

Tunable energy landscape of screw dislocation cores by compositional fluctuations in bcc high-entropy alloys from first-principles calculations

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The energy landscape of screw dislocation cores plays a central role in dislocation-mediated deformation mechanisms in body-centered cubic (bcc) metals. In bcc high-entropy alloys (HEAs), this energy landscape is modulated by local compositional fluctuations, which has important implications for deformation processes in these materials. Through first-principles calculations, this study investigates high-symmetry screw dislocation core structures in NbTaMoW and NbTaTiHf bcc HEAs. The results show that alloying group IV transition metals lead to large local lattice distortions at dislocation cores, which is demonstrated to be an important factor governing fluctuations in core configurations along a dislocation line. Importantly, group IV elements near the core induce features in the energy landscape that are exclusive for HEAs, specifically lowering the energy of core configurations that are unstable in elemental bcc metals. A combined influence of these chemical effects with crystallographic details enables the activation of {112} glide planes, a feature that has been linked to ductility improvements in bcc HEAs. These findings provide new insights into the atomic-scale mechanisms underlying dislocation mobility in bcc HEAs, offering a pathway for designing materials with tailored mechanical properties.

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I. INTRODUCTION

High-entropy alloys (HEAs), metallic alloys containing multiprincipal elements, have attracted considerable attention in research due to their nearly unlimited potential for designing materials with optimized mechanical properties for structural applications [1,2]. Among these, a specific class crystallizes as single-phase body-centered cubic (bcc) solid solutions [3], primarily composed of refractory transition metals of groups V (V, Nb, Ta) and VI (Cr, Mo, W) [4,5], as well as group IV elements (Ti, Zr, Hf) [6]. Depending on composition, bcc HEAs have been demonstrated to show outstanding mechanical properties such as high resistance to yield stress thermal softening [5], and retained tensile ductility even at low temperatures [7–9]. The unique performance of bcc HEAs arises from a complex combination of deformation mechanisms [7,10–12], in which $1/2 \langle 111 \rangle$ screw dislocations play a central role [13–16].

With the aim of establishing the link between deformation mechanisms and alloy chemistry, theoretical and computational work has examined the properties of screw dislocations [17–20]. At the atomic scale, where the properties

of these dislocations are controlled by their core structure [21], density-functional theory (DFT) calculations have been focused on ground state core configurations [17,20]. However, these calculations are insufficient to provide a detailed description of the dislocation core energetics, presenting a situation where the fundamental understanding of dislocation motion in bcc HEAs remains incompletely understood.

In the present work, we perform explicit DFT calculations of high-symmetry $1/2 \langle 111 \rangle$ screw dislocation core structures in NbTaMoW and NbTaTiHf bcc HEAs. These compositions are chosen to represent broader families of bcc HEAs, i.e., refractory and group IV element containing alloys, respectively. Results show that additions of group IV metals lead to appreciable distortion of the core structure, which has important implications for the fluctuations in core geometries due to variations in composition along a dislocation line. Importantly, we observe that the core energy is strongly influenced by its local chemical environment, and that group IV elements induce features in the core energy landscape that are unique to this family of alloys. We further correlate these findings with dislocation slip crystallographic details, and discuss the implications for strength and ductility.

II. METHODS

A. First-principles calculations

All first-principles calculations are performed within density functional theory (DFT) as implemented in the Vienna *ab initio* simulation package (VASP) code [22–24]. We employ the projector augmented wave (PAW) formalism [25,26], and

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the Perdew-Burke-Ernzerhof generalized gradient approximation (GGA-PBE) [27] to model the exchange-correlation potential. A plane-wave basis set with a kinetic energy cutoff of 600 eV is used, and in the k -point sampling we use the Methfessel-Paxton scheme [28] with a smearing of 0.2 eV to broaden the electronic occupation. The employed PAW potentials treat 4, 4, 11, 5, 6, and 6 electrons as valence for Ti, Hf, Nb, Ta, Mo, and W, respectively. Atomic relaxation is carried out at constant cell shape and volume at the equilibrium lattice parameter, until residual ionic forces have magnitudes below 10 meV/Å. To sample the Brillouin zone in the DFT calculations, we make use of a Γ -centered $2 \times 2 \times 16$ k -point grid.

