

# Direct atomistic simulation of dislocation climb in fcc Ni

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Dislocation climb is one of the key processes controlling the mechanical response and microstructure evolution of materials at high temperatures. The mechanisms of this phenomenon are still unclear due to its complex nature, which involves interactions between point defects and dislocations. Here we employed large-scale classical molecular-dynamics (MD) simulations to shed light on vacancy-driven dislocation climb in fcc Ni. A Ni crystal with dissociated dislocations was simulated under high-temperature vacancy supersaturation for multiple nanoseconds. A particular advantage of this method is the ability to reveal the underlying mechanisms of dislocation climb without prior knowledge. The study included three different dislocation characters: pure edge, mixed  $30^\circ$ , and  $60^\circ$ . We found that jog-pair formation initiated with vacancy clustering at partial dislocations, followed by the alignment of vacancies into linear clusters along the  $\langle 110 \rangle$  direction. This stage was clarified by a detailed analysis of vacancy segregation energies at dissociated dislocations for vacancy clusters of different sizes and configurations. Subsequent stages of jog-pair formation involved local reduction of the stacking-fault region and further jog-pair growth due to vacancy accumulation. From the MD simulations, we traced the full dislocation climb process and compared it with classical descriptions of dislocation climb in fcc metals. Detailed analysis of the MD results allowed us to resolve and describe all stages of dislocation climb from the perspective of dislocation reactions. Based on the changes in dislocation positions, we estimated the climb velocity for the considered dislocations driven by the osmotic force.

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## I. INTRODUCTION

Dislocation climb is a nonconservative motion that plays a fundamental role in determining the mechanical properties of metals and alloys at high temperatures. In contrast to dislocation glide, climb involves movement of dislocations in a direction normal to the glide plane. This becomes possible due to dislocation interaction with diffusing point defects [1]. In particular, vacancies can be absorbed at the dislocation, promoting its climb to the next atomic plane (i.e., positive climb).

The dislocation climb allows for a complex trajectory of dislocation motion. It is therefore crucial for dynamic and static recovery during annealing, where oppositely signed dislocations can annihilate by climb [2]. Similarly, it plays an essential role in dislocation creep, including glide-climb creep, as climb enables the bypassing of obstacles to glide [3]. Understanding the mechanisms of dislocation climb is of particular importance for materials subjected to high temperatures and loads, such as Ni-base superalloys [4,5] used for

turbine parts [6]. Vacancy-assisted climb of the dislocations in the Ni matrix (i.e.,  $\gamma$ -channels) surrounding the precipitates ( $\text{Ni}_3\text{Al}$  or  $\gamma'$ -phase) is considered to be one of the mechanisms that contributes to creep of single-crystal superalloys [7,8]. Thus, analysis of creep requires unraveling basic mechanisms of dislocations climb in Ni having face-centered-cubic (fcc) crystal structure.

In fcc metals, the process of climb is complicated by the dissociation of dislocation into partials bounding an intrinsic stacking fault (SF) region. Climb requires the complete transition of such planar configuration, including SF, to a parallel close-packed  $\{111\}$  plane. Practically, dislocation climb relies on the formation of a jog pair (or double jog)—a short segment of a dislocation that lies out of its slip plane [1,9]. A single jog can be considered as a step at dislocation line shifting dislocation from one atomic plane to another [10]. Such dislocation defects can be classified based on their “height”—the distance by which the dislocation line is displaced out of its original slip plane. A *unit-jog* is a step with a height equal to a single interplanar spacing, whereas a step with a height of several atomic layers is referred to as a *super-jog* [11]. For a dissociated dislocation, a jog can have a relatively complex atomistic structure [10,12]. This suggests that climb is more difficult for a dissociated dislocation than for a perfect one. Because of the limited possibilities for direct observation and the complex interactions between the involved defects, climb mechanisms in fcc metals continue to be actively discussed [10,13–18]. In particular, the mechanisms of jog pair formation on dissociated dislocations are not yet fully understood and require further explanation.

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Several theoretical studies [10,11,13–15,19–21] discussed possible ways of vacancy-driven nucleation of jogs at dissociated dislocations. For example, Escaig [19] suggested the formation of a vacancy prismatic loop on top of the stacking fault, and Kimura *et al.* [20] assumed the direct segregation of vacancies onto the partial dislocations together with a shift by  $1/12\langle 11\bar{2} \rangle$  of the stacking fault between the partials. According to Thomson and Balluffi [13], climb of a dissociated edge dislocation might start with the agglomeration of vacancies at one of the partial dislocations. These vacancy aggregates are equivalent to a prismatic vacancy loop with the same Burgers vector as the original dislocation. The vacancy loop interacts with the original partial dislocation and dissociates by glide. This process produces a complete jog pair consisting of an acute (extended) jog formed by a stair-rod dislocation dipole and an obtuse (constricted) jog formed by Hirth dislocations. As additionally suggested in [13], another way of jogs formation may rely on forming a platelet from vacancies directly in the SF plane leading to the growth of a Frank sessile loop. The concept of jog-pair formation through dissociation of a prismatic vacancy loop at the partial dislocation [13] has found its continuation in the analytical work by Grilhé *et al.* [14]. The research has focused on edge dislocation climb in Cu-Al alloys. The authors have estimated the size of a prismatic loop ensuring the formation of a stable double jog in the alloy. A critical number of vacancies for establishing the loop was assumed to be  $\sim 10^3$ ; more precise estimation was proportional to the material-specific SF width. The work [14] also proposed an extension of the theory to the mixed dislocations with various angles  $\theta$  between the Burgers vector  $\mathbf{b}$  and the line direction unit vector  $\vec{\xi}$ . One of the fundamental assumptions in [13,14] is that the dissociation width—the distance between partials—remains constant during jog formation.

An alternative view has been discussed by Stroh [10]: formation of jogs on dissociated dislocation was expected only after preliminary constriction of the SF. The constriction was determined as a local (i.e., occurring over a few atomic spacings) recombination of two partial dislocations. The change in dislocation configuration was only due to interactions between the partials; vacancies were not included in the consideration. As Stroh suggested, the constriction of the dissociated dislocations in fcc metals may be energetically favorable and hypothetically possible as a result of thermal effects. However, from estimates made for Al [10], even at temperatures close to melting, thermal fluctuations alone lead to a very low probability of dislocation constrictions. A steady climb process was supposed to rely on additional factors promoting local recombination of partials, such as applied stress.

The concepts outlined in Refs. [1,10,11,13–15] provide the theoretical framework for understanding the nuances of dissociated dislocation climb in fcc metals. However, the proposed climb mechanisms do not take into account dynamic changes in the dislocation structure and position due to its interactions with phonons [22]. These dynamic effects, however, impact the interaction between dislocation and vacancies. Incorporation of realistic dislocation configurations is also important for the description of dislocation mobility, vacancy segregation at dislocations, dislocation structure evolution in the presence of vacancies, and differences in atomic transport in bulk and

along dislocations. Some works [1,11,23] also highlighted the need to consider the role of superjogs in a climb process along with simpler unit jogs.

The atomistic mechanisms of climb-related processes in metals are a subject of significant interest [17,18,24–26]. In general, direct simulation of the climb process is considered challenging due to its complex displacive-diffusional mechanism and different characteristic time scales of the involved steps [25]. The latter generally include vacancy diffusion to/along the dislocation, jog-pair formation, and accompanying dislocation evolution. One way to deal with the time- and spatial-limitations of atomistic simulations is to focus specifically on the individual process steps. In addition, one can use accelerated atomistic simulation techniques and coupled methods that allow a combination of different time scales. Such approaches are illustrated by recent studies employing classical atomistic simulations [16–18,25] to investigate the realistic structure of dissociated dislocations and their interactions with point defects. Using diffusive molecular dynamics (DMD) [27], Sarkar *et al.* showed that when vacancies are manually placed at a partial-dislocation core of an edge dislocation in Cu, the intermediate jog-pair configuration postulated by Grilhé *et al.* [14] can be observed [25]. Jog formation in fcc metals was later studied in simulations by Abu-Odeh *et al.* [17]. The work focused on the aspects of vacancy absorption at edge dislocation in Cu and Al. It was shown that sequential segregation of single vacancies on partial dislocations leads to the formation of strongly oriented vacancy rows. Collision of such clusters is followed by constriction of the SF region [17]. The simulation results have been used to estimate the *climb efficiency*—a relationship between an ideal diffusion-limited climb velocity and an actual value, presumably reduced by low availability of jogs.

In Ref. [16], Baker and Curtin coupled two numerical methods to achieve a joint description of a single edge dislocation evolution and vacancy flow in fcc Al. The dynamics of a dislocation-containing region was treated with atomistic resolution by accelerated MD (AMD). At the same time, the discrete diffusion equation was used to model a long-range flow of vacancies in the lattice leading to vacancy transition to/from the AMD region. The work considered absorption of vacancies at the dislocation under vacancy supersaturation and showed the accommodation of multiple vacancies at the partial dislocations. Specifically, absorption of up to three vacancies led to the formation of a cluster at one of the partial dislocations, whereas absorption of five or more vacancies resulted in the formation of a distinct jog pair. The authors have shown the atomistic structure of the obtained jogs and discussed the evolution of the dislocation configuration corresponding to the initial stages of edge dislocation climb in fcc Al. The simulations also showed a strong attraction of vacancies to jogs, the latter being an effective vacancy sink. Another example of accelerated climb-related simulations has been reported by Fey *et al.* in [18]. The accelerated dynamics based on parallel trajectory splicing was used to study interactions between a vacancy and a jogged edge dislocation in Ni. They reported energy barriers for vacancy absorption/emission at the jog as well as for a pipe diffusion to the jog.

Current literature offers valuable perspectives on dislocation climb; however, the studies mostly rely on predefined

configurations that isolate specific events, such as jog nucleation. There is a notable lack of simulations that capture the continuous, long-term progression of the entire dislocation climb event. Furthermore, it would be interesting to consider the dependence of climb process on dislocation type, as suggested by previous research [1,14].

Climb is often the rate-limiting step in high-temperature deformation, which means that the dislocation climb rate  $v_{cl}$  is relevant for modeling dislocation creep. This includes discrete dislocation dynamics (DDD) methods acting at the mesoscale and used to describe dislocation evolution related to different conditions, including creep deformation. Some of the three-dimensional DDD models were proposed specifically for Ni-base superalloys [7,28]. An important question, however, deals with the model parametrization. For creep-related studies, DDD simulations need to include mobility laws governing climb of dislocation segments.

Analytical expressions for climb velocity derived from the second Fick's equation were previously discussed in a number of studies [1,7,29–31]. An important limiting case is vacancy supersaturation, in which the fractional vacancy concentration  $c_{vac}$  (number of vacancies per atom) is significantly higher than its equilibrium value  $c_{vac}^{eq}$ . In this case, the equation for the climb velocity  $v_{cl}$  was derived under the assumption that it is proportional to the product of the vacancy concentration near the dislocation core and the vacancy jump frequency [1]. The initial stage of the climb rate can be expressed using vacancy diffusion and  $c_{vac}$  as follows:

$$v_{cl} = \frac{8D_{vac}c_{vac}}{b \sin(\theta)}. \quad (1)$$

Here  $D_{vac}$  is a vacancy diffusion coefficient,  $b$  is the length of the Burgers vector of an edge dislocation, and  $\theta$  is a character angle between the Burgers vector  $\mathbf{b}$  and the line direction vector  $\vec{\xi}$ . In the subsequent steady regime, where the vacancy distribution around the dislocation is in local equilibrium, but the condition  $c_{vac} \gg c_{vac}^{eq}$  still holds far from the core, the dislocation climb is governed by the following equation [31]:

$$v_{cl} = \frac{2\pi D_{vac}}{b \sin(\theta) \ln(r_{\infty}/r_c)} (c_{vac} - c_{vac}^{disl}), \quad (2)$$

where the parameters  $r_{\infty}$  and  $r_c$  denote the outer radius at which the vacancy concentration is unaffected by the presence of the dislocation and dislocation core radius, respectively. The corresponding vacancy concentrations at these distances are  $c_{vac}$  and  $c_{vac}^{disl}$ , the latter being close to  $c_{vac}^{eq}$ . Thus, in the general case, under vacancy supersaturation, we suggest that the climb velocity can be expressed as

$$v_{cl} = \frac{\eta D_{vac} c_{vac}}{b \sin(\theta)}. \quad (3)$$

Here  $\eta$  is a numerical factor that accounts for the specific diffusion regime, initial and boundary conditions. In practice, high vacancy concentration can be achieved in many cases, such as quenching [1] or irradiation [32] of the material. Vacancy supersaturation also occurs due to the Kirkendall effect [33] or because of the appearance of superabundant vacancies caused by the presence of hydrogen [34].

Equation (3) is widely used for estimation of  $v_{cl}$  in fcc and bcc metals [23,31]. However, due to its formalism, the equation omits atomistic aspects dealing with dislocation structure. This includes the physical description of the core width for fcc lattice or anisotropic vacancy diffusion near a dislocation. Currently, there is an interest in incorporating the atomistic insights of the dislocation-vacancy interaction into the description of climb (and its rate  $v_{cl}$ ) used in mesoscale models, namely DDD. As was shown by Kabir *et al.* [24] and McElfresh *et al.* [35], kinetic Monte Carlo can be used to account for atomistic effects in dislocation climb. However, such studies have been done only for specific mixed dislocation in bcc Fe, and have not covered climb in fcc metals.

