

Vacancy-screw dislocation interactions in bcc Nb: A machine-learning potential investigation

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Vacancy-screw dislocation interactions in bcc Nb are studied with near density functional theory accuracy using a machine-learning potential, specifically a moment tensor potential (MTP), in large-scale atomistic simulations. The MTP predicts attractive vacancy-dislocation interactions with threefold symmetry in the (111) plane. These attractive interactions lead to a decrease in the Peierls stress by up to 28%, depending on the vacancy position relative to the dislocation. The interactions also lead to the formation of new complex topological defects (CTDs), when the vacancy is close to the dislocation core. A CTD can be geometrically characterized as a screw dislocation with *multiple kinks* and with a (partially) *dissociated* vacancy along the dislocation line. CTDs form under shear when the vacancy-dislocation distance is less than ~ 6 Å, providing a new mechanism for pinning screw dislocations. The formation of CTDs confirms theoretical predictions made in the early 1990s based on differential geometry and underscores the importance of machine-learning potentials and large-scale simulations for accurately describing the properties of extended defects in metals.

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I. INTRODUCTION

Lattice (point, line, and plane) defects significantly impact the mechanical properties of metals, such as plasticity and fatigue [1]. In particular, the plasticity of metals is controlled by the stress- and thermally-activated glide of line defects (dislocations) [1,2].

Dislocations in solids represent topological defects because they lead to lattice discontinuities, while point defects (e.g., vacancies, interstitials) are nontopological defects. Kröner [3] developed a combined differential-geometry theory of point and line defects. According to this theory, in the presence of a point defect, a dislocation ceases to be an autonomous physical object and instead couples with the point defect to form a new ‘point-line’ defect. We will refer to this point-line defect as a complex topological defect (CTD). The existence of such CTDs in body-centered cubic (bcc) or face-centered cubic (fcc) metals has not been, to the best of our knowledge, demonstrated experimentally or computationally to date. Related CTDs have been observed, for example, in graphene [4].

Molecular dynamics (MD) simulations offer a valuable atomistic perspective on dislocation-point defect interactions. Several MD studies, using classical interatomic potentials, reported the binding energies between a dislocation and a vacancy in bcc metals (W, Fe, Mo, Ta) [5–9]. The magnitude of the binding energies, however, varies from potential to potential in some of these studies [5,6,9], because classical

potentials generally have a limited capability for modelling defect properties.

Ab initio methods, such as density functional theory (DFT), provide the necessary accuracy in the atomic interactions. However, simulations of screw dislocations and vacancies require large supercells due to the long-range stress fields associated with both the screw dislocations and vacancies. Such simulations are still beyond the capability of current DFT methods, which are limited by their computational expense to a few hundred atoms and several thousand picoseconds.

Machine learning, on the other hand, has emerged as a new approach in materials science for constructing interatomic potentials, combining DFT accuracy with computational speed comparable to that of classical potentials. Recently, a moment tensor potential (MTP) has been developed for studying screw dislocation mobility in bcc Nb in the thermally and stress-assisted regime at low temperatures [10]. The MTP was built using an *extended* physically informed training set containing 316 configurations, including, in particular, several subsets with screw dislocations and a subset with vacancies. The vacancy formation energies, obtained with the MTP (2.51 eV for the relaxed vacancy; 2.82 eV for the unrelaxed vacancy), compare well with the DFT values (2.78 eV for the relaxed vacancy; 3.01 eV for the unrelaxed vacancy) [10]. The Peierls barrier, obtained with the MTP (31.5 meV/*b*, where *b* is the length of the Burgers vector), is in good agreement with our DFT estimate (32.7 meV/*b*) and previous DFT estimates (e.g., 36.0 meV/*b* [11]), while the Peierls barrier obtained using empirical embedded-atom model (EAM) potentials [12,13] gives significantly lower values (17.1 meV/*b* and 20.5 meV/*b*). The MTP also reproduces very well the tetragonal, orthogonal, and deformation paths [10], which play a key role in the proper description of the elastic properties of bcc metals. Thus the MTP from Ref. [10] is well-suited for probing dislocation-vacancy interactions in bcc Nb.

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However, neither this MTP nor any other machine-learning potential has been used so far to study dislocation-vacancy interactions in bcc Nb with supercells *large* enough to resolve CTDs and the effects of vacancies on the Peierls stress. Therefore, in the present paper, we address these points using MD simulations and the MTP from Ref. [10]. The continued interest in structural defects in bcc Nb originates not only from its technological importance, e.g., in superconducting radiofrequency cavities [14], as an alloying addition in superalloys and refractory-based high-entropy alloys [15], and from the role of dislocations in these alloys, but also from the fact that it exhibits several elastic and phonon anomalies not observed in other bcc metals (Ref. [10] and references therein).

II. COMPUTATIONAL METHODS

The present simulations were performed with LAMMPS [16]. The supercell was oriented as $X||[11\bar{2}]$, $Y||[111]$, and $Z||[1\bar{1}0]$ and had dimensions of $L_x = 163$ Å, $L_y = 57.5$ Å = $20b$, and $L_z = 188$ Å (Burgers vector: $b = 2.877$ Å), resulting in 96 000 atoms. A single $1/2\langle 111 \rangle\{110\}$ screw dislocation was introduced along the Y axis in the middle of the supercell ($X_D = 81.37$ Å and $Z_D = 92.4$ Å) by means of its isotropic elastic displacement using the ATOMSK [17] program. Periodic boundary conditions were applied along the Y axis, whereas nonperiodic boundary conditions were used along the X and Z directions. Supercells with the same orientation, but with different L_x , L_y , or L_z dimensions were used to check the convergence of the vacancy-dislocation binding energies and the depinning stress for selected vacancy positions.

Energy and force minimization of the ideal and defect supercells were performed using the Polak-Ribière version of the conjugate gradient algorithm implemented in LAMMPS [16]. A single vacancy was introduced by deleting an Nb atom in the *middle* of an atomic row parallel to the Y axis with given coordinates in the (111) plane. For selected vacancy positions in the core, it was cross-checked that the observed effects are independent of the initial vacancy position along the atomic row. The screw-dislocation core structure was analyzed using the program DDLOT [18]. Calculations of the local extrapolation grades per atom for selected CTD configurations, obtained from the LAMMPS simulations, were performed using the MLIP program [19]. Calculations of the per-atom Nye tensor α for selected CTD configurations were performed using the ATOMSK program [17]. The per-atom Nye tensor is a quantity related to the strain gradient $\mathbf{G}$ around each atom ($\alpha = -\nabla \times \mathbf{G}$) [20,21].