B. Atomistic calculations

Atomistic calculations are performed using the large-scale atomic/molecular massively parallel simulator (LAMMPS) package [29]. We use previously reported machine learning interatomic potentials for NbTaMoW [30] and NbTaTiHf [31], based on spectral neighbor analysis potential (SNAP) and atomic cluster expansion (ACE) formalisms, respectively. The atomic positions are relaxed using the conjugate gradient algorithm as implemented on LAMMPS, until the energy difference between two successive iterations divided by the magnitude of total energy is less than 10^{-8} eV, and residual ionic forces have magnitudes below 10^{-4} eV/Å.

C. Simulation cell

Chemical disorder is modeled using the special quasirandom structures (SQS) approach [32]. We use the MCSQS [33] package in the alloy theoretic automated toolkit (ATAT) to generate the SQS models, which are constructed to provide correlation functions for the first two neighbor shells that approximate a random solution for all constituent elements.

$1/2 \langle 111 \rangle$ screw dislocations are modeled using a quadrupolar arrangement with periodic boundary conditions [34,35]. The simulation cell periodicity vectors $\{\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3\}$ are $\mathbf{p}_1 = 5/2 \mathbf{u}_1 - 9/2 \mathbf{u}_2$, $\mathbf{p}_2 = 5/2 \mathbf{u}_1 + 9/2 \mathbf{u}_2$, and $\mathbf{p}_3 = \mathbf{u}_3$, where $\mathbf{u}_1 = a_0 [1 \ 1 \ 2]$, $\mathbf{u}_2 = a_0 [1 \ \bar{1} \ 0]$, and $\mathbf{u}_3 = a_0/2 [1 \ 1 \ 1]$ are the elementary vectors. This supercell geometry contains a total of 135 atoms, which is used to perform the DFT calculations. For the atomistic calculations, we replicate the geometry above 5, 5, and 100 times along $\mathbf{p}_1$, $\mathbf{p}_2$, and $\mathbf{p}_3$, respectively, yielding a final configuration with a total of 337 500 atoms. We note that the SQS models for DFT and atomistic calculations are generated independently. A dislocation dipole of Burgers vector $\vec{b} = -a_0/2 [1 \ 1 \ 1]$ is introduced in the simulation cell using anisotropic elasticity theory as implemented in the Babel package [36]. It is important that both dislocations composing the dipole relax toward the same configuration to obtain their core energy. After building the SQS models, we further impose a twofold rotational symmetry around $\mathbf{u}_1$ to ensure that both dislocations in the dipole observe the same local chemical environment [19].

III. RESULTS AND DISCUSSION

The following subsections are organized as follows. We first examine high-symmetry configurations of screw

dislocation cores, and analyze the effects of local lattice distortions. We study next variations of the core energy in the $\{111\}$ plane, focusing on the role of core position and local chemical environment. Further, we establish a link between features of the core energy landscape and dislocation slip details and ductility. At last, we assess the roughness of the dislocation line profile, and discuss correlations with strengthening models in the literature.

A. Screw dislocation core structure

We consider first high-symmetry core configurations of $1/2 \langle 111 \rangle$ screw dislocations, a property that critically controls the energy landscape of these dislocations [37]. Previous theoretical studies have identified three types of high-symmetry core structures [38]. The first case, referred to as the easy core, is the ground state configuration in elemental bcc metals [39]. The second case corresponds to an energy maximum, called a hard core [39]. Using differential displacements (DD) maps [40] for visualization, easy and hard cores correspond to dislocation positions at the gravity center of upward and downward triangles of $\langle 111 \rangle$ atomic columns, respectively (see Fig. 1). A third high-symmetry core configuration can be identified when the dislocation approaches a $\langle 111 \rangle$ atomic column, named as split core [37]. To obtain relaxed configurations of hard and split cores, we perform constrained ionic relaxations as described in Ref. [39].