The present work is devoted to the direct study of climb of split dislocations in fcc Ni driven by vacancy supersaturation. The simulated temperature regime is related to high-temperature creep and intersects with the area of application for Ni-based superalloys. We show that elementary stages of vacancy-assisted dislocation climb can be identified for different dislocation characters (e.g., edge and mixed). The structure of the paper is as follows. In Sec. II, we discuss methodology and the simulation setup, including a description of the interatomic potential and details of the atomistic configurations. In Sec. III, we report simulation results that range from the vacancy segregation energy at different dislocation configurations to the climb mechanisms and the instantaneous climb velocity  $v_{cl}$ . In Sec. IV, we analyze the MD simulation results regarding vacancy-driven climb and relate these observations to theoretical models of jog-pair formation.

## II. METHODOLOGY

This work is based on classical atomistic simulations using interatomic potentials. The main idea is to observe climb mechanisms directly by enhancing the processes in a physically sound way, i.e., by using high-temperature molecular dynamics at vacancy supersaturation. Throughout the work, we define a dislocation climb event as a complete transition of an initially jogless dissociated dislocation to another {111} atomic plane. Within such a setup, the formation of jog-pairs at dislocation due to absorption of vacancies at finite temperatures is observed as an intermediate stage.

The adequacy of the atomistic model strongly depends on the potential functions describing interatomic interactions in the material. We described Ni with the embedded-atom method interatomic potential of Du *et al.* [36]. The initial part of the work aimed at verification of high-temperature properties of Ni and, specifically, at dynamics of vacancy and self-diffusion. Another important block of simulations dealt with a study of vacancy segregation and clustering at dislocations (considering static calculations at zero temperature). Finally, we performed a direct simulation of the dynamic interaction of dislocations with vacancies at high temperatures following the framework of a numerical experiment. This led us to the observation of climb stages and estimation of *instantaneous* climb velocity. All simulations reported in the work have been carried out with the LAMMPS Molecular Dynamics Simulator [37].

TABLE I. Characteristics of the interatomic potential for Ni [36]: melting temperature  $T_m$  in K; stable intrinsic stacking fault energy  $\gamma_{sf}$  in mJ/m<sup>2</sup>; energies of a vacancy formation  $E_{vac}^f$  and migration  $E_{vac}^m$  (both in eV).

|             | $T_m$           | $\gamma_{sf}$       | $E_{vac}^f$ | $E_{vac}^m$ |
|-------------|-----------------|---------------------|-------------|-------------|
| Simulations | $1530 \pm 10^a$ | $102^b$             | $1.57^b$    | $0.98^b$    |
| Experiments | $1728^c$        | $120\text{--}130^d$ | $1.60^e$    | $1.30^e$    |

<sup>a</sup>This work.

<sup>b</sup>Reference [36].

<sup>c</sup>Reference [38].

<sup>d</sup>Reference [39].

<sup>e</sup>Reference [40].

### A. Climb-related properties of the potential

Table I summarizes the main features of the interatomic potential [36] relevant to MD simulations of high-temperature climb. In addition to the information reported in the original paper [36], we calculated the melting temperature  $T_m$  of Ni at zero pressure. More detail on the melting temperature calculations (and related to the data on lattice thermal expansion) is given in Appendixes A and B. For all dynamic simulations discussed here and below, the MD time step was set to 1 fs.

### B. Simulations of vacancy diffusion in bulk

The description of self-diffusion in the equilibrium state is a topic that deserves special attention while approaching dislocation climb. In Ni, self-diffusion is controlled by the formation and migration of single vacancies [41,42]. Comparison of vacancy formation and migration energies with the experimental values (as shown in Table I) can give the first impression of the potential accuracy. However, the energies alone do not provide enough data for evaluation of the high-temperature description of vacancy behavior. Properties of vacancies in a model at high temperatures can be understood by comparison with the experimental self-diffusion coefficient  $D_{self}$ . At a given temperature  $T$  it can be estimated from a combination of a single vacancy diffusivity  $D_{vac}$  and the equilibrium vacancy concentration  $c_{vac}^{eq}$ ; for details, see [41]:

$$D_{self} = D_{vac} c_{vac}^{eq}. \quad (4)$$

In general, the temperature dependence of the diffusion coefficients is often found to satisfy the Arrhenius formula [41]. For a vacancy diffusion, such dependence is written as  $D_{vac} = D_0 \exp(-E_{vac}^m/k_B T)$ , where  $D_0$  is a preexponential factor,  $E_{vac}^m$  is a vacancy migration energy, and  $k_B$  is the Boltzmann constant.

In MD,  $D_{vac}$  can be calculated directly from the trajectories of atoms in a simulated crystal containing a single vacancy. For Ni single crystal,  $D_{vac}$  was estimated as

$$D_{vac} = \sum_{i=1}^N \delta r_i^2 / 6t, \quad (5)$$

where  $\sum_{i=1}^N \delta r_i^2$  is the total squared displacements of all  $N = 2047$  atoms in a simulation box during the observation time  $t$ . We used the boxes with periodic boundary conditions (PBCs) in all directions. For all considered temperatures, the values of

$t$  were equal to 20 ns. The calculations were carried out in the NVE ensemble, and the volume  $V$  was adjusted for every  $T$  in accordance with the thermal expansion curve (for details, see Appendix A).

The equilibrium concentration of vacancies  $c_{vac}^{eq}$  contributing to  $D_{self}$  at given  $T$  was determined as follows:

$$c_{vac}^{eq} = \exp\left(-\frac{G_{vac}^f}{k_B T}\right) = \exp\left(\frac{S_{vac}^f}{k_B}\right) \exp\left(-\frac{H_{vac}^f}{k_B T}\right), \quad (6)$$

where  $S_{vac}^f$  is a vacancy formation entropy. Here we considered cases at zero pressure, hence  $H_{vac}^f$  was equal to  $E_{vac}^f$ . The numerical value of  $E_{vac}^f$  corresponding to the potential [36] is given in Table I. For the entropy term  $S_{vac}^f$  we used  $2.0k_B$ . This value was determined for Ni from different *ab initio* calculations [43,44]. Discussion of the simulation results is given in Sec. III A.

### C. Dislocation configurations

In this section, we describe the simulation boxes used throughout the work to represent dislocations in Ni. We considered different dislocation orientations: edge, mixed 60°, and mixed 30°. Dislocations were introduced into the ideal fcc Ni lattice according to the approach discussed in [45]. Dislocation lines were aligned along one of the box axes. All boxes have been built with PBCs in all directions. Due to this, the simulation setup results in dislocation dipole configurations shown in Fig. 1. The left panel in Fig. 1 shows a model of an edge dislocation dipole with Burgers vectors  $\pm \frac{a}{2}[110]$ , where  $a$  is atomic spacing. The other boxes shown in Fig. 1 were used for the study of mixed 60° and 30° dislocations. The pictures show dislocations in the dissociated configuration, after the relaxation performed with a Hessian-free truncated Newton algorithm implemented in LAMMPS [37] as the *hftn* minimizing algorithm. Atoms belonging to the SF regions are depicted, while atoms belonging to the fcc lattice are omitted in the visualization. The specific dislocations analyzed in the following sections are illustrated in Fig. 1, alongside their corresponding Burgers vectors and Thompson tetrahedron notation [46].

To study aspects of dislocation-vacancy interactions, we used two different types of classic simulations: static and MD. All simulations were performed with equilibrium lattice parameters corresponding to the given temperature. Specific details of the simulations based on the above-mentioned dislocation dipole configurations are discussed in the subsections below.

#### 1. Static calculations: Vacancy segregation at dislocations

In line with previous works [16,17], we studied vacancy segregation at the dissociated dislocations. To deepen our understanding of segregation patterns, we investigated specific vacancy clusters in addition to single vacancies. We utilized the simulation boxes illustrated in Fig. 1 to perform the necessary static calculations. The number of atoms in the models was  $\sim 10^6$ . The exact model sizes depend on the dislocation character; see Table II.

We evaluated the segregation behavior of a single vacancy to edge dislocations of varying geometries—including

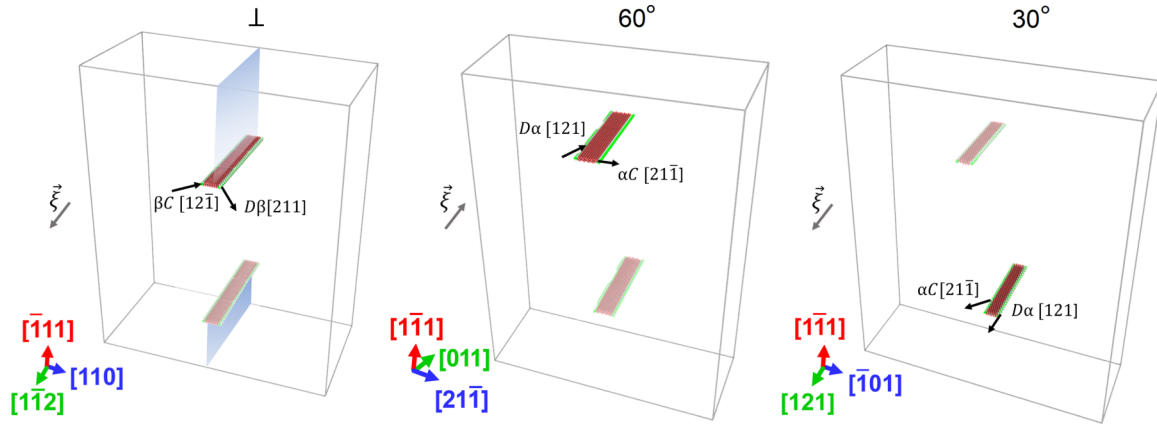


FIG. 1. The models of dislocation dipoles used in this work. Simulation boxes contain dislocations with different characteristic angles  $\theta$ :  $90^\circ$  (edge),  $60^\circ$ , and  $30^\circ$ . For edge dislocations, shaded blue regions show the position of the extra planes. Only atoms belonging to the stacking faults are depicted (in red). Green lines represent partial dislocations, and  $\xi$  is a dislocation line direction. The left-hand start-finish (LH/SF) convention is used for the Burgers circuit, and the Thompson tetrahedron notation [46] is used to label the dislocations. Here and below, color coding of the coordination axis is as follows: green, dislocation line direction; blue, glide direction; red, normal to the glide plane.

straight and jogged configurations—as well as at straight mixed dislocations. The jog-pair configuration was prepared for an edge dislocation with the Burgers vector  $\frac{a}{2}[110]$ . At the stage where the dislocation was introduced into a perfect fcc crystal, a segment of the dislocation line was shifted to the next atomic plane in the  $[\bar{1}11]$  direction. This modification promoted a stepwise dislocation line profile with a pair of unit jogs. The length of the dislocation segments between the jogs is equal to half of  $L_{[1\bar{1}2]}$ . After relaxation, the dislocation dissociates with the formation of the SF regions between the partial dislocations.

For the  $i$ th lattice site at the given dislocation we determine the vacancy segregation energy as the difference between two potential energies:

$$E_{\text{seg}}^i = E_{\text{vac}}^i - E_{\text{vac}}^{\text{bulk}}. \quad (7)$$

Here  $E_{\text{vac}}^i$  describes a system with a vacancy at the  $i$ th site belonging to the dislocation core or SF;  $E_{\text{vac}}^{\text{bulk}}$  is the energy for a system with dislocation and a single vacancy placed in a bulk region (i.e., away from the SF region and dislocation cores). For both cases, the total number of atoms in a system was the same. The values of  $E_{\text{vac}}^i$  and  $E_{\text{vac}}^{\text{bulk}}$  were determined with atomic relaxation.

In addition to the study of a single vacancy segregation, we paid special attention to vacancy clustering at straight edge dislocation. The possibility of vacancy ordering at the dissoci-

ated edge dislocation has been considered by Abu-Odeh *et al.* in the above-mentioned simulations [17]. In our work, we initiated the cluster construction by placing a single vacancy at one of the partial dislocations. To form a cluster of a given size, we sequentially deleted a line of neighboring atoms lying along the close-packed direction (i.e., along the  $\langle 110 \rangle$  direction) in the SF plane. In this way, we created a linear chain of vacancies that propagates into the SF region. The topology of such defects is reminiscent of so-called *vacancy tubes*—linear vacancy clusters generated from dislocation-cutting processes [47]. We also varied the cluster height in the  $[\bar{1}11]$  direction (i.e., perpendicular to the SF plane). The clusters with various heights are denoted as follows: 1T, for a line of single vacancies; 2T, for the tubes with a height of two atomic planes in the  $[\bar{1}11]$  direction; and 3T, for the tubes formed by a triple row of vacancies. The 1T configuration is similar to that discussed in [17] for Al and Cu. Also, such tubes have been found in atomistic simulations of work-hardening in fcc Cu [47].

We calculated the energy of vacancy tube formation ( $E_T^f$ ) at the edge dislocation for the 1T, 2T, and 3T clusters depending on the number of vacancies  $n$  in the cluster:

$$E_T^f(n) = E_n^{\text{disl}} + (n-1)E_0^{\text{disl}} - nE_{\text{vac}}^{\text{bulk}}. \quad (8)$$

Here the potential energies describe the following system states:  $E_n^{\text{disl}}$ , for a system with a vacancy cluster at the dislocation;  $E_0^{\text{disl}}$ , for a system containing only dislocation and no vacancies. All energy values were determined following atomic relaxation. This characteristic corresponds to the energy required for vacancy clustering on the dislocation, referenced to isolated, noninteracting vacancies in the bulk. The negative sign of this energy indicates a tendency for vacancy segregation.

