and on the loop surface for $V_4$. The only difference with the opposite motion is that the dislocation is consistently attracted by the loop surface once the separation distance between the two defects is less than 4 $b$. The dislocation pursues its gliding in its habit plane with a planar shape and leaves behind the faulted Frank loop with its previous orientation.

3.2.2. Unfaulnting with the formation of a bridge segment (Fig. 4)

Depending on the orientation of the loop, the unfaulnting mechanism can happen with a bridge created between the leading partial and the Frank loop. The removal of the faulted surface is made with the propagation of this segment all around the loop. On the other hand, when there is no such segment between the two defects, the successive passage of the leading and trailing partial on the Frank Loop conducts to a perfect loop of Burgers vector $\vec{b} = 1/2\langle110\rangle$. Specific cases where the Frank loop and the dislocation lay in the same habit plane led to change the habit plane of the former Frank loop.

This reaction is represented in Fig. 4. The leading partial approaches the loop and a bridge is created between the left arm of the leading partial and the top $(110)$ edge of the loop. This junction is apparently constituted of multiple cross slipped segments. When increasing stress, this bridge sweeps the upper loop and, simultaneously, the edge dislocation starts to bend. The remaining loop interacts with the trailing partial. The maximum stress due to

![Fig. 5. Configuration $V_1/M+$ at 300 K: snapshots are shown at 113 MPa, 520 ps (a) 217 MPa, 770 ps (b), 309 MPa (Critical stress), 1.02 ns (c) 239 MPa, 1.07 ns (d). The associated Stress–Strain curve is plotted on the right with its single edge dislocation response.](image)
Table 2

Resulting configurations between edge dislocation and the Frank loop ($D = 2$ nm) for the first passage with an $M^+$ dislocation motion. The above legend indicates the notation used in the table. The reaction is conducted at 300 K, 600 K and 900 K for three alloying random configurations. The loops have a $\langle 110 \rangle$ side and are hexagonal.

![Diagram](image)

Fig. 6. Cumulative ratio of interaction configurations (unfaulting, absorption or shear) at 300 K, 600 K and 900 K depending on the number of passages.

<table>
<thead>
<tr>
<th>Temp. (K)</th>
<th>Movement $M^+$</th>
<th>Orientation of the Frank loop</th>
<th>$V_1$</th>
<th>$V_2$</th>
<th>$V_3$</th>
<th>$V_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>300 K</td>
<td>Seed #1</td>
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<td></td>
<td>Seed #2</td>
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<td>Seed #1</td>
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<td>600 K</td>
<td>Seed #2</td>
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<td>Seed #3</td>
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<td>Seed #1</td>
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<td>900 K</td>
<td>Seed #2</td>
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<td>Seed #3</td>
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</table>
pinning is associated to the configuration represented in Fig. 4 (d) when a constriction around the two nodes is formed. In Fig. 4 (d), we can see that the lower part of the Frank loop has already its unfaulted behavior whereas the upper part has been turned into what appears to be a Stacking Fault Tetrahedron (SFT). This temporary configuration is consistent with the MD simulations realized by Kadoyoshi et al. [18] who established under stresses the formation of an incomplete SFT from a scalene hexagonal loop. This configuration induces a strong pinning on the trailing partial that is explained by a strong bowing of that partial. The dislocation core is released from the new perfect loop with \( b = \frac{1}{2}(110) \) and conserves a planar shape and its initial habit plane.

3.2.3. Absorption into a “superjog” (Fig. 5)

In this configuration, the upper part of the loop is absorbed with the creation of two junctions between the two partials and edges of the loop. The superjogs generated in this study are typically of acute type [17]. The orientation of the Frank loop \( (V_1) \) promotes the attraction of the leading partial by the Frank fault in the case of the \( M+ \) motion. Then the Frank loop is divided into two parts where the lower part is orientated in the BD direction and the upper part in the CD direction. Those two loops are connected by the leading partial following reaction in the Thompson notation:

\[
Ca \rightarrow aD + CD \rightarrow aB + CD + BD
\]  

After the interaction, the “superjog” remains dragged in its original configuration. One of the superjogs is dissociated in its ADC glide plane while the other is constricted in the AB segment. The segment between the “superjogs” has climbed by 6 \((11 \overline{1})\) planes and is extended in its new BCD glide plane. The dissociation of the extended “superjog” produces one \( \beta/CD \) Lomer–Cottrell stair-rod segments, visible on the right part of Fig. 5 (d).

3.2.4. Analysis of the 2nd and the 3rd passage (Fig. 6)

The simulations, which cover a statistic of 24 configurations, have been continued for a second and third passage, if the Frank loop had not been previously absorbed. In fact, as the probability
that a double “superjog” or a glissile loop may interact with a faulted or unfaulted loop is very low, the simulations are stopped once the defect has been partially or completely absorbed. A first analysis reveals that unfaulting and absorption are thermally activated and become predominant at 900 K. These observations are in accordance with the previous analysis made by Nogaret et al. [6], who noticed the removing of the Frank loops. This coincides with the observation of clear band in irradiated material. In this study, the absorption is observed for 80% of the total configurations. In the absorption process, it appears that the unfaulting is necessary for a next and likely absorption. However, 10% of the initial Frank loop conserved their faulted character and 50% of the interstitial Frank loops are still present at 300 K. The other new configurations exhibit unfaulted loops with a new Burgers vector \( \frac{1}{2}(110) \), which suggests absorption if the interactions were pursued.