Figure 1 shows DD maps of high-symmetry core structures in NbTaMoW and NbTaTiHf bcc HEAs. We observe that the core structures in NbTaMoW display features similar to an elemental crystal. Specifically, atomic displacements and Nye tensor components [41] found in the vicinity of the core are consistent with those produced by the insertion of a screw dislocation in the bcc lattice. In NbTaTiHf, by contrast, we observe pronounced displacements spread in the $\{111\}$ plane and even far from the core, introducing substantial perturbation in the calculation of the Nye tensor.

The different features of the core in the considered HEAs can be understood regarding the average local lattice distortions (LLDs) magnitude observed in these materials, i.e., the average atomic displacement away from the reference bcc lattice positions obtained from the structural relaxation of bulk alloy. In detail, DFT calculations [20] show that average LLDs can be more than three times larger in NbTaTiHf ($\simeq 0.13$ Å) compared to NbTaMoW ($\simeq 0.04$ Å). Further, using the anisotropic elasticity solution as reference [42], LLDs in NbTaTiHf can be as large as the absolute atomic displacements along the screw component produced by the dislocation at the vicinity of the core [43,44]. In this sense, we observe that group IV alloying elements induce appreciable distortions of the bcc lattice, and thus to the core structure of screw dislocations.

It is highlighted in Ref. [18] that LLDs in bcc HEAs containing group IV elements may be preferred (correlated) along the $\langle 111 \rangle$ direction, which coincides with the Burgers vector direction of screw dislocations, and could influence dislocation mobility. Additionally, atomistic simulations reports [45–47] show that an increase in bulk LLDs correlates with a decrease in the disparity between the mobilities of edge and screw dislocations [46]. This effect is attributed to