## 2. Dynamic simulations: Setup for high-temperature climb

Observing the dislocation climb in MD requires a proper choice of simulation parameters. Practically speaking, the simulation conditions should be chosen to match dislocation climb with spatial and temporal scales affordable by MD. As

TABLE II. Description of the simulation boxes used for static calculation of vacancy segregation energies: box side lengths  $L$  along specified  $x$ ,  $y$ ,  $z$  directions are in nm.  $N$  denotes the total number of atoms in a model (prior to introducing vacancies).

|                 | $x$                 | $y$                 | $z$           | $L_x$ | $L_y$ | $L_z$ | $N$    |
|-----------------|---------------------|---------------------|---------------|-------|-------|-------|--------|
| edge            | [110]               | $[\bar{1}\bar{1}1]$ | $[1\bar{1}2]$ | 14.9  | 18.2  | 4.7   | 117931 |
| edge (jog pair) | [110]               | $[\bar{1}\bar{1}1]$ | $[1\bar{1}2]$ | 14.9  | 18.2  | 4.7   | 117920 |
| $60^\circ$      | $[2\bar{1}\bar{1}]$ | [011]               | $[1\bar{1}1]$ | 12.4  | 5.0   | 17.8  | 101800 |
| $30^\circ$      | [121]               | $[\bar{1}01]$       | $[1\bar{1}1]$ | 4.7   | 14.0  | 17.2  | 104885 |

TABLE III. Description of the simulation boxes used for MD study of dislocation climb: box side lengths  $L$  along specified  $x$ ,  $y$ ,  $z$  directions are in nm.  $N$  is the total number of atoms in a model (prior to introducing vacancies).

|      | $x$           | $y$           | $z$           | $L_x$ | $L_y$ | $L_z$ | $N$    |
|------|---------------|---------------|---------------|-------|-------|-------|--------|
| edge | [110]         | $[\bar{1}11]$ | $[1\bar{1}2]$ | 30.4  | 37.2  | 9.7   | 946714 |
| 60°  | $[21\bar{1}]$ | [011]         | $[1\bar{1}1]$ | 26.0  | 10.2  | 36.2  | 827120 |
| 30°  | [121]         | $[\bar{1}01]$ | $[1\bar{1}1]$ | 9.7   | 29.1  | 35.6  | 867152 |

shown previously [24,25], increasing the vacancy concentration in a model is an efficient way to approach dislocation climb in atomistic simulations. In the absence of applied stresses, climb under vacancy supersaturation is driven by the osmotic force [29]. The latter is determined by the difference between the actual vacancy concentration  $c_{\text{vac}}$  and the equilibrium value  $c_{\text{vac}}^{\text{eq}}$ . The other important factor influencing the climb probability is vacancy diffusion. As discussed in Sec. II B, the diffusion coefficient  $D_{\text{vac}}$  increases exponentially with temperature. In light of this, high-temperature climb is well suited for direct atomistic simulations with appropriately chosen  $T$  and  $c_{\text{vac}}$ .

Sizes of the simulation cells used for dynamic simulations are given in Table III. The time lengths affordable for MD with models containing  $N \sim 10^7$  atoms were of the order of 10 ns. From preliminary tests, we determined the following conditions for Ni:  $T \geq 0.84T_m$  and  $c_{\text{vac}}/c_{\text{vac}}^{\text{eq}} \sim 10^3$ . In absolute values, it gives the simulation temperature  $T \geq 1300$  K and the actual vacancy concentration  $c_{\text{vac}} \sim (1-5) \times 10^{-3}$ . A fraction of  $N$  atoms in the simulation boxes were deleted to create given vacancy concentration. Since we did not consider specific stress-related driving forces, the simulation boxes containing dislocations and vacancies were mechanically equilibrated at  $T = 1300$  K with the *NPT* ensemble to maintain zero pressure in a system. Based on the geometry of the simulation cell, the dislocation density  $\rho$  was approximately  $2 \times 10^{15} \text{ m}^{-2}$ .

### 3. Detection of vacancy position at high temperatures

Our main goal was to observe the atomistic mechanisms of climb. Hence, tracing the exact positions of dislocations and vacancies during the MD simulations was of importance. For dislocations, the positions were determined with the help of the common neighbor analysis (CNA) and dislocation analysis methods [48] implemented in OVITO [49]. Using CNA, we kept track of the atoms in hcp ordering belonging to the SF region. The dislocation extraction algorithm (DXA) located the partial dislocation lines, as shown in Fig. 1. For vacancies, the detection of the exact positions was not that straightforward because of thermal fluctuations of atoms.

To overcome the problem of thermal noise, we traced the positions of the vacant sites with the help of a descriptor combining time-averaged atomic characteristics. Namely, values of atomic potential energy  $E_{\text{at}}$ , centrosymmetry (CS) parameter [50], and the CNA pattern for each atom in the model were calculated and averaged over time periods equal to 2000 MD steps (every 20 steps, in total 100 values). For the given interatomic potential [36], vacancy neighbor was characterized

by average energy  $E_{\text{at}}$  larger than  $-4.19$  eV,  $\text{CS} > 4.25$ , and  $\text{CNA} < 11.5$ . Based on these conditions, atoms surrounding the vacant sites were detected and visualized. Such filtering recognizes vacancies in hcp and fcc lattices and is also suitable for distinction of vacancy clusters. Examples of defect configurations detected in the MD simulations are shown in the next sections.

### 4. Dislocation climb velocity

To provide atomistically informed insights into the climb process in Ni, we calculated  $v_{\text{cl}}$  for the simulated dislocations. In the MD simulations, the dislocations climb under vacancy supersaturation is driven by the osmotic force. To study the dependence of the climb rate on  $c_{\text{vac}}$ , the MD setup was varied. Dislocation mobility due to climb was quantitatively characterized in terms of *instantaneous* climb velocities  $v_{\text{cl}}^{\text{MD}}$ :

$$v_{\text{cl}}^{\text{MD}} = d_{\text{cl}}/t_{\text{cl}}. \quad (9)$$

The value of  $v_{\text{cl}}^{\text{MD}}$  associated with a complete climb event was defined as the distance climbed by the dislocation  $d_{\text{cl}}$  divided by the simulation time  $t_{\text{cl}}$ . In other words, during the interval  $t_{\text{cl}}$ , the dissociated dislocation undergoes a complete transition between parallel {111} planes, recovering its jogless configuration. Subsequent vacancy absorption by the dislocation modifies the local environment. Specifically, a complete climb event changes the total vacancy concentration  $c_{\text{vac}}$  in the simulation box by 2–5 %, but the vacancy distribution around the dislocation can no longer be considered fully uniform. Thus, the MD simulation results are primarily associated with the first regime of dislocation climb under vacancy supersaturation conditions; that is, they are more consistent with Eq. (1) than with Eq. (2).

Another aspect worth mentioning is that climb may be governed by the nucleation and migration of different jog configurations, such as unit jogs or larger superjogs. This leads to intricate variations in the intermediate jogged states. As Geers *et al.* [30] demonstrated, dislocations of the same character but opposite sign are expected to climb with the same velocity. We used this fact to improve statistics by averaging over the estimated velocity  $v_{\text{cl}}^{\text{MD}}$  of two dislocations in the dipole.

## III. SIMULATION RESULTS

### A. Vacancy diffusion in bulk Ni

Vacancy diffusion coefficients calculated with Eq. (5) are plotted in Fig. 2. We also provided an analytic approximation of  $D_{\text{vac}}(T)$  with  $E_{\text{vac}}^{\text{m}} = 0.98$  eV estimated for Ni in static calculations [36]. The preexponential factor  $D_0 = (2.4 \pm 0.3) \times 10^{-6} \text{ m}^2/\text{s}$  was obtained by fitting the calculated  $D_{\text{vac}}(T)$  with the Arrhenius equation.

Combining  $c_{\text{vac}}^{\text{eq}}$  calculated with Eq. (6) and  $D_{\text{vac}}$  plotted in Fig. 2, we obtained the self-diffusion coefficient. The results are shown in Fig. 3. For more evident comparison with the experimental data, we present  $D_{\text{self}}$  in correlation with the reciprocal homologous temperature  $T_m/T$ . The values of  $T_m$  for experiments and simulations are summarized in Table I. The slope of the self-diffusion coefficients based on atomistic simulations of single vacancy diffusion agrees with reported experimental data [51–54]. The absolute values of the calcu-

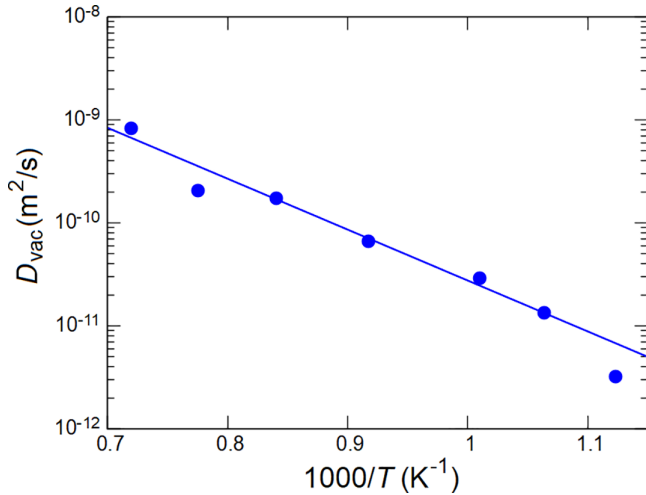


FIG. 2. Vacancy diffusion coefficient  $D_{\text{vac}}$  in fcc Ni (plotted against reciprocal temperature). Points—results of MD simulations at given  $T$ . Line—approximation with Arrhenius equation from this work (shown for  $D_0 = 2.4 \times 10^{-6} \text{ m}^2/\text{s}$ ).

lated  $D_{\text{self}}$  are also close to the experimental measurements. Based on the simulation results shown in Figs. 2 and 3, we can conclude that the interatomic potential of Du *et al.* [36] provides reasonable behavior of a vacancy in fcc Ni and produces the correct range of self-diffusion coefficients.

### B. Vacancy segregation at dislocations

In Fig. 4 we show how  $E_{\text{seg}}^i$  is distributed along the atomic sites at or near the straight dislocation cores. The values of  $E_{\text{seg}}^i$  were calculated with Eq. (7) for different dislocation orientations. Atomistic structures of the dislocations colored according to the CNA are shown in Fig. 4. As shown in Fig. 4, straight dislocations provide for a pronounced segregation of vacancies. For the partial cores belonging to the edge dislocation,

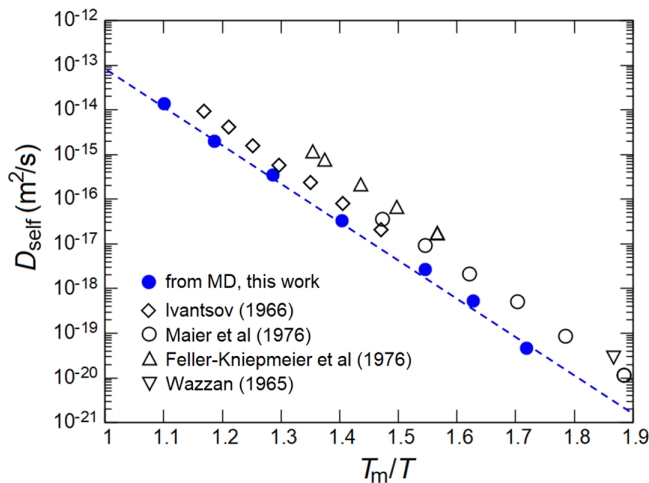


FIG. 3. Self-diffusion coefficient in fcc Ni (plotted against reciprocal homologous temperature). Filled symbols—results from this work. Empty symbols show experimental data from different sources: [51–54]. The dashed line is to guide the eye.

tion, vacancy segregation profiles are identical. For the mixed dislocations we observed an asymmetric distribution of  $E_{\text{seg}}^i$ , which may lead to a preferential arrangement of vacancies at one of the partial dislocation cores. From Fig. 4, vacancy segregation at the mixed dislocations relates to the edge character of the partial dislocations. Dislocation core with a larger edge Burgers vector component appears more preferential for vacancy segregation.

Numerically, the minimum values of  $E_{\text{seg}}^i$  for edge and  $30^\circ$  mixed dislocations are approximately  $-0.4 \text{ eV}$ . In the case of the  $60^\circ$  mixed dislocation, a slightly lower minimum of  $-0.45 \text{ eV}$  was observed at the partial with more pronounced edge character. Based on the calculated values of  $E_{\text{seg}}^i$ , vacancy segregation remains energetically favorable at elevated temperatures, potentially driving high-temperature climb. Consequently, jog formation may be triggered by the localized accumulation of vacancies starting at the partial dislocations. On this point we agree with a description proposed by Abu-Odeh *et al.* [17] based on static simulations of vacancy clustering at initially straight edge dislocations in Cu and Al.

In addition to straight dislocation, we studied segregation of a vacancy at an edge dislocation with unit-jogs. The structure of the jog-pair after relaxation is given in Fig. 5. The configuration includes one narrow and one expanded jog, in agreement with dislocation theory and profiles obtained previously in atomistic modeling [16–18]. In Fig. 5, we see significant segregation sites attributed to the jogs. At these specific sites, the values of  $E_{\text{seg}}$  may reach about  $-1.5 \text{ eV}$ . This value is similar to vacancy formation energy in Ni; see Table I. Hence, jogs act as prominent vacancy sinks promoting further attraction of vacancies and evolution of jogged dislocation. This observation agrees with a conclusion made by Baker and Curtin, based on atomistic simulation of jog formation in Al; see [16]. In addition to the discussion given in [16], we show that straight dislocation segments also noticeably contribute to vacancy segregation.

Based on the results for the edge dislocation plotted in Figs. 4 and 5, the values of  $E_{\text{seg}}$  at straight segments of dislocations do not depend noticeably on the presence of jog. For an edge dislocation, the minimum segregation energy  $E_{\text{seg}}$  is  $-0.36 \text{ eV}$  for a straight partial dislocation without jogs, and  $-0.4 \text{ eV}$  for a dislocation segment between jogs. Such result aligns with a conclusion made previously by Fey *et al.* [18]. That work has studied the interaction between a single vacancy and straight (or jogged) edge dislocation in Ni. According to simulations [18] performed with another interatomic potential [55], the energy describing the interaction of a vacancy with a straight segment of partial dislocation is irrelevant to the presence of jog.