Additional DFT benchmark calculations were performed with the Vienna *ab initio* simulation package (VASP [22]) using the Nb_pv projector-augmented wave (PAW) potential for Nb with the valence configuration of $4p^6 4d^4 5s^1$ (11 valence electrons), distributed with VASP. Except for the energy of the isolated Nb atom, we used non-spin-polarized calculations. We employed the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional. The plane-wave expansion cutoff energy was set to 520 eV, as in our previous work [10]. This cutoff energy ensures a high accuracy for the components of the stress tensor as well. To sample the Brillouin zone,

we used the Monkhorst-Pack method [23]. The first-order Methfessel-Paxton method [24] with a smearing width of 0.2 eV was used for integration in the Brillouin zone. During electronic relaxation, convergence was assumed when the energy variation between two subsequent electronic self-consistent steps was below 10^{-4} eV. The DFT calculations were performed on a skewed supercell containing 231 atoms and a pair of screw dislocations with opposite Burgers vectors (dipole) in a quadrupole arrangement [25]. The basis vectors of the supercell were $\mathbf{a}_1 = 7\mathbf{e}_1$, $\mathbf{a}_2 = 1/2(7\mathbf{e}_1 + 11\mathbf{e}_2 + \mathbf{e}_3)$, and $\mathbf{a}_3 = \mathbf{e}_3$, where $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$ are the basis vectors along the $[11\bar{2}]$, $[1\bar{1}0]$, and the $[111]$ directions, respectively. For comparison, the same supercell was also used for calculating the vacancy-dislocation binding energies with the MTP.

The degree of (de)localization of a vacancy in the dislocation core was quantified as follows. For a pure screw dislocation (no vacancy), an atomic row parallel to the *screw-dislocation line* (i.e., parallel to the Y axis in our setup) features first nearest-neighbor (NN) distances that are all equal to b . For a *localized* vacancy in the dislocation core, the distance between the first NNs of the vacancy becomes $2b$. These two limits motivate to quantify the degree of localization/delocalization of the vacancy along the Y axis by the *cumulative* vacancy fraction via the expression given in Ref. [6]:

$$v(m) = \sum_i [(y(i) - y(i-1))/b - 1], \quad (1a)$$

where $m = 1, 2, \dots, N$ is the number of an atom along the vacancy line (row), and the summation runs from 1 to m , while $y(i)$ refers to the y coordinate of the i 'th atom in the atomic row, and $y(0)$ is the periodic image of $y(N)$. In the case of a single vacancy, $N = L_y/b - 1$. A fully localized vacancy leads to a sharp jump of $v(m)$ from ~ 0 to 1 at the position of the vacancy. If the N atoms are *equally* spread along the vacancy line, $v(m)$ increases linearly from 0 to 1 with a slope of $1/N$ ($v(m) = m/N$). This state corresponds to a fully delocalized vacancy. A partially localized–partially delocalized (dissociated) vacancy leads to a gradual increase of $v(m)$. The degree of localization ξ is defined here as

$$\xi = S/S_0, \quad (1b)$$

where $S = \sum_m [v(m) - m/N]^2$ and $S_0 = \sum_m [v_0(m) - m/N]^2$, with $v_0(m)$ being the cumulative vacancy fraction for the fully localized state. In this definition, $\xi = 1$ for the fully localized state and $\xi = 0$ for the fully delocalized state.

For the determination of the Peierls stress, the shear strain along the positive (or negative) Y direction was increased incrementally, and an energy/force minimization was carried out at every step with LAMMPS [16]. The incremental shear strain step was $\Delta\gamma = 5.4 \times 10^{-5}$. The uncertainty $\Delta\tau$ in the resulting shear stress can be written as $\Delta\tau = \mu \Delta\gamma$, where μ is the shear modulus along the $[111]$ direction. Taking $\mu = 33$ GPa (see Ref. [10]), the applied shear strain increment leads to an uncertainty $\Delta\tau$ in the shear stress of about 0.002 GPa, which is smaller than the differences in the Peierls stress between the different vacancy positions in Table II. The Peierls stress was determined as the shear stress at which the screw dislocation starts to move irreversibly, as determined by the OVITO program [26]. The shear stress was taken as the

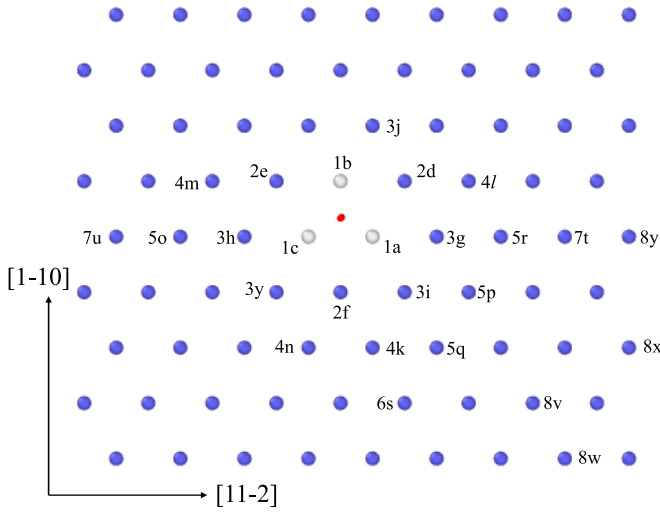


FIG. 1. Vacancy positions, listed in Table II, on the (111) plane. The atoms in the dislocation core are colored in white, while the bcc atoms are colored blue, as given by OVITO [26]. The position of the screw dislocation is marked with a red dot.

YZ component of the pressure tensor, computed by LAMMPS [16] as the pressure of the entire system of atoms.

The shear stress τ leads to a Peach-Köhler force [2] acting normal to the screw dislocation line along the positive (or negative) X direction for a positive or negative sense of shearing. For every resulting configuration, the position and the topology of the screw dislocation were determined using the dislocation analysis implemented in OVITO [26].

Convergence tests performed on models with different L_x , L_y , or L_z showed that the binding energy E_b and the depinning stress are converged for our setup [27]. The sites selected in Fig. 1 were chosen to capture the most important aspects of the vacancy-dislocation interactions.

The interaction between a dislocation and a vacancy is commonly characterized by the so-called binding energy E_b , defined here as

$$E_b = (E_{VD} - E_D) - (E_V - E_o), \quad (2)$$

where E_{VD} , E_D , and E_V are the total energies of the configurations containing both a vacancy and a dislocation, only a dislocation, and only a vacancy, respectively, while E_o is the total energy of the ideal supercell. According to this definition, the vacancy is attracted to the dislocation if E_b is negative. The binding energies represent the difference between several large total energy terms [see Eq. (2)]. Consequently, we used very high stopping tolerances for energy and forces, equal to 1×10^{-20} eV and 1×10^{-20} eV/Å, respectively.

III. RESULTS AND DISCUSSION

A. Core structure

The screw-dislocation cores for a model without a vacancy and a model with a vacancy localized at the 1a position are shown in Figs. 2(a) and 2(b), respectively.