The effect of alloying is also very strong on the reaction mechanism even if sometimes it appears there is a preferential orientation for a specific reaction. In this way, it can mean that the SFE
and/or friction stress is an important parameter to justify the new configuration adopted by the Frank loop. The effect of local alloying content has not been investigated here but recent studies led by Terentyev et al. [8] highlight the effect of Ni in a Fe FCC host matrix. It appears that increasing the SFE and the friction stress reduced the probability of absorption in the case of edge and screw dislocations. In that case, a possibility of absorption in temperature can be due to the decreasing of friction stress which allows the dislocation to cross-slip with the two arms of the leading edge dislocation that have acquired a screw character. Thus, the unfaulting mechanism becomes similar to the one occurring in pure metals [19,20].

3.3. Critical unpinning stress analysis

When a dislocation submitted to shear stress τ meets a point obstacle, it bows and the force exerted by the dislocation on the point defect is

\[ F = 2\Gamma \sin \left( \frac{\varphi}{2} \right) \]  

where \( \Gamma \) is the line tension of the dislocation, and \( \varphi \) is the bowing angle. In the simplest form, the line tension can be given by \( \Gamma = \mu b^2 / 2 \), where \( \mu \) is the shear modulus and \( b \) is the burgers vector modulus. Independently, the integration of the Peach and Koehler force along the dislocation gives

\[ F = (\tau - \tau_f) bL \]  

where \( L \) is the distance between two point obstacles and \( \tau_f \) is the friction stress of the dislocation. The yield strength is the critical applied stress \( \tau_c \) at which the dislocation can “break away” from the obstacle. Eqs. (3) and (4) lead to:

\[ \tau_c - \tau_f = \frac{\mu b^2}{2} \sin(\varphi^c) \]  

where \( \varphi^c \) is the critical angle at which the dislocation breaks away. The term \( \alpha = \sin(\varphi^c) \) represents the strength of the obstacle: it varies from 0 (no additional stress required to break through the obstacle) to 1 (obstacle by-passed by the dislocation).

In our case, the critical bowing angle is hard to determine as the curvature of the dislocation segments varies strongly in the vicinity of the obstacle. However, the strength \( \alpha \) can be determined from eq. (5):

\[ \alpha = \frac{(\tau_c - \tau_f) L}{\mu b} \]  

where \( \tau_c \) is the maximum of the stress–strain curve when the dislocation interacts with the defect, \( \tau_f \) is the maximum stress of the stress–strain curve in the absence of the defect and \( L = l_x - D \) is the difference between the box size \( l_x \) and the obstacle diameter \( D \). The shear modulus is defined here as the average of two extreme cases, the Reuss average (\( \mu = 60 \) GPa) and Voigt average (\( \mu = 88 \) GPa) limits (\( \mu = 74 \) GPa here).

The influence of temperature, loop morphology and random generator has been investigated on the unpinning stress for dislocation to overcome the Frank loops strength. The strength \( \alpha \) of the obstacle has been subdivided into three classes depending on the temperature, four classes depending on the orientation of the Frank loop and three other classes based on the alloying random generator. The strength of the 2 nm Frank loop is represented in Figs. 7 and 8 and in Fig. 9 in the case of the 10 nm Frank loop. The influence of temperature on \( \alpha \) is not similar for the different orientations and sizes of the Frank loops. However, in the case of the 10 nm size, where shearing is the only mechanism that is observed, the strength of the obstacle tends to decrease systematically with the temperature. Thus, the interaction mechanism types strongly influence the strength of the obstacle, even more than temperature. Depending on the Frank loop size, the 10 nm Frank loop gives a
higher strength by a factor of ~33%.

3.4. Averaging obstacle strength

In all cases, reactions observed for the interactions between dislocation and the Frank loop are similar as those found in Refs. [6,7,20]. The absorption mechanism is a thermally activated process, which becomes the major outcome after the third interaction. The Unfaulting mechanism appears to be a prerequisite for the absorption of the Frank loop. For the shearing mechanism, the reconstruction of the sheared Frank loop, which occurs via the migration of the 1/2[110] step formed in the shear reaction over the loop, is systematic for the 2 nm size and never observed for the 10 nm size. In the case of the 2 nm Frank loops, the combination of the probability of the outcome reactions and the average strength $\pi$ of the obstacle can constitute a constitutive law which can be employed at a higher simulation scale, for example in Dislocation Dynamics. The average strength of the obstacle and the outcome of the interaction are gathered in Fig. 10 for the three main sets of interactions.

4. Conclusion

The interaction between edge dislocation with the Frank loops in a random solid solution Fe–Ni100Cr20 has been studied. The interaction has been carried out using a constant strain rate loading conditions corresponding to a dislocation velocity of ~55 m s$^{-1}$. For the 2 nm size, the interaction mechanism between the edge dislocation and the Frank loop can be categorized into three sets: shearing, unfaulting and absorption. The majority of the Frank loop are absorbed in the third passage, where unfaulting of the Frank loop appears to be a prerequisite. The absorption of nearly all the obstacles is in agreement with the experimental observations where the presences of clear bands or free obstacle channels are revealed. The unfaulting of the Frank loop always happened with a direct contact between the Frank loop and edge dislocation and the faulted Frank loop is turned into a perfect loop of $b = 1/2\langle110\rangle$. For a 10 nm size of Frank loop, only shearing is identified leaving behind a stable step on the Frank loop, which means for large loops, the edge dislocation do not play a crucial role in clear channeling.

From a mechanical point of view, the 10 nm Frank loop exhibits a higher strength than the 2 nm loop. In the case of the 2 nm size, the unfaulting mechanism is the most strengthening mechanism compared to shearing, which lead to the least strengthening. The temperature affects strongly the strength of the obstacle for some orientations. However, for the 2 nm loop, the decreasing of obstacle strength is not systematic. This can be partly explained by the unfaulting mechanism, which is a thermally activated process, and is associated to a higher strength. The combination of data on the average strength of the obstacle and the probability of the outcome reaction could lead to a constitutive law useful for the Dislocation Dynamics.

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