For the vacancy clusters, the formation energy is plotted in Fig. 6. Here we compare the results obtained for tubes of 1T, 2T, and 3T types containing up to 12 vacancies. For clarification of cluster geometry and related classification, see the explanation in Sec. II C and illustrations in Fig. 6. The snapshots illustrate tube configurations after atomic relaxation. Negative values of  $E_{\text{T}}^f$  confirm the tendency for vacancy clustering at the dissociated dislocation. For relatively small clusters containing  $n < 4$  vacancies, the 1T configuration is preferable. With further increase in a cluster size,  $E_{\text{T}}^f(n)$  for 2T becomes lower than that for 1T, making the for-

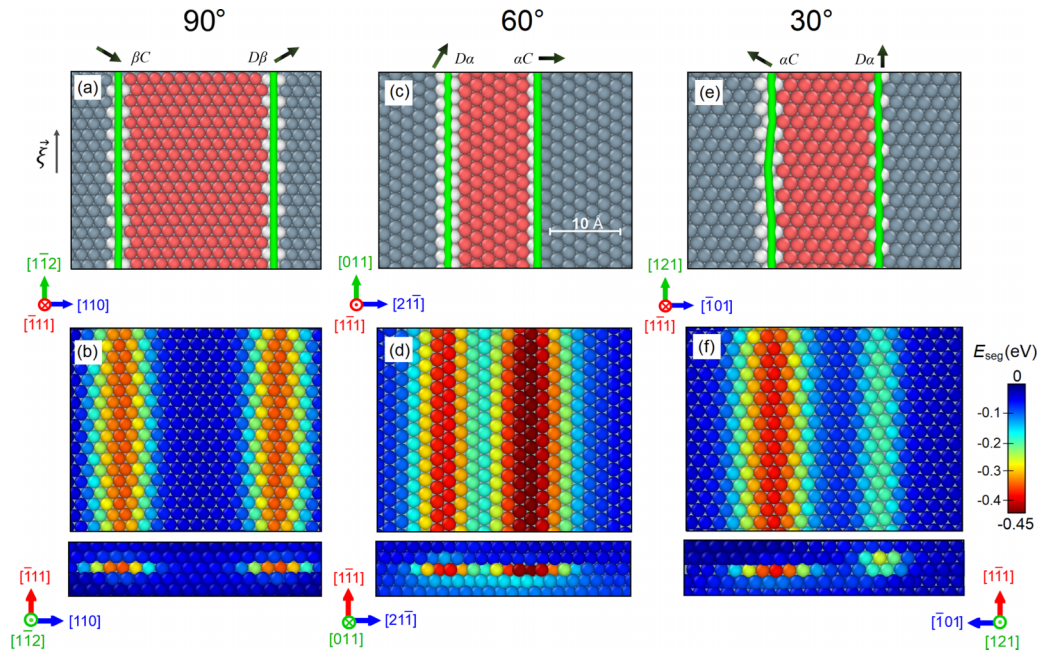


FIG. 4. Dislocation configurations (top row) and distribution of vacancy segregation energies for the straight edge and mixed dislocations. Results of static calculations at  $P = 0$  and  $T = 0$ . For the structure snapshots (a), (c), (e) atoms are colored according to CNA [49]: red—hcp lattice (SF), gray—fcc lattice, white—other symmetry (defects). Snapshots (b), (d), (f) show segregation energies  $E_{\text{seg}}$  calculated at each atomic site in the top view and viewed along the dislocation line direction (the bottom row of snapshots). The planes depicted in views (b), (d), (f) correspond to the middle of the lower snapshots. Dislocation description is given in Thompson tetrahedron notation [46], viewed from outside the Thompson tetrahedron.

mation of the 2T cluster energetically favorable. From the hierarchy of tube formation energies, the 3T clusters are the least stable.

A detailed discussion of the dislocation evolution upon interaction with multiple vacancies is given in the following subsection, which is focused on dynamic simulations of climb in Ni.

### C. Observation of dislocation climb

We directly simulated the high-temperature evolution of dissociated dislocations in the presence of diffusing vacancies, treating the simulation as a numerical experiment. Using the dynamic setup described in Sec. II, we examined the fundamental mechanisms of dislocation climb with respect to thermal effects. Considered dislocation types and the model dimensions are summarized in Table III. Specifically, all dislocations utilized for these dynamic simulations had a length of  $\sim 10$  nm. This subsection highlights several key features characterizing the climb process at finite temperatures, specifically focusing on atomistic insights gained from MD.

#### 1. Edge dislocation

Figure 7 shows the evolution of edge dislocation due to the interaction with diffusing vacancies. For efficient visualization, the depicted area is limited to 1.5 nm width in the  $[\bar{1}11]$  direction. The snapshots are taken from the MD simulation at  $T = 1300$  K, equal to  $0.85T_m$  for Ni. At this high temperature, the partial dislocation lines fluctuate and the entire dislocation can move within its glide plane without externally applied shear stress. For an additional visualization of the

dynamic simulation of edge dislocation climb, the reader is referred to Supplemental movie 1 provided in the Supplemental Material [56].

In Fig. 7(a) one can see positions of partial dislocations and vacancies shortly after the start of simulations. Despite high temperatures and the dislocation fluctuations, vacancies segregate at the partial dislocations. This observation agrees with the calculated segregation energies, cf. Fig. 4. As segregation [as seen in Fig. 7(a)] proceeds, vacancies gather into the tubes oriented along the  $\langle 110 \rangle$  directions. Snapshots (b) and (c) in Fig. 7 show the formation of 2T tubes. Once formed, vacancy tubes remain immobile and grow in the closed-packed direction. As observed in the simulations, the occurrence of vacancy tubes typically correlates with the appearance of a stacking fault and a partial dislocation (having the same Burgers vector as the original) lying in a parallel  $(\bar{1}11)$  plane, distinct from the original dislocation glide plane. Such configuration is seen for example in Figs. 7(b) and 7(c), where segments of the SF colored in green (“outside” the vacancy clusters) are two layers above the initial SF position (colored in blue).

Figure 7(c) further explains how a strong directional growth of the vacancy clusters leads to their interconnection. Once the vacancy tubes intersect, a jog is formed at the point of intersection. According to the DXA, dislocation loops with  $\pm\beta A$  (Burgers vector along the original line direction, in the glide plane) can be observed at the vacancy tubes. The retraction of the  $\wedge$ -shaped structure formed by two interacting vacancy tubes—visible in panel Fig. 7(d)—corresponds to the motion of a  $\beta A$  prismatic loop between the left and right partial dislocation. Detailed views of the dislocation structure

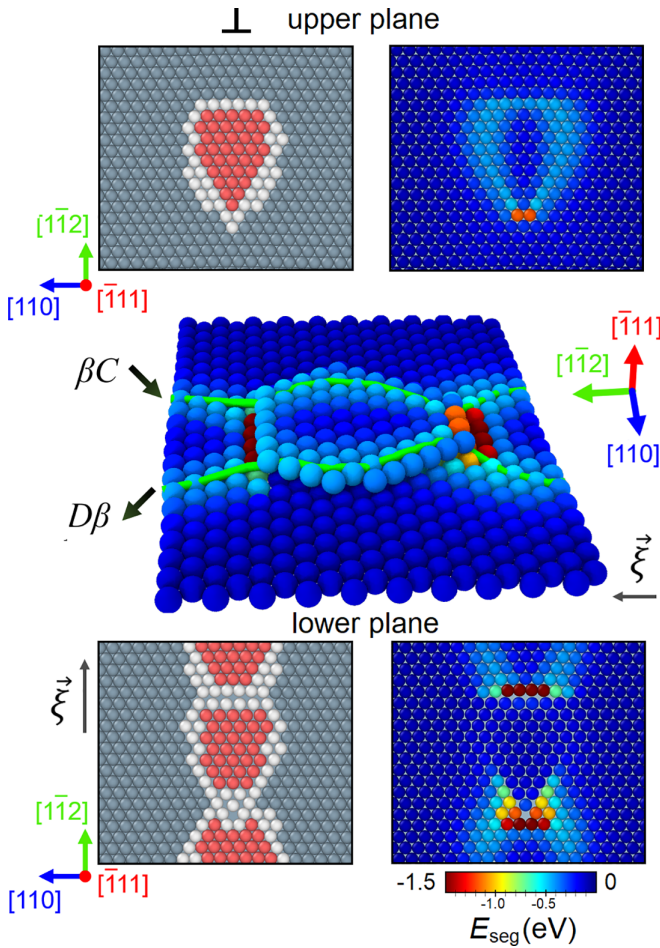


FIG. 5. Vacancy segregation energies  $E_{\text{seg}}$  at jogged edge dislocation, calculations for  $P = 0$  and  $T = 0$ . The panels show structure of atomic planes and corresponding values of  $E_{\text{seg}}$ . For the structure snapshots: atoms belonging to the SF (hcp) are in red, fcc lattice—gray, other symmetry (defects)—white. Dislocation description is in Thompson tetrahedron notation [46].

at this stage are provided in the inset of Fig. 7(d), where partial dislocations and the prismatic loop are color-coded and labeled with their respective Burgers vectors. Once the vacancy tubes have fully retracted, the other part of the jog pair is formed. With absorption of vacancies accumulated in the vacancy tubes and formation of a jog-pair, the dislocation evolves into the intermediate jogged configuration. This stage of the climb is shown in Fig. 7(e).

After formation of the jog pair, dislocation evolution is governed by the following vacancy segregation at the created jogs, as well as at the other dislocation segments. Segregation of vacancies at the jogged dislocation changes the jog positions along the dislocation line and promotes the dislocation climb. Practically continuing absorption of vacancies can lead to motion of existing jogs and growth of new jog-pairs. Figure 7(f) shows a situation where dislocation lines are located in three different atomic planes connected by jog pairs. The following stages of dislocation climb are shown in Fig. 7, panels (g) and (h).

A three-dimensional representation of the dislocation structures characterizing the climb process is provided in

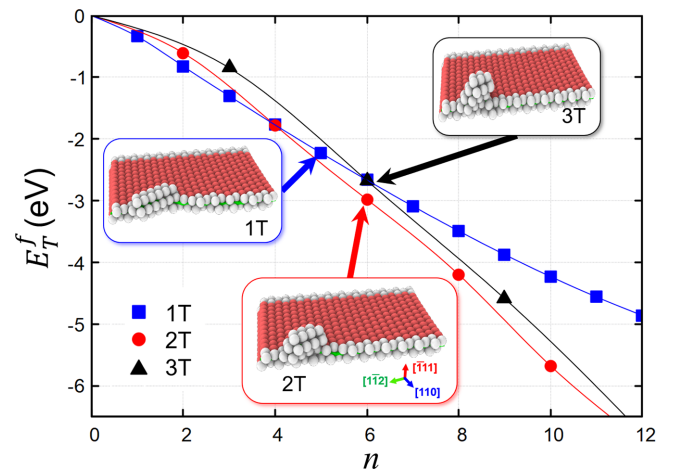


FIG. 6. Formation energy for vacancy tubes at split edge dislocation. The tubes contain  $n$  vacancies and are arranged along the close-packed  $\langle 110 \rangle$  direction with different height in the  $\bar{1}11$  direction: 1T—a line of single vacancies, 2T and 3T—tubes formed by double and triple rows of vacancies, respectively. For the atomistic snapshots: red atoms—hcp, white atoms—surrounding defects (vacant sites and dislocation lines). The configurations are shown after energy minimization.

Fig. 8, depicting edge dislocation configurations after energy minimization. Specifically, the snapshots illustrate the positions of partial dislocations and attributed SF regions, which are situated in parallel  $\bar{1}11$  planes. Detailed examples of vacancy clusters observed at high temperatures are shown in the left column. The character of vacancy clustering is consistent for different  $c_{\text{vac}}$ . We can also observe single vacancies segregating to the dislocations at various time intervals. Following the classification of vacancy tubes introduced in this work, the clusters shown for Ni in Figs. 8 and 7(b) are identified as 2T type. Estimates for the observed amount of vacancies accumulated in a single stable tube are in the range from 10 to 20. As demonstrated, in the process of vacancy-driven climb, the edge dislocation can evolve with formation of different jog-pair combinations. The latter includes unit jogs and super-jogs. Examples of super-jog are seen in Fig. 8 for the cases of  $c_{\text{vac}} = 2 \times 10^{-3}$  and  $4 \times 10^{-3}$ . Coexistence of two unit jogs and one super-jog can be seen for a dislocation at  $c_{\text{vac}} = 3 \times 10^{-3}$ .

According to Fig. 7 we consider the transition from stage (a) to stage (h) taking 2.86 ns as a complete dislocation climb event. As the MD simulation continues, the next climb event goes through similar stages. The only difference is in the time required, since the area around the dislocations is depleted of vacancies after their annihilation during the first act of dislocation climb [as seen in Fig. 7, cf. panels (a) and (h)]. Therefore, further accumulation of vacancies at the partials requires a preliminary diffusion of vacancies from the bulk to the dislocation region. The evolution of the other edge dislocation within the dipole follows the same process.