The differential displacement map for the model without a vacancy is consistent with a nonplanar nondegenerate type of core structure, in qualitative agreement with previous DFT calculations (e.g., Ref. [11]). The presence of a vacancy in the

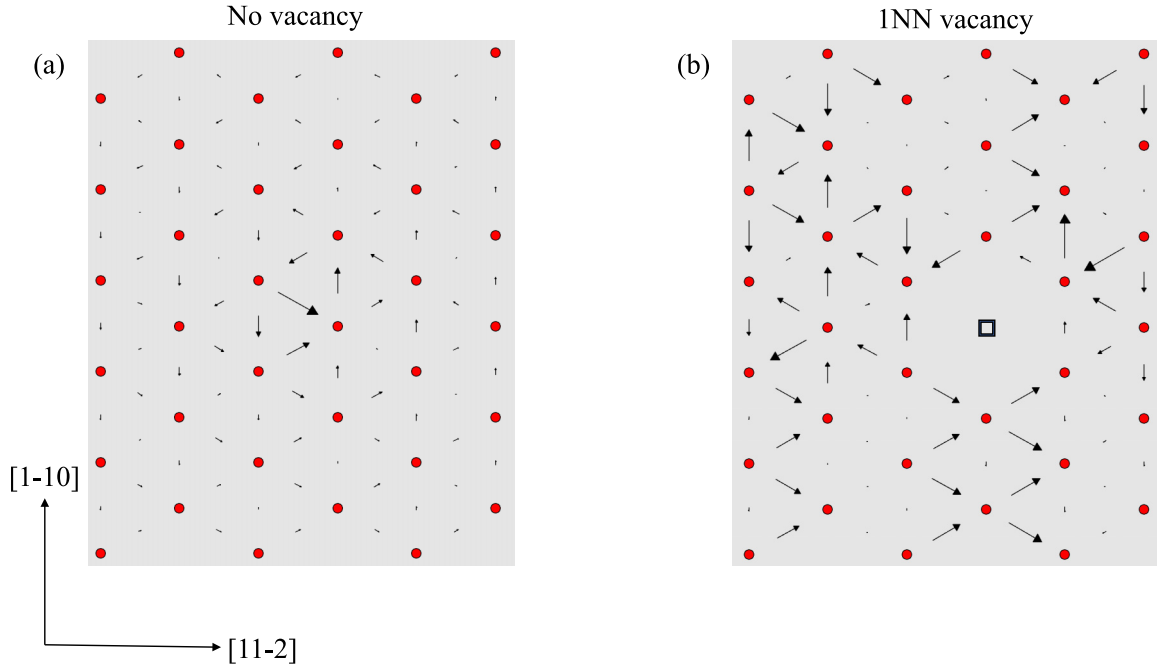


FIG. 2. Differential displacement maps showing the *screw* components in the dislocation core, obtained with the MTP, projected on the (111) plane using the DDPlot program [18]: (a) without a vacancy; (b) with a localized first nearest-neighbor vacancy. For clarity, only the atoms belonging to the layer with the vacancy are shown. The length of the arrows in the plot is proportional to the atomic displacements of the atoms in the core, relative to their positions in the ideal crystal.

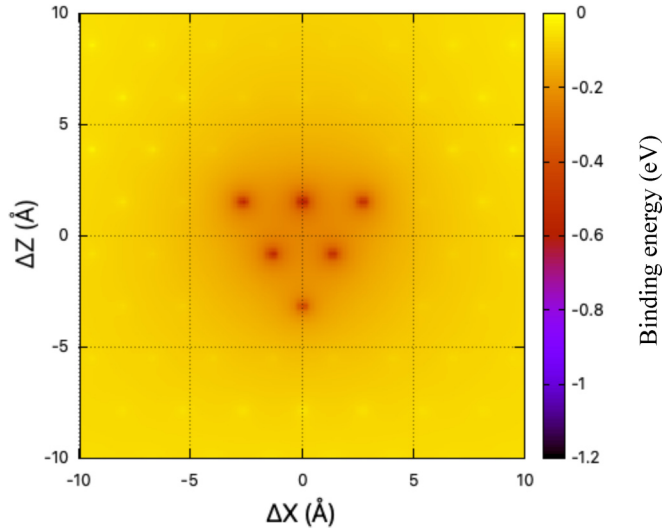


FIG. 3. Vacancy-dislocation binding energy map. The vacancy positions are given relative to the screw dislocation at (0,0). The X axis is parallel to the $[11\bar{2}]$ crystallographic direction, and the Z axis is parallel to the $[1\bar{1}0]$ crystallographic direction.

dislocation core leads to the removal of the threefold symmetry, an increase in and slower decay of the screw components with increasing distance from the center of the screw dislocation core, reflecting the long-range stress field of the localized vacancy. Similarly, the edge components in the dislocation core increase significantly in the presence of a vacancy.

B. Vacancy-dislocation binding energies

The binding energies E_b as a function of the vacancy position in the (111) plane, calculated with the MTP, are shown in Fig. 3. The binding energies are all negative for $R < 10$ Å and rapidly decrease towards zero beyond the third nearest neighbor (NN) of the dislocation ($R > 4.0$ Å), indicating that the vacancy is *attracted* to the dislocation. Negative binding energies for bcc Nb up to the third NN were also reported using DFT calculations on a dislocation dipole with only 135 atoms [28] (see Fig. 4).

At larger distances ($R > 10\text{--}12$ Å), the E_b map exhibits very weak ($|E_b| < 0.01\text{--}0.03$ eV) *alternating* positive and negative regions with threefold symmetry [27], arising from the dilation field of the screw dislocation [29]. The E_b map has an almost perfect $3m$ point group symmetry in accordance with the Neumann-Curie principle. In contrast, similar simulations performed with a classical EAM potential for bcc Nb [12] exhibit vacancy-dislocation interactions with only mirror symmetry parallel to the Z axis (point group m [27]). The E_b values for the 1NN and the 2NN vacancies, obtained with the MTP and from our DFT calculations, using the 231-atom supercell for both, are similar within error limits (see Fig. 4), demonstrating the extrapolation reliability of the MTP potential. The errors in Fig. 4 are taken as the standard deviations of E_b , averaged over all nearest neighbors in a given coordination shell.