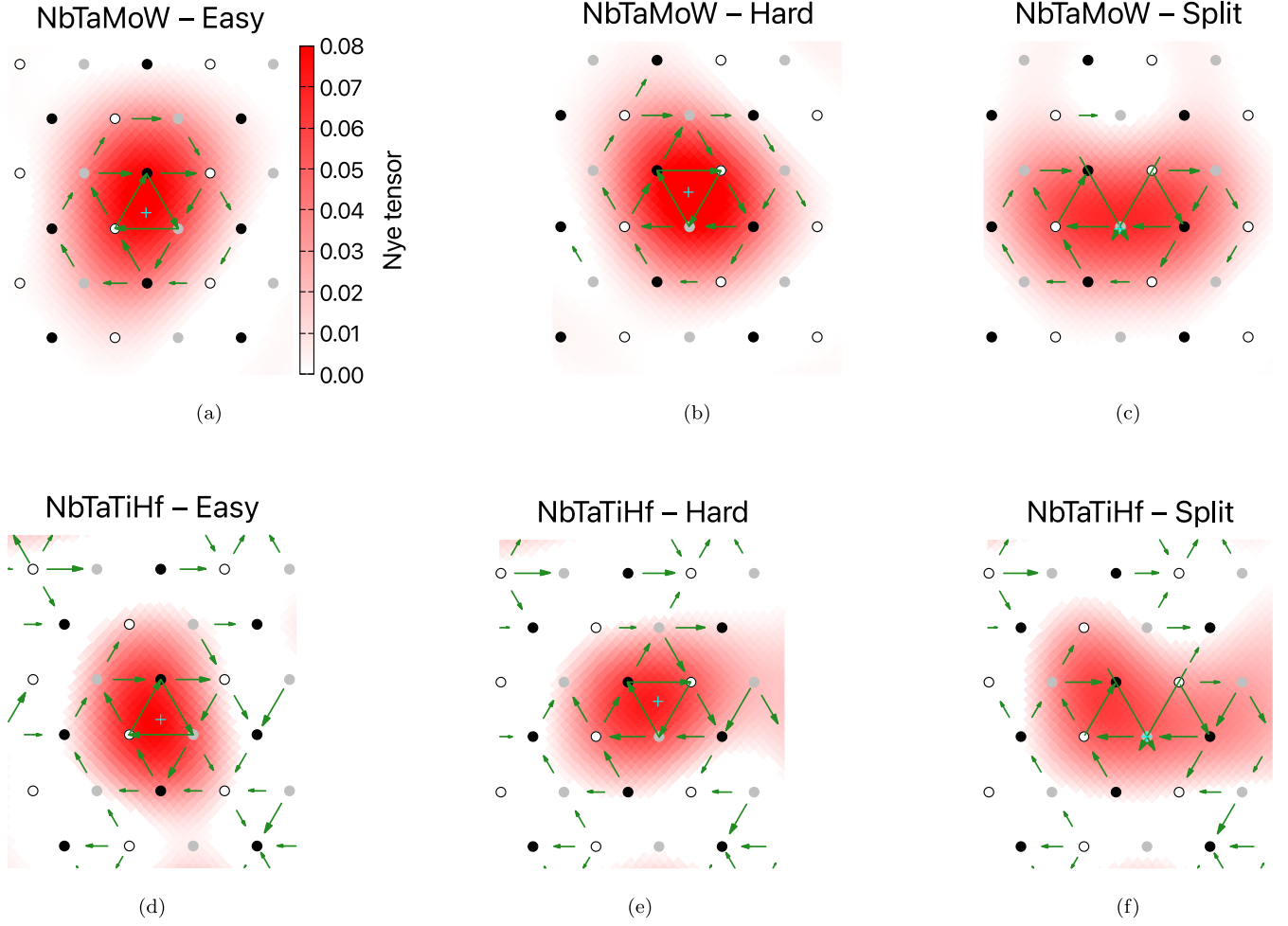


FIG. 1. First-principles calculated screw dislocation high-symmetry core structures in bcc HEAs. Differential displacement maps of high-symmetry configurations of $1/2 \langle 111 \rangle$ screw dislocation cores in (a)–(c) NbTaMoW and (d)–(f) NbTaTiHf. (a), (d) Easy and (b), (e) hard cores correspond to dislocation positions at the gravity center of upward and downward triangles of $\langle 111 \rangle$ atomic columns, respectively, and the (c), (f) split core corresponds to the dislocation position at the vicinity of a $\langle 111 \rangle$ atomic column. The atomic structure is projected in the $\{111\}$ plane, and white, gray, and black circles indicate original $\{111\}$ planes in a perfect bulk bcc crystal. Arrows are drawn proportional to the relative displacement normalized by $b/2$ between neighboring $\langle 111 \rangle$ atomic columns along the Burgers vector direction, and are omitted if they are smaller than $b/12$. The contour map shows the screw component of the Nye tensor, and cyan crosses indicate the dislocation position.

significant lattice friction experienced by edge dislocations due to chemical disorder (see below).

B. Screw dislocation core energy landscape in the $\{111\}$ plane

We consider next the energy landscape of $1/2 \langle 111 \rangle$ screw dislocations, which is closely correlated with details of dislocation slip [37,48]. In principle, the dislocation can assume any position in the $\{111\}$ plane, leading a two-dimensional Peierls potential [37]. The high-symmetry core configurations presented in the previous subsection are expected to be a local energy extremum of this potential [38], providing valuable insight into the fundamental dislocation mobility.

To elucidate alloying effects, we calculate the relative energies of hard (E_H) and split (E_S) cores with respect to the easy core in elemental bcc metals, which are defined as

$$E_H = 1/2(E_{\text{hard}}^{\text{dipole}} - E_{\text{easy}}^{\text{dipole}}), \quad (1)$$

$$E_S = 1/2(E_{\text{split}}^{\text{dipole}} - E_{\text{easy}}^{\text{dipole}}), \quad (2)$$

where $E_{\text{easy}}^{\text{dipole}}$, $E_{\text{hard}}^{\text{dipole}}$, and $E_{\text{split}}^{\text{dipole}}$ are DFT calculated energies of the dipole supercell with easy, hard, and split core configurations, respectively. We highlight that group IV metals show an unstable bcc lattice at zero temperature [49], which challenges the calculation of relaxed core structures in these materials. We therefore approximate the core energies for Ti and Hf using the relaxed atomic positions obtained for Nb in the DFT calculations. Although these results are not quantitatively accurate for Ti and Hf, core energies for these metals are nevertheless included to discuss trends across transition metals of groups IV, V, and VI.