## 2. 60° mixed dislocation

The evolution of 60° mixed dislocations due to the vacancy-driven climb is illustrated in Fig. 9. Here we discuss

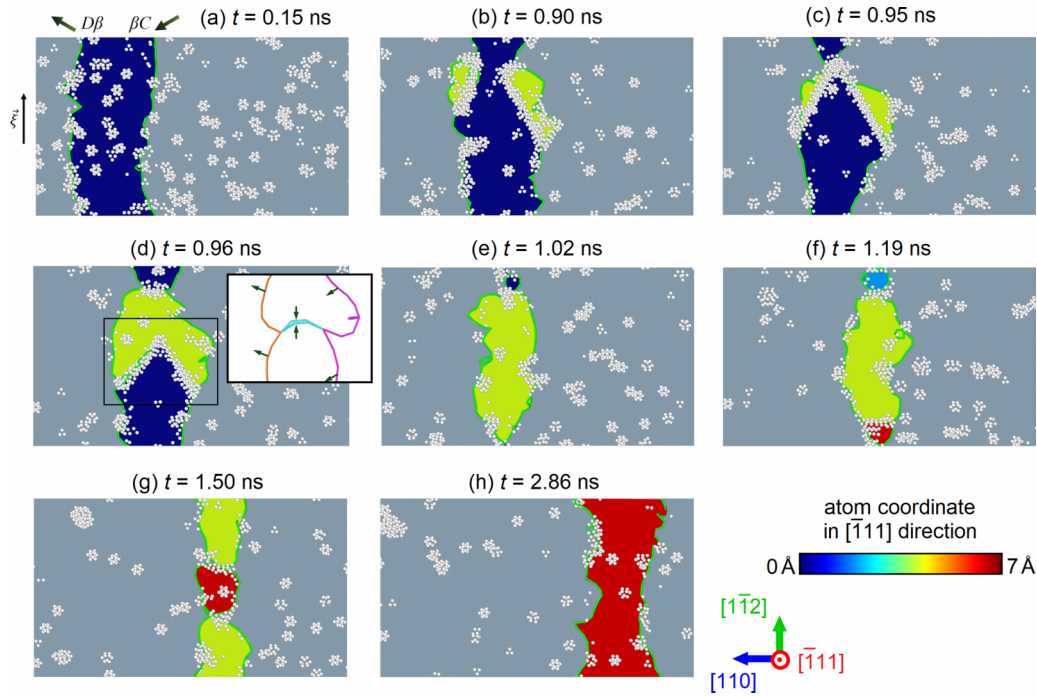


FIG. 7. Evolution of edge dislocation in Ni due to interaction with diffusing vacancies: observation from MD at  $T = 1300$  K,  $c_{\text{vac}} = 4 \times 10^{-3}$ . Climb of a dislocation with a length of 9.7 nm proceeds in the  $\bar{1}\bar{1}1$  direction, advancing toward the viewer. The stacking faults are color-coded according to the related atomic coordinates in climb direction (see legend). The top row of panels shows the stages of vacancy segregation at dislocation and their clustering along  $\langle 110 \rangle$  direction (into the *vacancy tubes*). Contact of the two vacancy tubes (c) initiates formation of a first jog pair (i.e., super-jogs) on the edge dislocation [panels (d), (e)]. An inset in panel (d) shows in detail fragments of the partial dislocation lines and a formed dislocation loop, with Burgers vectors. Panel (f) shows how the dislocation configuration develops after subsequent formation of pairs of unit jogs. The bottom panels depict the intermediate stages of the jogged dislocation (g) until it realigns into a different atomic ( $\bar{1}\bar{1}1$ ) plane via climb (h). Only atoms belonging to the vacancy surroundings are depicted explicitly (in white). Green lines indicate partial dislocations. Gray color is for parts of the simulation box with fcc lattice.

the MD simulation performed at  $T = 1300$  K for initial vacancy concentration  $c_{\text{vac}} = 4 \times 10^{-3}$ . In the snapshots Figs. 9(a)–9(c) we observe stages of vacancy segregation and clustering at the dislocation. Fluctuations in the partial dislocation lines are visible, reflecting thermal noise at finite temperature. Supplemental movie 2 provides an animation of the dynamic simulation of  $60^\circ$  mixed dislocation climb, see the Supplemental Material [56].

For the  $D\alpha$  partial dislocation, we observed vacancy clustering; however, these clusters do not form stable vacancy tubes. This stands in clear contrast to the other partial,  $\alpha C$ , which has pure edge character. At  $\alpha C$ , distinctive vacancy tubes are visible, as illustrated in Figs. 9(b) and 9(c). In the snapshot shown in Fig. 9(b), we identify a vacancy cluster of the 1T type. At a later stage, the dislocation evolves into a configuration with a more stable 2T-type vacancy tube, as illustrated in Fig. 9(c). The tubes are oriented along the close-packed lattice direction coinciding with the  $[011]$  dislocation line direction. Similarly to the observations made from the simulations of edge dislocation in Sec. III C 1, the occurrence of vacancy tubes correlates with the appearance of a stacking fault and a partial dislocation (having the same Burgers vector as the original) lying in a parallel ( $\bar{1}\bar{1}1$ ) plane, distinct from the original dislocation glide plane. Such peculiarity is seen in the Figs. 9(b)–9(d), where the SF regions corresponding to a new glide plane are shown in yellow and red, compared to the initial position of the SF (in blue).

The stage preceding a jog-pair formation is shown in a snapshot Fig. 9(d). Here we see how the left partial dislocation  $D\alpha$  interacts with the vacancy tube, leading to the absorption of vacancy cluster and the formation of a super-jog pair, Fig. 9(e). In the panel Fig. 9(d) we observe mixed dislocation realigned after it climbed two atomic layers relative to the initial ( $\bar{1}\bar{1}1$ ) plane. The second dislocation of the dislocation dipole shows the same characteristic processes.

### 3. $30^\circ$ mixed dislocation

Climb process observed in MD for  $30^\circ$  mixed dislocation is shown in Fig. 9. Compared to the observations made from simulations of edge and  $60^\circ$  dislocations, the climb of the  $30^\circ$  dislocation proceeds much faster. Figure 10 illustrates results for a calculation performed at  $c_{\text{vac}} = 2.5 \times 10^{-3}$ . The full climb for  $30^\circ$  mixed dislocation for this  $c_{\text{vac}}$  and  $T = 1300$  K took about 0.86 ns. An animation of the dynamic simulation of  $30^\circ$  mixed dislocation climb is provided in Supplemental movie 3; see the Supplemental Material [56].

In agreement with the analytical expression for the splitting distance [1], the partial dislocations are more closely spaced than in the case of the edge and  $60^\circ$  dislocations (cf. Figs. 7 and 10). In the snapshot Fig. 10(a) we show initial stages of the dislocation-vacancy interactions, with partial dislocations exhibiting visible thermal fluctuations. Figure 10(b) illustrates the character of vacancy clustering. In contrast with the other

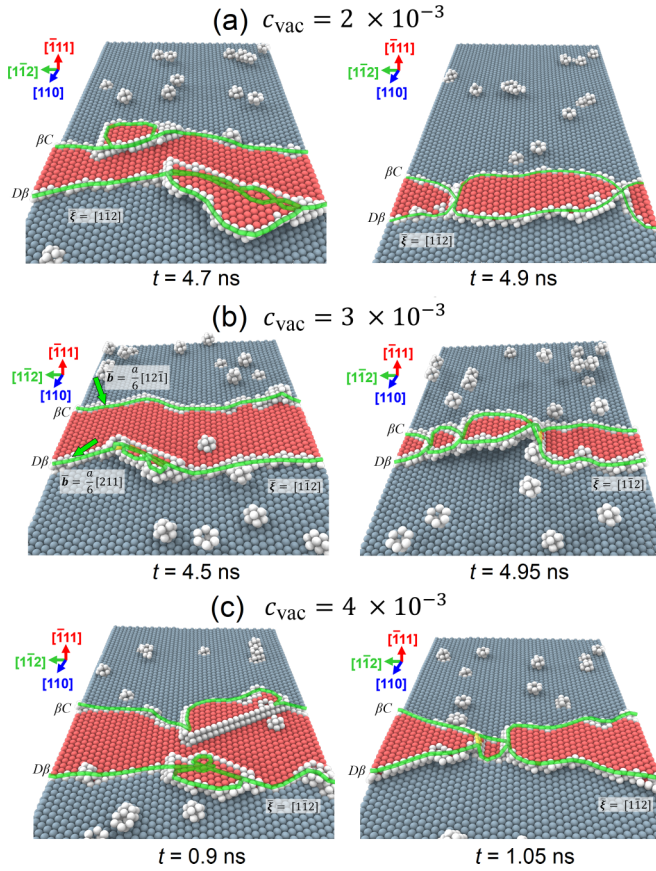


FIG. 8. Stages of jog-pair formation at edge dislocation in Ni for different vacancy concentration  $c_{\text{vac}}$ . Dislocation length equals 9.7 nm. The snapshots on the left show linear vacancy clusters growing at partial dislocations. The images on the right show the dislocations after the formation of jog pairs. Green lines indicate Shockley partial dislocation lines as identified by DXA; short yellow segments at the jogs are identified as  $\frac{1}{3}\langle 100 \rangle$  Hirth dislocations. Gray atoms—fcc lattice, red—hcp (stacking fault), and white are the surroundings of vacant sites. The models are shown after energy minimization to reduce thermal noise.

cases considered above, no clear  $\langle 110 \rangle$  oriented vacancy tubes were detected in the simulations. The constriction of the dissociated  $30^\circ$  dislocation, as seen in Fig. 10(c), precedes the formation of a jog pair. The latter is clearly visible in Fig. 10(d). Here, we observe a case of super-jogs with a height of two atomic planes. Figure 10(d) illustrates the growth of this super-jog, accompanied by the formation of an additional unit-jog pair.

#### D. Rate of dislocation climb

A summary of instantaneous climb velocities  $v_{\text{cl}}^{\text{MD}}$  obtained from the dynamic simulations is plotted in Fig. 11. These velocities characterize the first full dislocation climb event, as discussed in Sec. II C 4 explaining methodology. The values of  $v_{\text{cl}}^{\text{MD}}$  shown in Fig. 11 represent an average over two dislocations in the given dipole configuration. The symbols show the values of  $v_{\text{cl}}^{\text{MD}}$  obtained with Eq. (9). For dislocations forming a dipole, the observed difference in velocity was about 0.01 m/s.

TABLE IV. Parameters describing dislocation climb observed in MD at  $T = 1300$  K; for comments, see Eq. (3).

| Climb parameters                           | Values based on MD     |
|--------------------------------------------|------------------------|
| $D_{\text{vac}}$ ( $\text{m}^2/\text{s}$ ) | $3.8 \times 10^{-10}$  |
| $c_{\text{vac}}$                           | $(1-6) \times 10^{-3}$ |
| $b$ (nm)                                   | 0.253                  |
| $\eta$                                     | 32.0                   |

For the edge dislocation, we investigated the sensitivity of  $v_{\text{cl}}^{\text{MD}}$  to the simulated dislocation length. Specifically, two simulation box widths were tested: the original  $L_y \sim 10$  nm (as specified in Table III) and a reduced width of  $0.5L_y$ , while  $L_x$  and  $L_z$  remained constant. As shown in Fig. 11, within the range of model sizes considered, the climb rate appears to be independent of the dislocation length.

In addition to the direct MD simulation results, Fig. 11 presents the analytical dependence of  $v_{\text{cl}}^{\text{MD}}$  on  $c_{\text{vac}}$  based on Eq. (3). The simulated case is well suited for the application of this equation, since  $c_{\text{vac}}^{\text{eq}} \approx 6.0 \times 10^{-6}$  estimated with Eq. (6) for  $T = 1300$  K is several orders of magnitude lower than  $c_{\text{vac}}$ . Table IV summarizes the numerical values for all parameters relevant to Eq. (3) at  $T = 1300$  K. The value of  $D_{\text{vac}}$  was calculated for a dislocation-free Ni single crystal. Details are provided in the first part of our work devoted to validating the interatomic potential. The only unknown parameter in Eq. (3) is the factor  $\eta$  that accounts among others for the geometry of the flux field. Fits to the edge dislocation climb velocity results provide  $\eta = 32.0$ . This value exceeds the value of 8 in Eq. (1), which is commonly used in analytical description of the initial stage of climb under vacancy supersaturation. Thus, dislocation climb is a factor of four faster than predicted for the assumptions behind Eq. (1). Kabir *et al.* [24] already noticed that vacancy diffusivity near dislocation cores in bcc Fe exceeds that in regions unaffected by the core, due to a reduction in migration barriers in the vicinity of the dislocation. Similarly, Burke and Nix [57] also showed that the elastic interaction between the vacancy and dislocations can lead to an increase in the climb velocity by 30%. Other factors that may contribute to the high value of  $\eta$  include the discrete nature of the crystal lattice, pipe diffusion, and temperature-induced fluctuations in the dislocation position, which could increase the rate of capture of vacancies.