The E_b values of Tsuru *et al.* [28] for the 3NN are comparable to our MTP results, but the E_b values in the dislocation core (1NN and 2NN) are higher. The main reasons for this

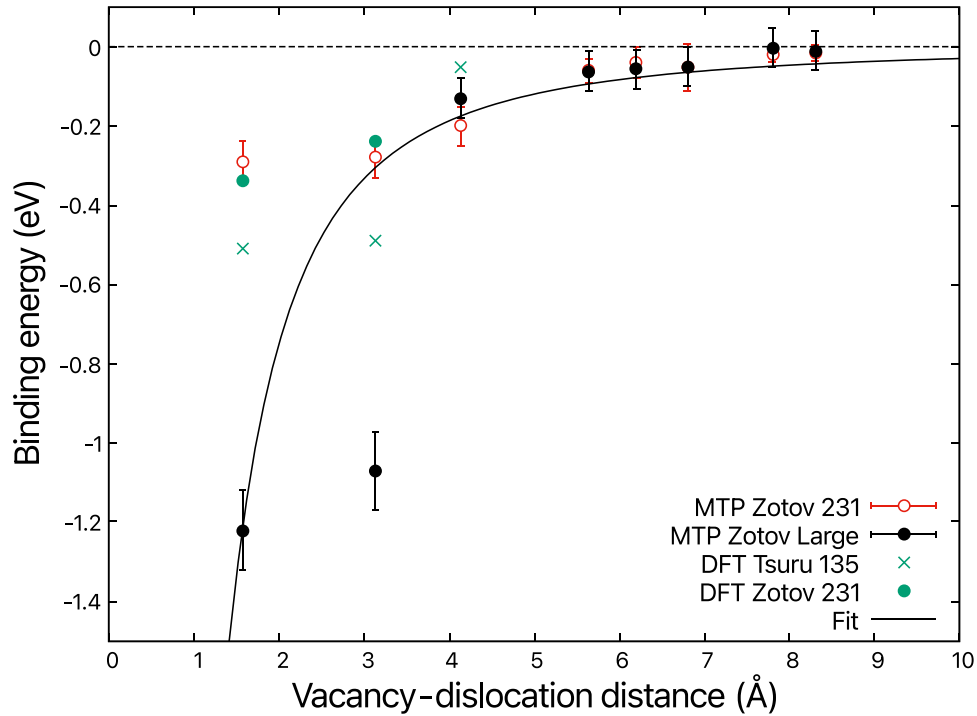


FIG. 4. Dependence of the binding energies on the vacancy-dislocation distance obtained with: the MTP using the 231-atoms supercell (red empty circles), the MTP using a large supercell (black full circles), DFT calculations on a 135-atoms supercell [28] (green $\times$ symbols) and DFT calculations on the 231-atoms supercell for the 1NN and 2NN (green full circles) from the present study. The full black line is a fit of Eq. (3b) through the MTP data for the large supercell. The dashed line is only a guide for the eye.

discrepancy are the small size of the supercell along the Z axis in Ref. [28], which leads to a different size and shape of the screw dislocation core-vacancy configuration, compared to those in the large supercell, and the interaction of the two screw dislocations in the dipole. This is clearly seen from our calculations using the 231-atom supercell as well. The binding energies for the 3NN and beyond, obtained with the small supercell (231 atoms) and the large supercell (96 000 atoms) are within error limits the same. However, the binding energies in the dislocation core for the small supercell are higher than the MTP values for the large cell, similar to the results of Tsuru *et al.* [28].

Several kinds of interactions exist between a point defect and a screw dislocation in the framework of classical elasticity theory [30]: a first-order size interaction arising from the interaction between the long-range stress field of the dislocation and the atomic displacements around the point defect, a second-order size interaction arising from the nonlinear elastic properties of the crystal, and a second-order inhomogeneity interaction arising from the difference between the elastic constants of the crystal and those associated with the point defect. The spatial form of the first-order size interaction is [30]

$$E_1 = -A_1/R, \quad (3a)$$

while the spatial form of both second-order interactions is [30]

$$E_2 = -A_2/R^2. \quad (3b)$$

The constants A_1 and A_2 depend on the sense of the dislocation, the elastic constants of the crystal, the Poisson ratio ν , and the radius r_0 of the unrelaxed vacancy [30]. In the case of a screw dislocation and a spherical point defect $A_1 = 0$. The A_2 constant in the case of the second-order size interaction is a complex function of the elastic constants and takes a simpler form, $A_2 = 5\mu b^2(1-\nu)r_0^3/2\pi(7-5\nu)$, in the case of the second-order inhomogeneity interaction. The MTP data are best fitted by Eq. (3b) with $A_2 \sim 3 \text{ eV } \text{\AA}^2$ (see Fig. 4), indicating that mainly second-order interactions govern the vacancy-dislocation interaction in bcc Nb at the MTP level. Larger deviations from the elasticity prediction are observed when the vacancy is in the dislocation core (2NN). Similar observations were also made for bcc W using empirical potentials [5].

Negative binding energies were reported for tungsten (W) as well, using several classical potentials: the Finnis-Sinclair [5], bond-order (BOP) [5,8], and EAM potentials [7,8]. On the other hand, both positive and negative binding energies, even in the dislocation core, were reported for α -Fe [6,9], Mo [6], and Ta [6].

C. Formation of complex topological defects

The attractive binding energies (Fig. 3) suggest that vacancies could affect both the screw dislocation topology and its mobility. We demonstrate in this section that the presence of a vacancy leads to significant changes in the screw dislocation topology.

In models without a vacancy, the screw dislocation line is straight before and after the jump from one Peierls valley to another. When a vacancy is introduced in the dislocation

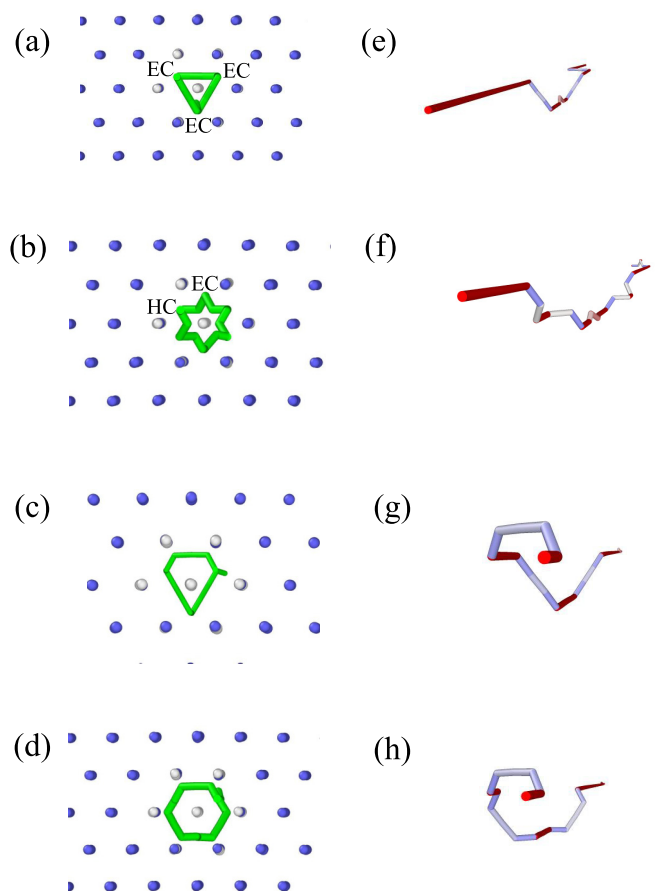


FIG. 5. Complex topological defects (CTDs): (a) trigonal; (b) star; (c) pentagonal, (d) hexagonal configurations of the screw dislocation (in green), projected on the (111) plane, with the vacancy in the dislocation core at the 1a position (cf. Fig. 1). The atoms in the dislocation core are colored in white, while the bcc atoms are colored blue. The corresponding multiple kinks along the screw dislocation lines are shown in (e)–(h), respectively. Screw components colored in red, edge components colored in blue, as given by OVITO [26].