Table I presents first-principles calculated hard and split core energies for elemental bcc metals. Results show that whereas the easy core corresponds to local energy minima in elements of groups V and VI, the split core is the low energy

TABLE I. First-principles calculated screw dislocation core energies in elemental bcc metals. Energies of hard (E_H) and split (E_S) cores with respect to the easy core, all of which are expressed in units of meV/b. Results for Ti and Hf are approximated using relaxed atomic positions obtained for Nb in the DFT calculations.

	E_H	E_S
Ti	46	-13
Hf	40	-27
Nb	61	67
Ta	45	60
Mo	94	147
W	130	203

configuration in group IV metals. We note that results obtained for group V and VI elements are in excellent agreement with previous DFT [37] reports within 5%.

To obtain the core energy landscape in NbTaMoW and NbTaTiHf, we calculate the core energy in various positions in the {111} plane, sampling the effects of local chemical environment on high-symmetry core configurations. We define a reference (zero) energy level as the average of easy core energy values for each HEA. We highlight that our study provides details of core energetics beyond those presented in previous DFT reports [17,19,50], by considering high-energy core structures in addition to those corresponding to Peierls valleys. Additionally, we note that although a single SQS model is used for each alloy composition, the effects of

compositional fluctuations are sampled by surveying various core positions in the {111} plane, which mimics corresponding fluctuations across different SQS models. Since the DFT calculations are performed in relatively large cells (135 atoms), this strategy allows the most optimal use of computational resources.

Figure 2 shows the first-principles calculated screw dislocation core energy landscape in NbTaMoW and NbTaTiHf bcc HEAs. We observe that the core energy is strongly influenced by its position in the {111} plane, showing a maximum energy difference between the highest and the lowest energy values of 530 meV/b and 247 meV/b in NbTaMoW and NbTaTiHf, respectively. To obtain further insight into fluctuations in the energy landscape, we calculate the root mean square (RMS) average of core energies (E_i) defined as

$$RMS = \sqrt{\frac{1}{n} \sum_{i=1}^n E_i^2}, \quad (3)$$

and obtain 186 meV/b and 76 meV/b for NbTaMoW and NbTaTiHf, respectively. Such large RMS values have strong implications for the dislocation line, which may adopt a wavy profile in order to minimize its energy [10]. To complement the statistical analysis of these energy fluctuations, the average and standard deviation of hard and split core energies in NbTaMoW and NbTaTiHf are presented in Table II. We note that the complete distribution of core energies used in these statistical analyses are presented in Fig. 2.