The set of parameters summarized in Table IV can also adequately describe the velocities of the mixed dislocations. As Fig. 11 shows, the velocities estimated for  $30^\circ$  and  $60^\circ$  mixed dislocations using Eq. (3) with parameters from Table IV agree with the directly calculated  $v_{\text{cl}}^{\text{MD}}$ . In general, we see that for Ni the values of  $v_{\text{cl}}^{\text{MD}}$  estimated for different dislocation orientations are comparable:  $\sim 10^{-1}$  m/s for the tested vacancy concentration range,  $c_{\text{vac}} \sim 10^{-3}$ . Based on a detailed comparison of the considered dislocations, we establish the hierarchy of climb velocity depending on  $\theta$ : the  $30^\circ$  mixed dislocation shows the fastest climb, followed by the  $60^\circ$  and edge dislocation. The parametrization of Eq. (3) reflects an interest in bridging atomistic insights with analytical models [58] following the discussion reported by Clouet [59] and the implementation of kMC data for description of dislocation climb in Fe [24]. However, care must be taken to

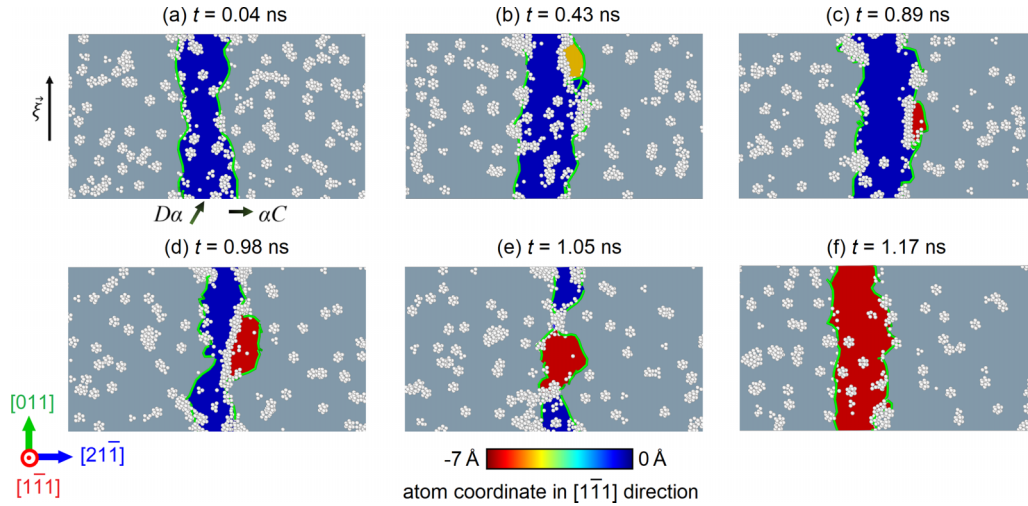


FIG. 9. Evolution of  $60^\circ$  mixed dislocation due to interaction with diffusing vacancies: observation from MD at  $T = 1300$  K,  $c_{\text{vac}} = 4 \times 10^{-3}$ . Dislocation climb proceeds in the negative  $[1\bar{1}1]$  direction, moving away from the viewer into the plane of the image. The stacking faults are color-coded according to the related atomic coordinates (see legend). The top row of panels shows the stages of vacancy segregation (a) and clustering (b), (c) at partial dislocations. For  $\alpha C$  partial dislocation we observe the formation of different vacancy tube configurations: 1T (b) or 2T (c) coaligning with the  $[011]$  dislocation line direction. The bottom row depicts interaction between the 2T vacancy cluster and  $D\alpha$  partial (d) followed by formation of a superjog-pair (e). The last panel (f) shows the mixed dislocation realigned after it climbed two atomic layers relative to the original  $(1\bar{1}1)$  plane. Only atoms surrounding the vacancies are shown (in white). Dislocation lines are depicted in green. The atoms belonging to fcc or hcp lattices are not visualized. Dislocation description is given in Thompson tetrahedron notation [46], viewed from inside the Thompson tetrahedron.

apply values for climb velocities and mobilities in mesoscale models only to exactly the same situation from which they were obtained (in our case, this corresponds to the initial climb rate in Ni strongly supersaturated with vacancies at very high temperatures). Experimental conditions can deviate strongly from such idealized cases, e.g., by having curved dislocations and different dislocation densities.

The melting temperature predicted by the interatomic potential should also be taken into account when interpreting the climb kinetics. The simulation temperature of 1300 K corresponds to approximately  $0.85T_m$  for the model, whereas the same absolute temperature corresponds to a lower homologous temperature in experimental Ni. At the same time, Fig. 3 shows that the temperature dependence of the calculated

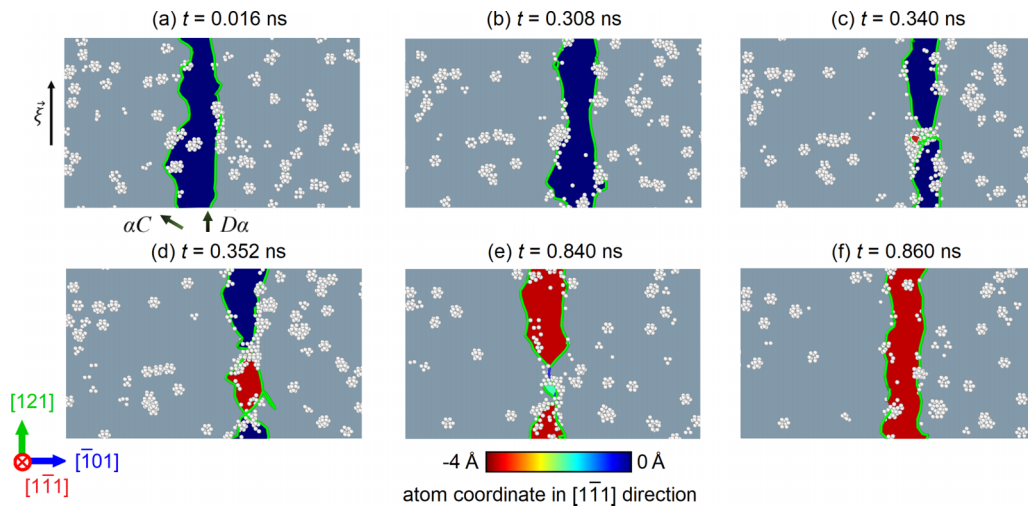


FIG. 10. Evolution of  $30^\circ$  mixed dislocation due to interaction with diffusing vacancies: at  $T = 1300$  K,  $c_{\text{vac}} = 2.5 \times 10^{-3}$ . Dislocation climb proceeds in the  $[1\bar{1}1]$  direction, moving towards the viewer into the plane of the image. The SF for different atomic planes containing dislocation are color-coded by related atomic coordinates in the  $[1\bar{1}1]$  direction, see the legend. The top row of panels shows vacancy segregation at partial dislocations [cf. panels (a), (b)] and the initial stage of jog-pair formation (c). The row below depicts the progression of a partially climbed dislocation in different atomic planes (d), (e), which leads to a full dislocation climb (f). Only atoms surrounding the vacancies are shown (in white). Dislocation lines are depicted in green. Note the different range of atomic coordinates in  $[1\bar{1}1]$  direction compared to Figs. 7 and 10.

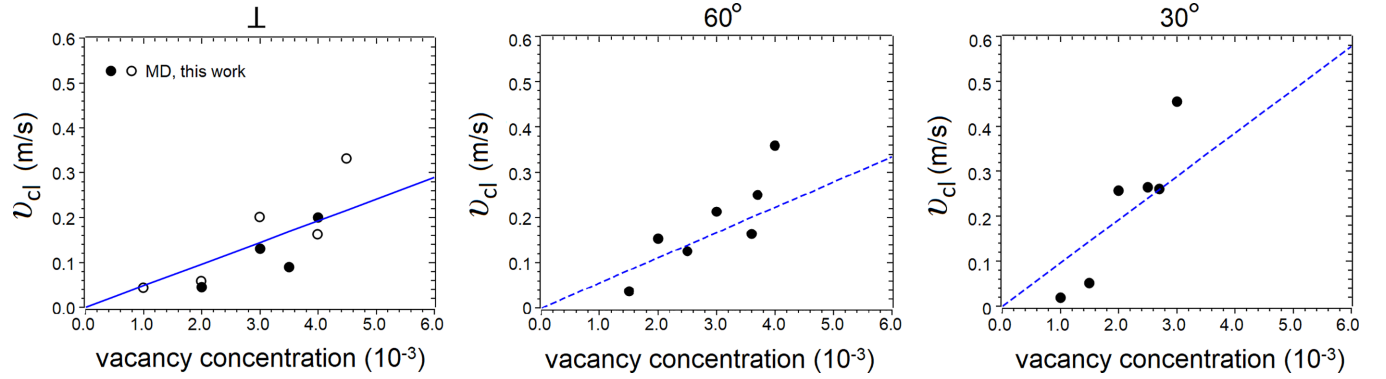


FIG. 11. Climb velocities estimated in this work for different types of dislocations. Symbols—instantaneous velocities obtained directly from MD models with different dislocation lengths:  $\circ$ , 5 nm;  $\bullet$ , 10 nm. Solid line—analytical estimation obtained with Eq. (3) based on parameters extracted from MD and a fitted  $\eta$ , as given in Table IV. Dashed lines—analytical estimation made for the mixed dislocations respecting dislocation orientation via  $\sin(\theta)$ , see Eq. (3).

self-diffusion coefficient agrees well with the experimental data when expressed as a function of homologous temperature. Therefore, the climb velocities reported here should be interpreted as model-scale values representative of Ni at high homologous temperature, rather than as direct quantitative predictions for experimental Ni at the same absolute temperature.

#### IV. DISCUSSIONS

##### A. Vacancy-related aspects of climb

Summarizing the MD results for dissociated dislocations, vacancy-driven climb proceeds through multiple stages associated with jog-pair formation. The subsequent evolution of the jogged dislocation promotes rearrangement of the dissociated dislocation in a parallel glide plane (i.e., climb). Our results show that climb for dissociated dislocations in fcc metals is a collective process involving vacancy clusters or dislocation loops. This differs from the case of the bcc lattice, where climb is primarily driven by the interaction of dislocations with single vacancies [59].

From the considered examples of edge and mixed dislocations, we see that accumulation of vacancies at partial dislocations serves as the first step of jog-pair creation. Vacancy segregation patterns can be dislocation-specific, as supported by dynamic simulations and segregation energies  $E_{seg}^i$  computed from the static relaxation. For edge dislocations, we found that both partial dislocations can equally absorb vacancies. For the mixed dislocations, we show that segregation profiles are asymmetric, leading to preferential absorption of vacancies at one of the partials.

As seen in the simulations, the accumulation of vacancies at dislocations promotes local growth of vacancy clusters. Specifically, stable vacancy clusters oriented along the close-packed lattice direction  $\langle 110 \rangle$  can be observed. Spatial configurations of such defects probably range from 1T to 2T, depending on cluster size. The occurrence of vacancy tubes typically correlates with the appearance of a stacking fault and a partial dislocation (having the same Burgers vector as the original) lying in a parallel  $\langle \bar{1}11 \rangle$  plane, distinct from the original dislocation glide plane. In the case of edge dislocation, vacancy tubes are oriented towards each

other, following the lattice symmetry. For  $60^\circ$  mixed dislocation growth of vacancy tubes is aligned with the dislocation line direction (coinciding with  $\langle 110 \rangle$ ). In accordance with the asymmetric pattern seen from  $E_{seg}^i$  calculated for this dislocation orientation, the vacancy tubes are observed at the partial having edge character. Nevertheless, less ordered (and probably less stable) agglomerations of vacancies are visible for the other partial. The latter is relevant for a case of  $30^\circ$  mixed dislocation showing no stable vacancy tubes. At the same time, local agglomeration of vacancies is probably more prominent for one of the partials. Namely, the dislocation core with the larger edge Burgers vector component appears preferential for vacancy segregation.

According to the simulations, the formation of a jog-pair can be initiated after reaching a critical size of the vacancy cluster  $\sim 10$  vacancies (see, for example, the illustrations for  $60^\circ$  mixed dislocation, Fig. 9). Additionally, the collision between the tubes growing on different partial dislocations can facilitate the process of jog-pair formation. At this stage of the climb process, observed after the intersection of vacancy clusters, the partial dislocations approach each other, reducing the stacking fault (SF) width

As we show for the edge dislocation, once the vacancy tubes intersect, a jog is formed at the point of intersection. Depending on the configuration of the agglomerated vacancy clusters, the resulting jog pair can have different characteristics and may consist of various combinations of unit- and super-jogs. The examples are shown for edge dislocation in Fig. 8. The formation of such super-jogs probably comes from absorption of vacancies gathered in more stable 2T clusters. Further growth of the created jog-pair occurs because of the continuing segregation of vacancies to the dislocation. As we show in Fig. 5, the unit-jogs create significant segregation sites for vacancies, where the values of  $E_{seg}^i$  can locally reach values comparable to the vacancy formation energy in Ni. Hence, jogs act as prominent vacancy sinks promoting further attraction of vacancies and growth of the created jog-pair. Additionally, the process of vacancy absorption at jogs is accompanied by continuing vacancy segregation at the other dislocation segments. Such complex processes can lead to parallel elongation of existing jog-pairs together with formation of new ones.

The observed mechanisms of dislocation climb do not fall strictly into one of the concepts proposed for fcc metals in the classic works. Specific differences in the jog-nucleation stage are discussed in Sec. IV B from the point of view of the dislocation reactions. From atomistic simulations, we confirm that the first stage of climb resembles the formation of a prismatic loop on one of the partial dislocations, as described by Thomson and Balluffi. However, as MD shows, the segregation of vacancies has a specific character and alignment depending on the dislocation orientation. The size of vacancy clusters required for the jog-pair formation depends on the stacking-fault width and is therefore expected to be material-specific. Considering the possibility of oriented vacancy tubes and the influence of thermal fluctuations, the number of defects required for jog-pair formation may be significantly lower than that proposed previously by Grilhé [14].

Another aspect revealed by the simulations is the importance of accounting for thermal and correlation effects when considering dislocation climb at finite temperatures, particularly under supersaturated conditions. Specifically, the behavior of vacancies in the vicinity of the dislocation is likely to differ from random diffusion in a defect-free crystal. Both the interaction radius of point defects [60,61] and the dislocation-defect capture radius [62,63] can reach effective values on the order of 4–5 nm. Consequently, vacancy migration within the stress field of a dislocation core is expected to be more correlated and faster than in a perfect crystal. Diffusion barriers for vacancy near the dislocation core were shown to be lower than in bulk [24]. This may partially explain why the calculated climb rate exceeds the value predicted by Eq. (1) when using the bulk coefficient  $D_{\text{vac}}$ . In other words, using the bulk value of  $D_{\text{vac}}$  in this analysis effectively yields a fitted value of  $\eta$  that is higher than the classical theoretical value of 8 [1]. Additionally, the estimated  $\eta$  may reflect dynamic effects associated with defects motion and the discrete nature of the crystal lattice. On the other hand, the MD results show very good agreement with the analytical functional dependence of the climb rate on  $\sin(\theta)$ . Therefore, Eq. (3) remains a useful tool for estimating the order of magnitude of the climb velocity.