core (e.g., positions 1a–1c, see Fig. 1), a segment of the screw dislocation bows out towards the vacancy already at zero external shear stress, indicating that the vacancy induces a high stress on the dislocation line. However, at zero external shear stress, the vacancy remains fully localized [$\xi = 1.0$; Fig. 6(a), black curve]. Already a small external shear stress leads to the formation of multiple kinks along the dislocation line with threefold symmetry [“trigonal” configuration, Fig. 5(a)] and the vacancy is dissociated with a degree of localization $\xi = 0.18$ [Fig. 6(a), red curve]. The multiple kinks position parts of the screw dislocation in the three-neighboring easy-core (EC) positions. With increasing shear stress, a “star” configuration with a sixfold symmetry is formed [Fig. 5(b)], and the vacancy is dissociated with a degree of localization $\xi = 0.32$ [Fig. 6(a), blue curve]. In this configuration, parts of the screw dislocation are placed at alternating EC–hard core (HC) lattice positions. As the screw dislocation has a higher energy at the HC positions than at the EC positions [31], this explains the appearance of the “star” configuration at higher shear stress. With a further increase in shear stress, first a “pentagonal” configuration [see Fig. 5(c)] with $\xi = 0.41$

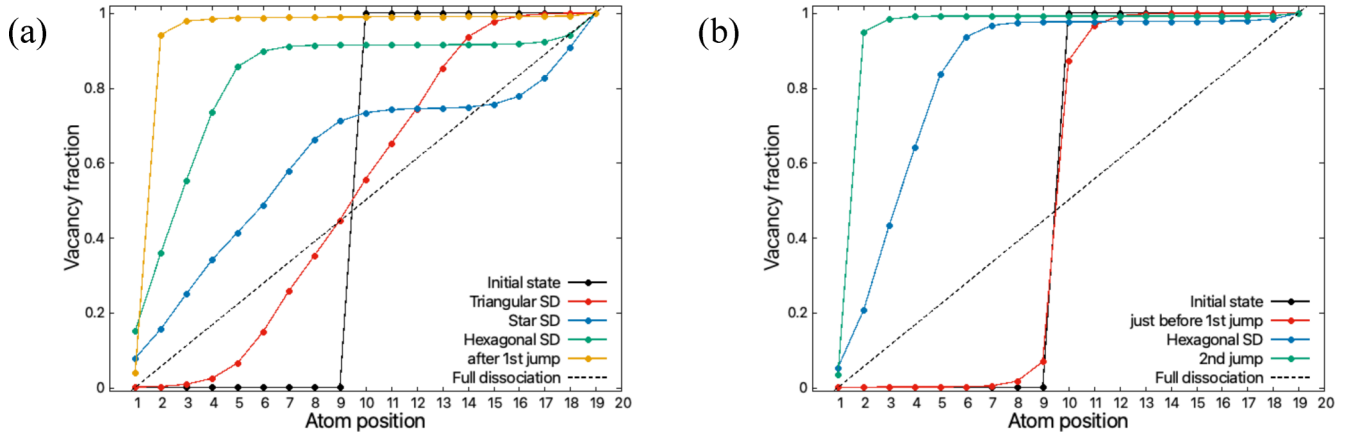


FIG. 6. Cumulative vacancy fractions for the: (a) initial fully localized state (black line); trigonal CTD (red line), star CTD (blue line), hexagonal CTD (green line), and localized state just after the first jump (brown line) at the 1a position; (b) initial fully localized state (black line); before the first jump (red line), hexagonal CTD (blue line) and localized state after depinning (green line) at the 3i position. The dashed black lines show the fully delocalized state.

and then a “hexagonal” configuration [Fig. 5(d)] form. In the hexagonal configuration, the vacancy is partially dissociated and partially localized with a degree of localization $\xi = 0.46$ [Fig. 6(a), green curve]. The screw dislocation remains *strongly* pinned in the “hexagonal” configuration until the first jump, after which a straight screw dislocation at a neighboring EC position and a *localized* vacancy are observed again [$\xi = 0.92$, Fig. 6(a), brown curve]. In this process, the vacancy jumps from the middle to the first position in the atomic row. These simulations confirm the suggestion of Thomson and Balluffi [32] that vacancies could dissociate along the screw-dislocation line.

Several topological characteristics of the CTDs at the 1a and 2d positions are given in Table I. The straight screw dislocation line is initially positioned in the center of the dislocation core (see Fig. 1). The formation of CTDs involves the nucleation of multiple kinks, inclined with respect to the dislocation direction [see Figs. 5(e)–5(h)] as a result of which the dislocation line spirals around the vacancy row. The number of kinks increases from 3 in the trigonal CTD to 12 in the star CTD (see Table I). In the trigonal CTD, the height of the three kinks is $h \approx 2.74 \text{ \AA}$. The components of

the Nye tensor are $\alpha_{ij} = b_i \rho_j$, $i, j = 1, 2, 3$, where $\mathbf{b}$ is the Burgers vector and $\boldsymbol{\rho}$ is a vector of the dislocation length per unit volume, which depends on the screw-edge character of the dislocation on each site [20]. For the large supercell, $\mathbf{b}$ is parallel to the Y axis, thus the only nonzero components of $\boldsymbol{\alpha}$ are α_{2j} , $j = 1, 2, 3$. The α_{22} component reflects the screw character, while $\alpha_{\text{Edge}} = (\alpha_{21}^2 + \alpha_{23}^2)^{1/2}$ reflects the edge character [20]. The introduction of a vacancy as a 1NN or 2NN of the screw dislocation leads to the formation of kinks with an edge component [see Figs. 5(e)–5(h)] and correspondingly, to a significant increase and redistribution of the α_{Edge} tensor components along the vacancy rows in the corresponding CTDs. The *maximum* values of α_{Edge} are listed in Table I. Since the Nye lattice *curvature* tensor $\boldsymbol{\kappa}$ is related to the Nye tensor $\boldsymbol{\alpha}$ by $\boldsymbol{\kappa} = \boldsymbol{\alpha} - \frac{1}{2} \text{Tr}(\boldsymbol{\alpha}) \mathbf{1}$ [33], where $\mathbf{1}$ is the identity tensor, the above results imply a significant increase of the α_{21} and α_{23} components of the lattice curvature tensor in the CTDs, with the largest values obtained for the trigonal CTD at the 2d position. The multiple kinks in these defect configurations spread over lengths ranging from $\sim 5b$ in the trigonal CTD and the hexagonal configuration to about $16b$ in the star configuration, thus increasing the end-to-end length

TABLE I. Topological characteristics of the CTDs.