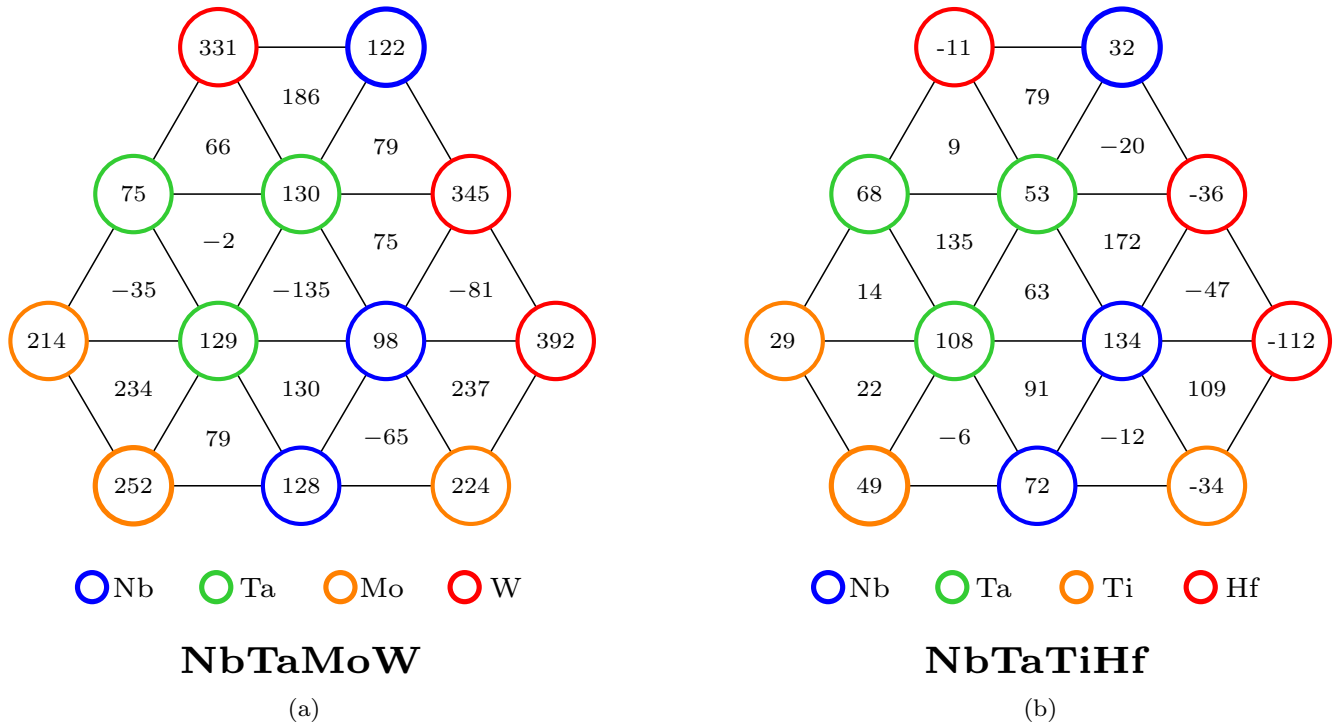


FIG. 2. First-principles calculated energy landscape of screw dislocation cores in bcc HEAs. Schematic representation of the $1/2 \langle 111 \rangle$ screw dislocation core energy landscape in the {111} plane in (a) NbTaMoW and (b) NbTaTiHf. The zero-energy level is defined as the average of easy core energy values for each HEA, and annotated values in the plots above indicate relative energy differences with respect to this reference energy level at respective positions in the {111} plane. All energies are given in units of meV/b. Atoms are color coded by element: Nb (blue), Ta (green), Mo (orange), W (red), Ti (orange), and Hf (red).

TABLE II. Average and standard deviation (std. dev.) of hard and split core energies in NbTaMoW and NbTaTiHf of core energy distributions shown in Fig. 2. All energies are given in units of meV/b.

		Average	Std. dev.
NbTaMoW	Hard	143	95
	Split	203	107
NbTaTiHf	Hard	102	51
	Split	29	68

We undertook an effort to develop a lattice model for the core energies based on the site occupation dependency on the local chemical environment in the vicinity of the core. However, our analysis revealed that this model was unable to reproduce the results obtained from the DFT calculations. This discrepancy highlights the fact that the core energy landscape is influenced by pairwise and multibody interactions between atoms within the core. Further, we verified that the core energetics cannot be approximated using rule of mixtures approaches based on core energies computed for elemental bcc metals. These findings show that the core energy landscape strongly depends on the synergies arising from compositional complexity around the core, which can only be obtained through explicit DFT or atomistic approaches.

Importantly, we observe that while local minima of the energy landscape are found at easy core positions in NbTaMoW, these local minima may occur either at easy or split core positions in NbTaTiHf. Moreover, low-energy split core positions in NbTaTiHf correspond to an atomic column of group IV elements, notably Hf, highlighting the key role of the local chemical environment on the core energy.

In this sense, composition can be tuned to control the energy landscape of screw dislocations, leading to features that are unique to HEAs. Specifically, the addition of group IV alloying elements enables to relatively lower the energy of split cores, which might have strong implications for the dislocation motion. Figure 3 schematically illustrates the dislocation slip crystallographic details, showing that two consecutive easy cores are directly connected along $\{110\}$ planes, and are connected through the hard or split cores along $\{112\}$ planes. Further, $\{112\}$ planes show twinning/antitwinning asymmetry, an intrinsic property of the bcc lattice [51], in which the twinning direction correspond to a softer path through the split core [48].

As a result, a combination of chemical effects and crystallographic details may constrain dislocation slip along $\{110\}$ planes in NbTaMoW, while in NbTaTiHf, by contrast, an increased participation of $\{112\}$ planes might be observed. Additionally, DFT calculations in Ref. [20] show that group IV element additions induce isotropy between $\{110\}$ and $\{112\}$ planes in terms of unstable stacking fault energies, a property linked to dislocation mobility [52,53]. The activation of $\{112\}$ slip has been correlated with improvements in ductility by experimental reports [18,54], and is considered a key factor underlying the enhanced damage tolerance observed in bcc HEAs containing group IV elements [20].