As discussed, individual steps of the proposed climb schematics intersect with previous works studying specific details of edge dislocation climb in fcc Ni, Al, or Cu. Comparing with the theoretically discussed mechanisms of a jog-pair formation, the simulations performed in this work for Ni add to the existing concepts and create a new interpretation of the climb in fcc metal.

### B. Dislocation theory interpretation

The results of the atomistic simulations obtained for fcc Ni can be interpreted from a point of view of dislocation reactions. To enable easier comparison with the existing literature on dislocation climb mechanisms, we switch for this section from the actual crystallographic orientation of the dislocations used in the simulations to crystallographically equivalent orientations that are always shown from outside the Thompson tetrahedron. While vacancy segregation to partial dislocations takes place for all studied dislocation characters, the mechanism and observed dislocations that lead to jog pair

formation on the different dislocation characters are clearly distinct.

The current textbook understanding of jog-pair formation for dissociated edge dislocations [1] is based on the mechanism proposed by Thomson and Balluffi [13], which was studied by Grilhé *et al.* [14] in 3D and used to compute the jog pair nucleation energy as function of stacking fault energy and who determined a critical jog size. This mechanism is depicted in Fig. 12. In it, vacancies segregate onto the line of one of the equivalent partial dislocations. These correspond to (or form) a so-called prismatic vacancy selfdislocation loop with the same Burgers vector as the original dislocation. This loop then reacts with the original dislocations and dissociates by glide. Further glide produces a complete jog pair, with an acute extended jog made of a stair rod dislocation dipole and an obtuse constricted jog by Hirth dislocations. Exactly these dislocation configurations were observed in DMD simulations when vacancies were manually introduced on the dislocation line [25]. If vacancies are, however, allowed to their minimum energy position one after the other as in the work of Abu-Odeh *et al.* [17], the formation of  $\langle 110 \rangle$  oriented vacancy tubes was observed, which did not directly lead to well-formed jog pairs, but required additional vacancies and thermal energy to lead to jog pairs as shown in Fig. 5.

The observed mechanism for jog-pair formation on a dissociated edge dislocation in the simulations, Fig. 7, diverges from the mechanism proposed by Thomson and Balluffi in multiple aspects: (i) vacancies align along  $\langle 110 \rangle$  directions and not along the original dislocation line direction; (ii) vacancies segregate to both partial dislocations, climb takes place at both dislocations, and only through their concerted motion do the two partial dislocations form a jog pair; (iii) a dislocation configuration similar to Fig. 7(c) is not observed; instead, partial dislocations with Burgers vector parallel to the original line direction (corresponding to  $D\gamma$  in the orientation of Fig. 7) are observed to play an important role in the formation of the jogs.

Based on the observations, Fig. 7, we suggest the following new mechanism for jog-pair formation on dissociated edge dislocations, see Fig. 13: in agreement with [17], vacancies segregate in tubes along  $\langle 110 \rangle$  directions, forcing the partial dislocation lines locally along these directions [Fig. 13(a)]. These vacancies can—at least in part—be described by prismatic *partial* dislocation vacancy loops of the type  $B\alpha$  or  $\beta A$ , i.e., dislocations which were not present before. Alternatively, these partial dislocation loops can be thought of as nucleated at the vacancy tube. The fact that these are partial dislocation dipoles by topology implies that they are bounded by stacking faults on two different parallel planes, see Fig. S1 in the Supplemental Material [56]. These loops react with the initial partial dislocations leading to stair rod dislocations  $\alpha\gamma$  or  $\gamma\beta$  [Fig. 13(b)]. The upper part of the partial dislocation loops decomposes to also form a stair rod dislocation ( $\gamma\alpha$  or  $\beta\gamma$ ) and the partial dislocations corresponding to the initial partial dislocations ( $B\gamma$  and  $\gamma A$ )—just parallel to initial plane. This situation corresponds exactly to Fig. 7(b). Please note that the formation of the stair rod partial dislocation dipoles is only possible due to the orientation of the vacancy tubes along the  $\langle 110 \rangle$  directions  $BD$  and  $AD$ , the intersection lines of the  $(c)$  plane with the  $(a)$  plane and the  $(b)$  plane, respectively. The

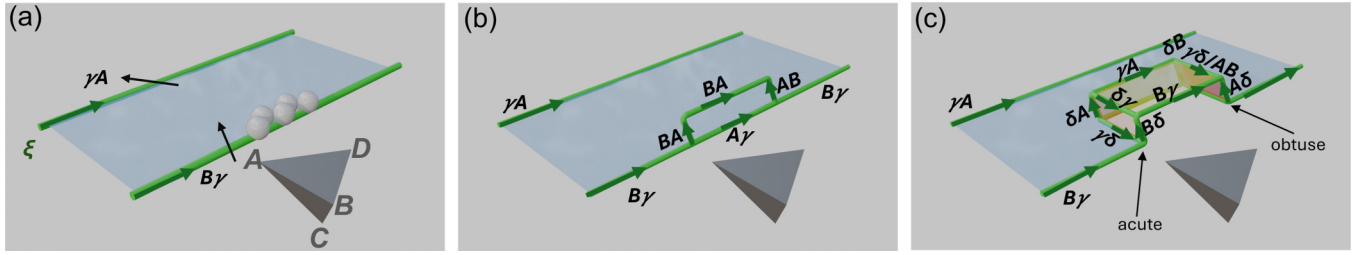


FIG. 12. Current text-book model for the nucleation of a jog pair on the edge dislocation  $BA(c)$  by vacancy absorption according to [1] and following [12–14,25]. To form a self-dislocation vacancy loop  $BA$ , two staggered rows of vacancies along  $[\bar{1}\bar{1}\bar{2}]$  corresponding to the two inserted  $(\bar{1}10)$  planes need to be present [see (a)]. The prismatic vacancy loop  $BA$  reacts with the partial dislocation  $B\gamma$  at which it formed, resulting in  $A\gamma$  (b). The full Burgers vectors then dissociate on the different glide planes and react according to the Burgers vector algebra in the Thomson tetrahedron notation, resulting in an acute jog formed by a pair of stair rod dislocations  $\gamma\delta$  and an obtuse jog, which is made up of a pair of Hirth dislocations  $\gamma\delta/AB$  (c). Green lines correspond to partial dislocation lines with green arrows representing the line direction  $\xi$ . Intrinsic stacking faults are shown as semitransparent planes. Gray—Thompson tetrahedron provides information on the crystallographic orientation.

occurrence of the  $D\gamma$  dislocations observed in simulations which are necessary to form the jogs can be explained by the nucleation of another prismatic partial dislocation vacancy loop  $\alpha D$  (or  $D\beta$ ) at the vacancy tubes, see Fig. 13(d). Together with the stair rod dislocations, these result in  $D\gamma$  dislocations on both planes [Fig. 13(e)]. Due to their line sense, they annihilate each other, leaving only the full dislocations  $BA$ , which is dissociated in  $\gamma A$  and  $B\gamma$  on the top (c) plane and dissociated into partial dislocations and stair rod and Hirth dislocations on the (d) planes, respectively; see Fig. 13(f).

For the  $60^\circ$  dislocation, the climb process observed in Fig. 9 matches in part with the one proposed by Thomson and Balluffi for the edge dislocation. In this case, vacancy segregation takes place only on the partial

dislocation with edge character and the preferred  $(110)$  direction of the vacancy tube corresponds with the line direction [Fig. 14(a)]. The vacancy loop in this case can be described by a full prismatic self-dislocation loop  $AB$  [Fig. 14(b)]. It reacts with the partial dislocation  $\gamma B$  forming  $A\gamma$ , which can easily be annihilated by the original partial dislocation with  $30^\circ$  character, while the upper dislocation  $AB(c)$  dissociates again in  $\gamma B$  and  $A\gamma$ , Fig. 14(c).

In the case of the  $30^\circ$  dislocation, the entire climb process is much faster than for the edge and  $60^\circ$  dislocations. Also the partial dislocations are closer together, making the exact details of the jog pair formation more difficult to observe (Fig. 10). It can, however, be safely assumed that vacancy segregation takes place mostly at the partial dislocation with

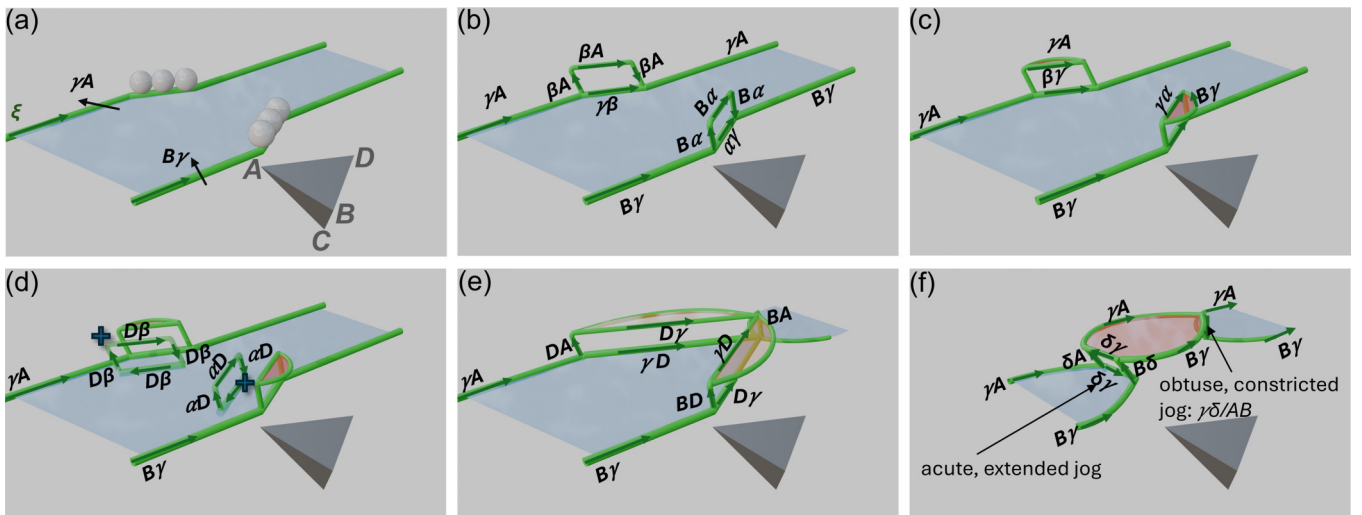


FIG. 13. Suggested model for jog-pair nucleation on an extended edge dislocation  $BA(c)$ , explaining the observations in Fig. 7. Vacancy rows along the close-packed  $(111)$  directions  $AD$  and  $BD$  form on *both* partial dislocations [see (a)]. These vacancy tubes can lead to prismatic *partial dislocation* vacancy loops (b). The upper parts of the loops can decompose into stair rod dislocations that form dipoles at the vacancy tube, and the appropriate partial glide dislocations (c). The formation of partial dislocations with Burgers vectors  $\pm D\gamma$  as observed on both partial dislocations of the original dislocation can be explained by the formation of additional prismatic partial dislocation loops  $D\beta$  and  $\alpha D$  (d). Together, the short segments of the total prismatic loops form full dislocations  $DA$  and  $BD$ , while the long segments on both original partial dislocations both become  $D\gamma$  (e). The full dislocations can react with each other, forming  $AB(d)$ , which decompose into an acute, extended jog with stair rod dislocations  $\pm\delta\gamma$  and an obtuse, constricted jog with Hirth dislocations  $\pm\gamma\delta/AB$  (f). See Fig. 12 for the explanation of the symbols. Please note dislocation slip system is different from Fig. 7 but crystallographically equivalent.

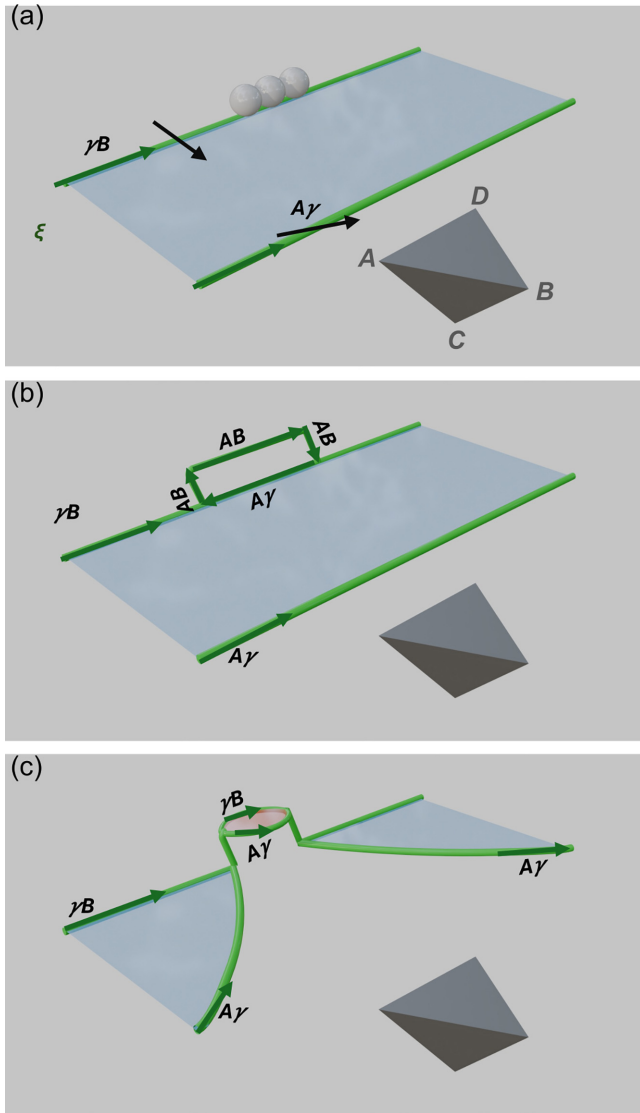


FIG. 14. Mechanism of jog pair formation on the  $60^\circ$  dislocation  $AB(c)$ , based on the simulation results, see Fig. 9. Segregation of vacancies on the dislocation line with edge character only and formation of a  $[\bar{1}\bar{1}0]$  vacancy tube (a), which can be represented by a full vacancy prismatic self-dislocation loop  $AB$  (b). Dissociation of the upper dislocation segment into  $\gamma B$  and  $A\gamma$ ; annihilation of the lower segment of the dislocation loop with the right partial dislocation  $A\gamma$ . Green lines correspond to partial dislocation lines with green arrows representing the line direction  $\xi$ . Intrinsic stacking faults are shown as semitransparent planes. Please note the dislocation slip system is different from Fig. 9 but crystallographically equivalent.