State	Kinks	Dislocation Density $\times 10^5 \text{ (\AA}^{-2}\text{)}^a$	$\alpha_{\text{Edge}}^{\text{max}} \text{ (\AA}^{-1}\text{)}$	$\langle \delta \rangle$
<u>1a position</u>				
Dislocation + localized vacancy	0	3.56	0.002	2.6 ± 4
Trigonal CTD	3	3.61	0.08	2.0 ± 2
Star CTD	12	3.68	0.10	2.0 ± 2
Pentagonal CTD	5	3.63	0.08	2.3 ± 5
Hexagonal CTD	9	3.69	0.07	2.4 ± 6
<u>2d position</u>				
Dislocation + localized vacancy	0	3.63	0.013	2.5 ± 4
Trigonal CTD	3	3.61	0.13	2.0 ± 3
Pentagonal CTD	5	3.63	0.12	2.1 ± 4
Hexagonal CTD	9	3.67	0.08	2.4 ± 6

^aDislocation density per unit dislocation length $= L_{\text{SD}}/V$, where L_{SD} is the total length of the screw dislocation, as determined from the OVITO program [26], where V is the volume of the supercell.

of the screw dislocation and the corresponding dislocation density (see Table I). DFT calculations with a periodic length typically of only $1b$ along the dislocation line [28] cannot properly capture the nature of these extended defects.

Table I includes also the average extrapolation grades, $\langle\delta\rangle$, for the different CTD configurations at the 1a and 2d positions. Benchmark calculations with only a localized vacancy give $\langle\delta\rangle = 0.9 \pm 2.2$ and with only a straight dislocation $\langle\delta\rangle = 1.6 \pm 1.2$. The average local extrapolation grades with *both* a screw dislocation and a dissociated vacancy are below 3 within error limits, indicating *reliable* extrapolation according to the classification given in Ref. [19], thus confirming further the robustness of the observed CTDs.

When the vacancy is at a larger distance ($R > R_{2NN}$), but its angular position is relatively close to the screw dislocation trajectory ($|\Theta - \Omega| < 20^\circ$, e.g., position 3i, see Fig. 1), the behavior is different (Θ is the angle between the radius vector of the vacancy and the direction of the Peach-Köhler force; $\Omega = -60^\circ$ [10] is the average angle of the dislocation trajectory with respect to the $+X$ axis). At zero external shear stress, the vacancy is fully localized [$\xi = 1.0$; Fig. 6(b), black curve]. There is no or only a small initial bow-out of the dislocation, because the stress produced by the vacancy decreases as $\sim 1/R^3$ with increasing vacancy-dislocation distance R [2]. The screw dislocation remains straight and the vacancy relaxes slightly with a degree of localization $\xi = 0.85$ [Fig. 6(b), red curve], as long as $R > 6 - 7 \text{ \AA}$. When the screw dislocation *approaches* the vacancy ($R < 6 \text{ \AA}$), it is attracted to it, bows out and a “hexagonal” CTD with a degree of localization $\xi = 0.50$ [Fig. 6(b), blue curve] is formed. The screw dislocation remains weakly pinned in this state until the next jump of the screw dislocation, after which the vacancy becomes localized again [$\xi = 0.94$, Fig. 6(b), green curve]. Similar vacancy-fraction curves are obtained also for, e.g., the 4k and 5q positions. For vacancy positions like 3h, 4n, 5o, etc., no dissociation of the vacancy and no formation of multiple kinks are observed.

Such screw-dislocation topologies have not been reported in any previous simulation study of vacancy-dislocation interactions in bcc metals. Dissociation of a vacancy in the screw dislocation core at *zero* shear stress has been reported in models of α -Fe, Mo, and Ta [6] using classical potentials. The present results demonstrate that this process is more general and that the degree of vacancy dissociation depends on the vacancy position, the applied shear stress, and the dislocation topology.

The *simultaneous* nucleation of multiple kinks with three-, five-, or sixfold symmetry and the dissociation of the vacancy in models with *both* a screw dislocation and a vacancy, as described above, represent the formation of *coupled defects*. These coupled defects disappear *simultaneously* after the screw dislocation is depinned from the vacancy, and they can be conceptualized as complex topological defects (CTDs). Due to their extended nature, CTDs are observed in atomistic models with a dislocation length of $\geq 5b$. The formation of these CTDs confirms the theoretical predictions made by Kröner [3] and Thomson and Balluffi [32] unambiguously.

The different CTDs and the corresponding pinning regimes are summarized in Fig. 7. When the vacancy is in the dislocation core ($R \leq R_{2NN}$), several different CTDs are ob-

served. For distances in the range from 3NN to 5NN (and $-90^\circ < \Theta < 30^\circ$), the formation of only hexagonal CTDs is observed. The different CTDs have different ranges of mechanical stability with increasing shear stress. The forces acting between n interacting kinks must be balanced by the applied shear stress in order for the system to be in mechanical stability. The minimum shear stress necessary for the mechanical stability of a given CTD should increase with increasing number of kinks, as observed qualitatively from the atomistic simulations: In the case of 1NN, a trigonal CTD appears at very low shear stress, a pentagonal CTD at about 0.2 GPa, and a hexagonal CTD at about 0.76 GPa. In the case of 2NN, a trigonal CTD forms at about 0.14 GPa, a pentagonal CTD at about 0.23 GPa, and a hexagonal CTD at about 0.74 GPa. In the case of 3NN-5NN, only a hexagonal CTD is formed at even higher shear stresses. For vacancy positions at larger distances ($R > 7 \text{ \AA}$), but relatively close to the dislocation trajectory ($|\Theta - \Omega| < 20^\circ$, e.g., positions 8v, 8w), a hexagonal CTD is also formed when the dislocation approaches the vacancy.

The topology of the screw dislocation in the hexagonal CTD resembles a *single* “helical turn” [see Fig. 5(b)]. The presence of multiple vacancies could lead to the interaction of hexagonal CTDs and the formation of a helical-like dislocation (see Fig. 8). The helical-like dislocation in Fig. 8 was generated by simultaneously introducing three vacancies along the 1a atomic row, separated by distances of $L_y/3$.

The formation of helical dislocations at *large* chemical stresses, produced by high vacancy concentrations, has been theoretically analyzed (e.g., Weertman [34]) and experimentally observed in different neutron-irradiated materials (Ref. [35] and references therein). It should be noted, however, that (1) the force produced by the chemical stress on the dislocation and, correspondingly, the number of helical turns are temperature dependent in these models and should be zero at 0 K [34]; (2) both the concentration of vacancies and the helical pitch (λ) in neutron-irradiated materials are quite large (typically vacancy concentration $\sim 10^4$ vacancies/helical turn and $\lambda \sim 500\text{--}700 \text{ \AA}$); (3) the absorption of vacancies, produced by irradiation, in pre-existing screw dislocations and the formation of helical dislocations by dislocation climb typically take place at zero shear stress and ambient (or higher [35]) temperature. Here, we demonstrate that helical-like screw dislocations could be formed at much lower vacancy concentrations (1 vacancy/helical turn) in nonirradiated materials at 0 K under shearing due to the interaction of hexagonal CTDs.