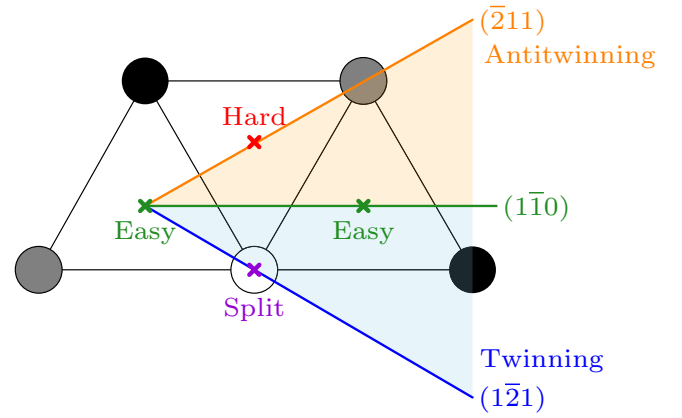


FIG. 3. Dislocation slip crystallographic details. Projection of the bcc lattice in the $\{111\}$ plane showing high-symmetry easy, hard, and split core positions. $\{110\}$ and $\{112\}$ slip planes are shown using straight lines, and twinning and antitwinning regions are shown as shaded areas in blue and orange, respectively.

C. Screw dislocation line profile

As discussed in the previous subsections, details of the local chemistry are shown to induce fluctuations in the core energy landscape and distortions of the bcc lattice, both which can lead to rugged dislocation lines [55]. To study the line profile of screw dislocations in the considered HEAs, we perform atomistic relaxations of a straight dislocation segment using previously reported machine-learning interatomic potentials (see Methods). These calculations are performed at zero temperature and zero stress, and models an energy minimum configuration closest to a straight line dislocation.

Figure 4 shows the screw dislocation line profile obtained for NbTaMoW and NbTaTiHf bcc HEAs. We observe that major features of the line profile reflect the details of the core structure discussed above. Specifically, we find that the line profile is substantially more distorted in NbTaTiHf compared to NbTaMoW, consistent with the larger magnitude of LLDs found in the group IV element containing alloy. Additionally, DFT calculations in the previous subsection (see Fig. 2) show that while low energy core positions are found only at the center of triangles of $\langle 111 \rangle$ atomic columns in NbTaMoW, local energy minima can also be located at the vicinity of $\langle 111 \rangle$ atomic columns in NbTaTiHf, enhancing the waviness of the line profile in this alloy. We therefore conclude that LLDs and lowering of split core energies play an important factor governing fluctuations in core configurations along a dislocation line in NbTaTiHf.

We note that previous reports have shown spontaneous kink formation in screw dislocation lines [56], which was not observed in our atomistic relaxations. These structures may be found by further sampling dislocation lines, which could benefit of increasing the line length in the simulations and by performing heat treatments to allow the system to realize states away from the local energy minima configurations close to straight lines.

The roughness of the dislocation line is suggested to have strong implications for its mobility [57]. Specifically, an enhanced concentration of equilibrium kinks may promote the dislocation motion *via* the nucleation of new kinks [58],

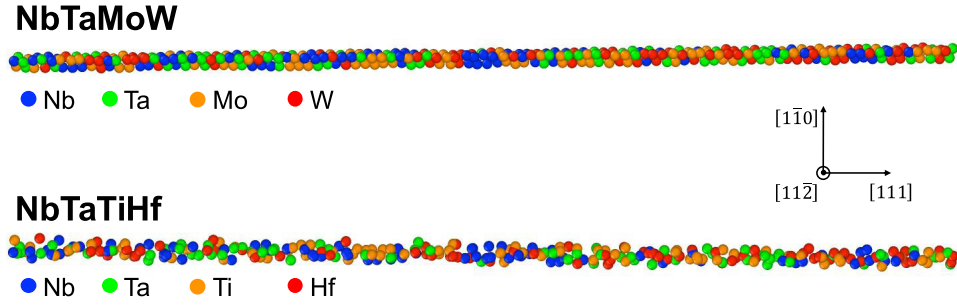


FIG. 4. Atomistic calculated screw dislocation line profile in bcc HEAs. Line profile of $1/2 \langle 111 \rangle$ screw dislocations in (top) NbTaMoW and (bottom) NbTaTiHf. The profiles are obtained using atomistic calculations of a dislocation line segment with a length equals to 100 times the Burgers vector. Atoms are color-coded by element: Nb (blue), Ta (green), Mo (orange), W (red), Ti (orange), and Hf (red).