$60^\circ$  orientation ( $B\gamma$  in Fig. 15) rather than at the partial dislocation with screw orientation. The observed formation of a stacking fault on a parallel plane to the original stacking fault and to the left of it [Fig. 10(c)] can again be explained by the nucleation of a prismatic *partial* dislocation vacancy loop  $B\alpha$  at the vacancies [Fig. 15(b)]. This reacts with the original partial dislocation  $B\gamma$  to form a stair rod dislocation  $\alpha\gamma$ , while the upper partial dislocation dissociates into the corresponding upper stair rod dislocation  $\gamma\alpha$  of a stair rod dipole and the upper leading partial dislocation  $B\gamma$ , see Fig. 15(c). The trailing original partial dislocation with screw

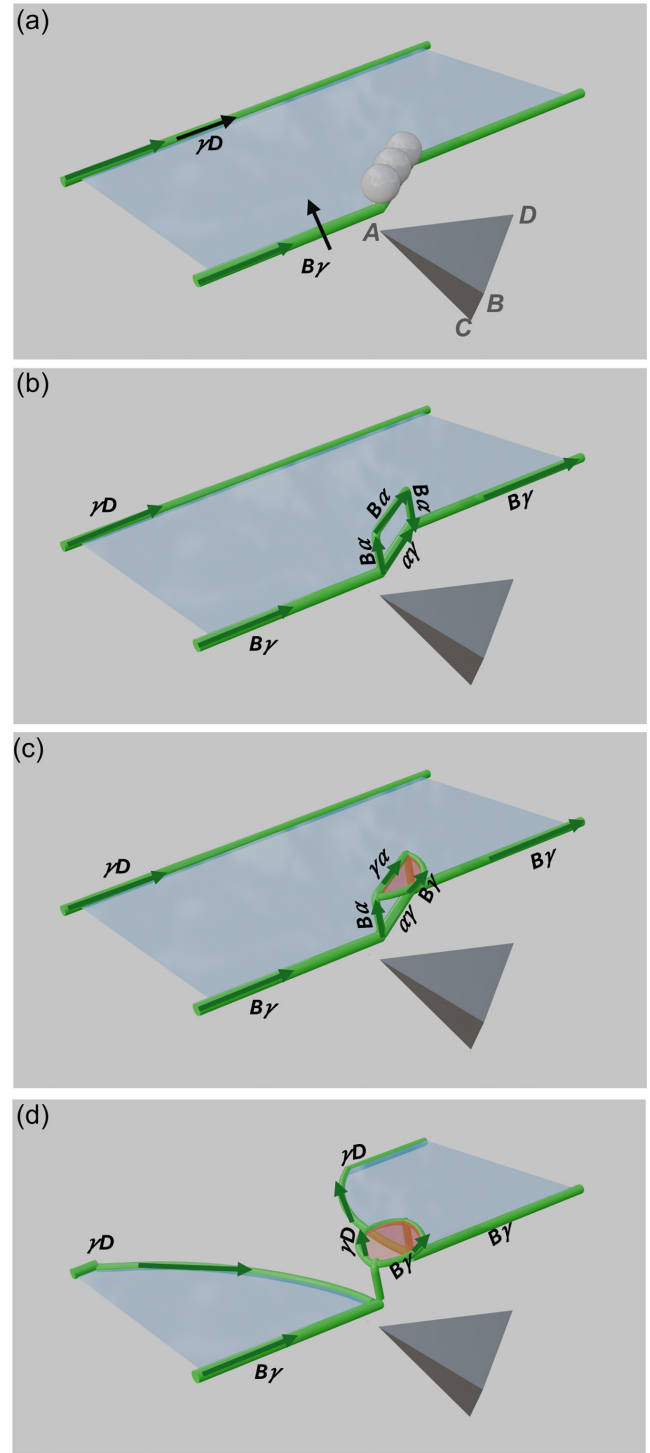


FIG. 15. Mechanism of jog pair formation on the  $30^\circ$  dislocation  $AB(c)$ , based on simulation results, see Fig. 10. Segregation of vacancies takes place only on the partial dislocation with nonscrew character, which can be represented by a vacancy prismatic partial self-dislocation loop  $B\alpha$  (b). Dissociation of the upper dislocation segment into  $B\gamma$  and  $\gamma\alpha$  (c). Contact of the screw partial dislocation  $\gamma D$  with the remaining lower segment of the dislocation loop  $\alpha\gamma$  and double cross slip through the Fleischer mechanism with the two stair rod dislocation  $\alpha\gamma$ ,  $\gamma\alpha$ , forming the trailing partial dislocation on the jog  $\gamma D$ . See Fig. 12 for the explanation of the symbols. Please note dislocation slip system is different from Fig. 10 but crystallographically equivalent.

character,  $\gamma D$  can glide towards  $\alpha\gamma$  and react to  $\alpha D$ , similar to the Fleischer mechanism of dislocation cross-slip [64,65]. This partial dislocation can then double cross-slip by reacting with  $\gamma\alpha$  to  $\gamma D$ , the original trailing partial dislocation, just now on a parallel plane, see Fig. 15(d).

It is important to note that in the simulations, the driving force for climb was purely due to vacancy supersaturation. The application of stresses could affect the jog-pair formation energies and mechanisms. The above-described mechanisms were observed at very high concentrations of superabundant vacancies, which can only be reached in the most extreme irradiation regimes (high dose rate and low temperature). Whether they are relevant at typical creep conditions is an open question. However, the fact that vacancy tubes at partial dislocations form preferentially along close-packed  $\langle 110 \rangle$  directions is independent of vacancy concentration [17]. The suggested mechanisms of jog pair formation that include *partial* dislocation vacancy loops and stair-rod dislocation dipoles along  $\langle 110 \rangle$  should therefore still remain valid. Furthermore, the subsequent nucleation of *partial* dislocation vacancy loops should be energetically more favorable than the nucleation of a *full* dislocation vacancy loop. These considerations suggest that the mechanisms introduced here are not an artifact of the high vacancy concentrations employed, but may also operate under typical creep conditions at lower vacancy concentrations and temperatures. Their inclusion in dislocation dynamics models like [7,23,29,35,66–73] or phase field models [74–80] might improve the generality and accuracy of these mesoscale models under creep, annealing, and irradiation conditions.

## V. SUMMARY AND CONCLUSIONS

Using large-scale MD simulations, we provide an alternative perspective on vacancy-driven climb in fcc Ni. By directly simulating dissociated dislocations under high-temperature vacancy supersaturation, we resolved the atomistic stages of the climb process. Our results demonstrate that vacancy-driven climb relies on the specific segregation of vacancies at partial dislocations, leading to the formation of stable vacancy clusters. Such clusters (or “vacancy tubes”) align with close-packed lattice directions and can grow until they reach a critical size (approximately 10–15 vacancies) or intersect with one another, leading to the nucleation of unit- or super-jogs. Our results indicate that the nucleation of single- and super-jogs is linked to the type of vacancy tubes (i.e., T1 or T2) contributing to a given dislocation climb event. We find that the details of cluster formation are sensitive to dislocation type. While edge dislocations exhibit symmetric vacancy segregation and cluster growth across both partials, mixed dislocations show a distinct asymmetry, with preferential vacancy accumulation at the partial possessing greater edge character.

Distinct jog-pair formation pathways were observed for different dislocation characters. While the  $60^\circ$  dislocation partly follows the mechanism originally proposed for edge dislocations by Thomson and Balluffi [13] and later detailed in three dimensions by Grilhé [14], this framework does not capture the processes observed for dissociated edge dislocations. We therefore propose an alternative mechanism for jog-pair

formation on dissociated edge dislocations in fcc metals. Central to this mechanism—and to a newly identified mechanism for  $30^\circ$  dislocations—is the formation of partial dislocation vacancy prismatic loops, rather than full dislocation vacancy prismatic loops as assumed in the classical picture. These partial loops naturally account for the occurrence of stair-rod dislocation dipoles and for stacking faults on two parallel planes, both of which are directly linked to the  $\langle 110 \rangle$  vacancy-tube intermediates.

We used results from MD simulations to estimate the climb rates of the considered dislocations under vacancy supersaturation. The observed rates exceed classical predictions by a factor of 4 when the vacancy diffusion coefficient in defect-free bulk is used as an input parameter. Nevertheless, a discrepancy of only a factor of a few between fully analytical theory and direct large-scale simulations represents a significant achievement for such a complex process. An important aspect of this comparison is that both simulation and theory predict the same functional dependence of the climb rate on dislocation orientation. Specifically, the following hierarchy of climb rates was observed: the  $30^\circ$  mixed dislocation shows the fastest climb, followed by the  $60^\circ$  and edge dislocation.

These findings provide a physically based framework for incorporating atomistic mechanisms of vacancy-mediated climb into mesoscale models. Such an approach is important for enhancing the predictive capabilities of simulations describing high-temperature deformation and irradiation-driven microstructural evolution in fcc metals.

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## DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

## APPENDIX A: THERMAL EXPANSION

The lattice thermal expansion of the Ni model was verified by calculating equilibrium lattice parameters for a single crystal at various temperatures. A model containing 1372 Ni atoms in a fcc lattice was equilibrated at the given temperature  $T$  and zero pressure. Namely, MD simulations were carried out with the  $NPT$  ensemble with the lattice parameter set to condition of  $P = 0$ . We used the boxes with PBC in all directions. In Fig. 16, we show the relative linear thermal expansion with

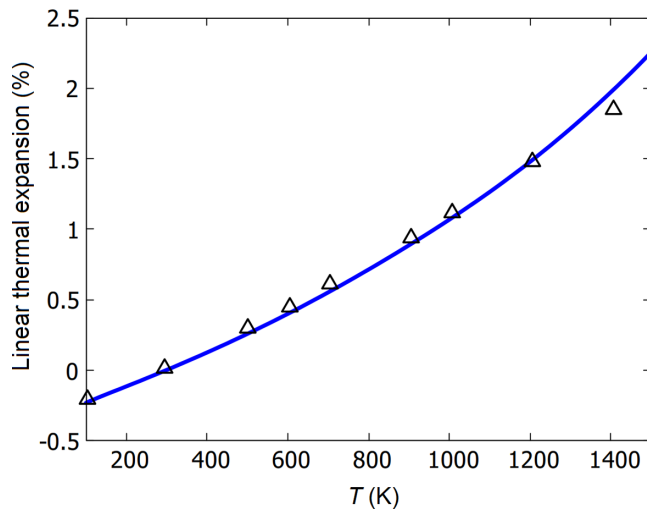


FIG. 16. Linear thermal expansion coefficient of fcc Ni. Triangles—experimental data from [81], line—results of this work, molecular dynamics with an interatomic potential [36].

respect to the Ni lattice parameter at 298 K. In the temperature range up to  $T_m$  (see Table I), thermal expansion of the model corresponds to the experimental data for Ni [81].

## APPENDIX B: MELTING TEMPERATURE

To calculate the melting temperature  $T_m$  reported in Table I, we used two different methods that yielded largely consistent results. In the first simulation method, we used a model of fcc Ni with open surfaces. The simulation box

was built periodic in directions [010] and [001] and had surfaces in the [100] direction. The number of Ni atoms in simulation was equal to 3146. The model was slowly heated at a rate of 0.1 K/ps. During the heating, zero pressure was maintained in the periodic directions using a Nose-Hoover thermostat/barostat. In such a case, the liquid phase formed spontaneously at the surfaces as a result of premelting [82]. The value of melting temperature was determined from a change in a slope of potential energy depending on the simulation time (and related model temperature). The described simulation setup accounted for an initial phase of melting and aimed to avoid an overestimation of the melting point  $T_m$  due to overheating of a crystal [83]. This method yielded a melting temperature of  $1530 \pm 10$  K.

Additionally, as a further validation test, we estimated  $T_m$  using the two-phase simulation method [84]. This method is based on the direct simulation of a solid-liquid interface. The computational cell was constructed with one part occupied by liquid Ni and the other by fcc Ni. The model contained 7718 atoms, and PBCs were applied in all directions. Simulations were performed at zero pressure for a series of trial temperatures. Depending on the temperature, the interface migrates so that either the solid or liquid phase grows at the expense of the other. At temperatures close to the melting point, the interface velocity becomes too small to be resolved on the timescale accessible to atomistic simulations, and the interface therefore appears stationary within the statistical uncertainty. For each trial temperature, the simulation was continued for 5 ns. The melting temperature was determined by tracking the interface displacement and identifying the temperature interval between simulations that resulted in crystallization and those that resulted in melting. Using this criterion, the two-phase simulations gave  $T_m = 1545 \pm 15$  K for Ni at zero pressure.

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