D. Peierls and depinning stresses

Probably the most important physical quantity that determines the dislocation mobility is the Peierls potential and the corresponding Peierls stress (τ_p) [2]. In atomistic simulations, the shear stress at which the screw dislocation starts to move is commonly identified as the Peierls stress. The Peierls stress of the investigated supercell model of bcc Nb in the absence of a vacancy is 1.27 GPa.

The results presented in Sec. III C show that, when the vacancy is closer to the screw dislocation, it can lead to pinning of the screw dislocation during shearing, and it is necessary to

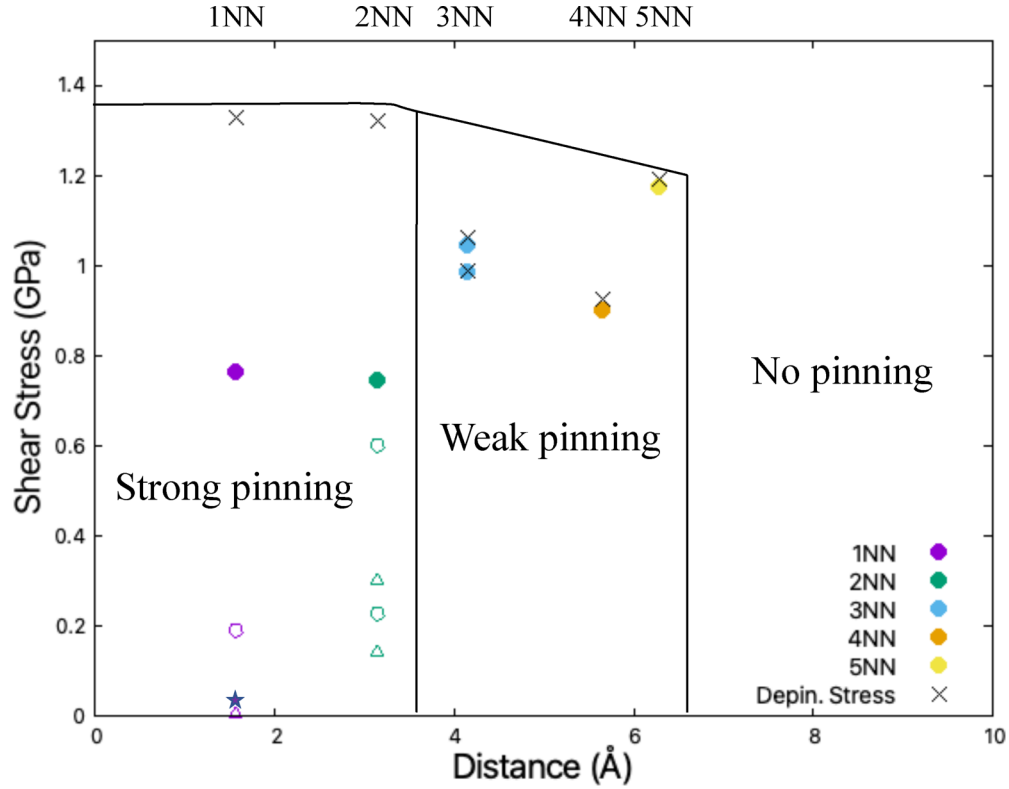


FIG. 7. Dependence of the depinning stresses (x) and the *minimum* shear stresses necessary for the formation of the corresponding CTDs on the vacancy-dislocation distance: trigonal CTD (empty triangles), star CTD (star), pentagonal CTD (empty pentagons), and hexagonal CTD (full circles). The black lines are only a guide for the eye.

distinguish between Peierls and depinning stresses. We denote as the Peierls stress the stress needed to move the dislocation from its *initial* position in the simulation cell (regardless of the relative position of the vacancy), while the depinning stress is the stress required to move the dislocation *away from a*

vacancy after pinning (regardless of the actual step during the simulation). When the vacancy is in the dislocation core (e.g., positions 1a-2f), the screw dislocation is strongly pinned at the vacancy, and much higher shear stress is necessary for depinning. In this case, the Peierls stress and the depinning stress are equal.

For vacancy-dislocation distances in the range $R_{3NN}-R_{5NN}$ and $|\Theta-\Omega| \leq 50^\circ$ (e.g., positions 3i, 3g, 4k, 5p, 5q), formation of a hexagonal CTD and weak pinning are observed *after* the onset of screw dislocation movement. The shear stresses required for depinning from the hexagonal CTD are higher than the corresponding Peierls stresses (see Table II). For vacancy-dislocation distances in the range $R_{3NN}-R_{5NN}$ and $|\Theta-\Omega| > 50^\circ$ (e.g., positions 3y, 4n, 5r), weak pinning *without* the formation of CTDs is observed *after* the onset of screw dislocation movement. Finally, when the vacancy is at a larger distance ($R > 7$ Å) and away from the dislocation trajectory ($|\Theta-\Omega| \geq 50^\circ$, e.g., positions 5o, 7t, 7u, 8x, 8y), no formation of CTDs and no pinning are observed.

The depinning stresses τ_D are approximately equal (1.31 ± 0.03 GPa) regardless of the vacancy position (see Table II). On the contrary, the Peierls stresses depend sensitively on the vacancy position, relative to the screw dislocation. Physically, in all cases, the screw dislocation is attracted to the vacancy. However, when the radius vector of the vacancy and the initial bow-out are approximately parallel to the glide direction [Fig. 9(a)], the attraction leads to a smaller Peierls stress. Vice versa, the vacancy *pulls back* the dislocation and leads to a larger Peierls stress, when the radius vector of the vacancy

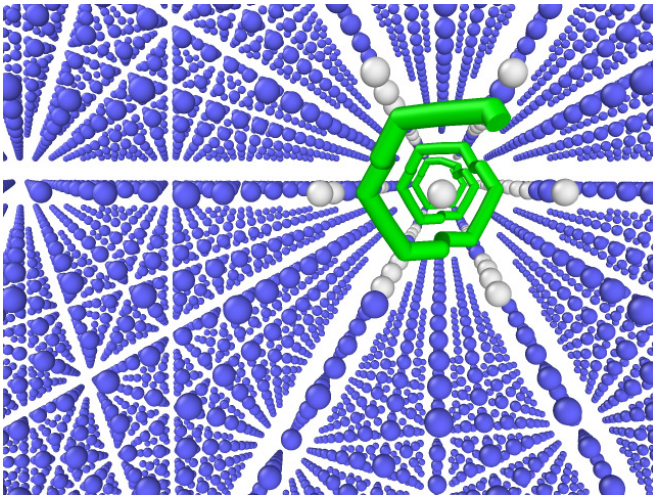


FIG. 8. Helical-like screw dislocation with helical pitch $\lambda \sim 19$ Å and radius ~ 2.1 Å, formed under shear in the presence of three vacancies in the 1a row. The atoms in the extended dislocation core are colored in white, while the bcc atoms are colored blue, as given by OVITO [26].