different from the mechanism generally observed in elemental bcc metals, in which motion is controlled by kink migration (lateral motion) [59]. As such, dislocations in HEAs may observe significant lattice friction during motion, and might even be pinned by local compositional fluctuations [14,60].

This discussion can be extended to edge dislocations, and has been considered a central hypothesis for the development of strengthening models in the literature [61]. To obtain quantitative estimates for strengthening effects in HEAs, theoretical studies [62] have been using a misfit parameter (δ) based on atomic radius differences, which is defined as

$$\delta = \sqrt{\sum_{i=1}^N c_i \left(1 - \frac{r_i}{\bar{r}}\right)^2}, \quad (4)$$

where c_i and r_i are the concentration and atomic radius of the i th specie, respectively, and $\bar{r}$ is the concentration-weighted sum of the elemental atomic radii. The atomic radii are obtained using DFT calculated equilibrium atomic volumes for the elemental metals in a bcc structure assuming a hard sphere model, consistent with previous reports in the literature [43,62]. In detail, the calculated radius for Ti, Hf, Nb, Ta, Mo, and W is equal to 1.59 Å, 1.74 Å, 1.64 Å, 1.63 Å, 1.55 Å, and 1.56 Å, respectively. As a result, the misfit magnitudes are equal to 2.4% and 3.3% for NbTaMoW and NbTaTiHf, respectively.

While a larger misfit in NbTaTiHf correlates with a rougher dislocation line profile found in this alloy compared to NbTaMoW (see Fig. 4), the difference in misfit values between these two HEAs does not correlate with experimental reports of tensile yield stress. Specifically, reported yield stress magnitudes at room temperature are approximately equal to 1400 MPa [63] and 600 MPa [9] for NbTaMoW and NbTaTiHf, respectively. In this sense, NbTaMoW exhibits a yield stress more than twice larger than NbTaTiHf, regardless of featuring a significantly smaller misfit. Additionally, softening of the yield stress induced by increasing temperature does not correlate with the misfit parameter. In detail, reported yield stress magnitudes at 800 °C are about 900 MPa [63] and 400 MPa [9] for NbTaMoW and NbTaTiHf, respectively, both corresponding to a decrease close to 35% with respect to room temperature values. In this sense, the experimental findings suggest that strengthening and softening factors such as cross-kink formation and jog collapse [56,64], respectively, might

play an important role on the alloy strength. Improving the understanding of these dislocation structures would benefit of further atomistic simulations beyond the scope of the current work.

IV. CONCLUSION

In summary, we present a detailed investigation of the effects of core configuration and local chemical fluctuations on the energy landscape of $1/2 \langle 111 \rangle$ screw dislocations in NbTaMoW and NbTaTiHf bcc HEAs. Rugged dislocation lines reflect large lattice distortions, arising from additions of group IV transition metals. However, analyses of the line profile alone are insufficient to fully explain the strengthening mechanisms in these HEAs. We further show that the core energies are strongly influenced by the atoms near the core, which can induce features in the energy landscape that are unique for HEAs. Specifically, the core energy in the vicinity of an atomic column is lowered by the presence of group IV metals, locally stabilizing core configurations that are unstable in elemental bcc metals or refractory HEA compositions. When combined with the inherent twinning/antitwinning asymmetry of the bcc lattice, these features enable the elemental dislocation motion through $\{112\}$ planes in addition to the conventional $\{110\}$ system found in alloys without group IV metals. The participation of high-order planes in dislocation-mediated deformation processes has been linked to enhanced damage tolerance in bcc HEAs, such that the results presented here offer insight into the underlying physics governing the mechanical behavior in these materials.

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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.

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