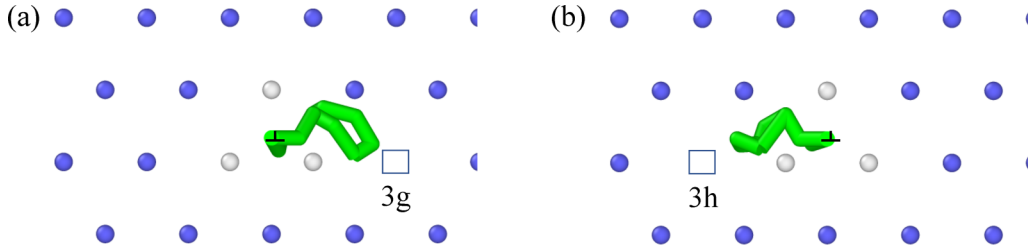


FIG. 9. Initial bow-out of the screw dislocation, when (a) the vacancy is at the 3g position and (b) the vacancy is at the 3h position. The position of the initial straight screw dislocation is marked with $\perp$. The atoms in the dislocation core are colored in white, while the bcc atoms are colored blue, as given by OVITO [26].

and the initial bow-out are approximately opposite to the glide direction [Fig. 9(b)].

This is well exemplified by the Peierls stresses at positions 3g and 3h, or at position 5o, compared to positions 5p and 5q. This effect was further cross-checked by changing the sense of shearing. Changing the sense of shearing leads to the transformation $\Theta \rightarrow 180 - \Theta$ and the Peierls stress should increase (decrease) respectively. Indeed, the Peierls stress, with the vacancy at, e.g., the 3g position, is 1.19 GPa for positive sense of shearing, but increases to 1.28 GPa for negative sense

TABLE II. Radial (R) and angular (Θ) coordinates of the vacancy and the corresponding Peierls and depinning stresses (in GPa). The vacancy-dislocation distances R are given with respect to the screw-dislocation position. Θ is the angle between the radius vector of the vacancy and the $+X$ direction. Positive angles are defined as being anti-clockwise, and vice versa for negative angles.

NN	Position	R (Å)	Θ (°)	Depinning stress	Peierls stress
1	a	1.57	-29.3	1.34	1.34
	b	1.58	89.6	1.34	1.34
	c	1.55	209.9	1.33	1.33
2	d	3.15	30.2	1.32	1.32
	e	3.13	149.7	1.34	1.34
	f	3.13	-89.3	1.33	1.33
3	g	4.15	-10.7	1.31	1.19
	h	4.13	190.7	—	1.31
	i	4.14	-49.0	1.32	0.99
	j	4.16	70.8	—	1.27
	y	4.13	229.1	1.26	1.12
4	k	5.64	-76.0	1.33	0.93
	l	5.66	16.2	1.31	0.91
	m	5.64	163.7	—	1.27
	n	5.63	256.2	1.34	1.14
5	o	6.80	186.5	—	1.28
	p	6.27	-29.8	1.30	1.19
	q	6.82	-53.3	1.32	1.19
	r	6.83	-6.5	1.30	1.27
6	s	8.28	-70.8	1.32	1.27
7	t	9.53	-4.6	—	1.28
	u	9.51	184.6	—	1.27
8	v	11.30	-43.8	1.30	1.27
	w	13.90	-46.9	1.30	1.27
	x	13.38	-24.11	—	1.27
	y	12.24	-3.6	—	1.27

of shearing. Similarly, the Peierls stress, with the vacancy at the 4k position, is 0.93 GPa for positive sense of shearing, but increases to 1.13 GPa for negative sense of shearing.

Nb specimens, used for the experimental determination of the Peierls stress and the temperature dependence of the flow stress, are commonly prepared through cyclic plastic deformation [36]. The vacancy concentration in these specimens [36] was not specified. However, it has recently been demonstrated experimentally that such procedures lead to high concentrations of *nonthermal* vacancies in both fcc (Al, Ni, Cu) and bcc (Fe, Nb, W) metals at room temperature [37]. The present simulations show that the presence of vacancies in real materials could lead either to a slight increase of the Peierls stress by pinning or to a decrease of the Peierls stress, depending on the predominant arrangement of the dislocation-vacancy complexes.

IV. CONCLUSIONS

We have studied vacancy-screw dislocation interactions in bcc Nb using a state-of-the-art moment tensor potential (MTP) with near DFT accuracy. Additional validation of the developed MTP was made against DFT calculations using a quadrupole supercell containing both screw dislocations and a vacancy. It has been demonstrated that vacancy-dislocation interactions are attractive and have almost perfect threefold symmetry (point group $3m$) in the (111) plane. In contrast, similar simulations performed with a classical EAM potential for bcc Nb [12] exhibit vacancy-dislocation interactions with only mirror symmetry parallel to the Z axis (point group m). The knowledge obtained from the present high-accuracy results thus opens an interesting direction of future investigations, namely the construction of symmetry-based EAM potentials for bcc metals, as proposed for fcc Cu [38].

The attractive vacancy-dislocation interactions lead to (1) a slight reduction in the Peierls stress, which depends sensitively on the position of the vacancy relative to the screw dislocation, and (2) the formation of complex topological defects (CTDs), which were predicted theoretically in the early 1990s using differential geometry. The CTDs consist of screw dislocations with multiple kinks and a (partially) dissociated vacancy along the dislocation line. The formation of CTDs constitutes a new mechanism for pinning screw dislocations. The presence of several hexagonal CTDs could lead to the formation of helical-like screw dislocations under shear, at much lower vacancy concentration compared to that in neutron-irradiated materials. The formation and subsequent

disappearance of the CTDs under shearing also lead to jumps of the vacancy along the dislocation line, thus providing a possible mechanism for fast (pipe) diffusion of nonthermal vacancies at *low* temperatures during plastic deformation.

The *extended* nature of the CTDs underlines the necessity of using large atomistic models and dedicated machine-learning potentials for an accurate description of the defect properties of metals. Extension of the present work could be the investigation of CTD formation in the case of $1/2\langle 111 \rangle\{112\}$ screw dislocations, which exhibit twinning-anti-twinning asymmetry, higher Peierls stresses, and different dislocation trajectories [10], as well as further characterization of these new topological defects using differential geometry.

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DATA AVAILABILITY

Data will be made available upon a reasonable request.

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