

Atomic cluster expansion potentials for screw dislocations in BCC refractory metals

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Accurate atomistic modeling of screw dislocations in body-centered cubic (BCC) metals remains challenging because their plasticity is governed by complex dislocation glide behavior due to their compact threefold symmetric core structure and a strongly temperature-dependent flow stress induced by the large Peierls barrier. In the context of group 5 (V, Nb, and Ta) and group 6 (Mo and W) refractory metals (RMs), both classical interatomic potentials and some machine-learning potentials consistently fail to reproduce density functional theory (DFT) Peierls barriers and the glide plane. Here, we developed an array of atomic cluster expansion (ACE) potentials for these RMs by extending an existing DFT database. The developed ACE potentials significantly improve the description of screw dislocation properties, showing good agreement with the DFT references for Mo and W and substantial improvement for V, Nb, and Ta. The results show that transferability to screw dislocation behavior depends sensitively on both database composition and element-specific energetics and that achieving a single-humped Peierls barrier alone is not a sufficient validation metric for accurate prediction of dislocation glide. For Nb, Mo, and W, the developed ACE models also enable reliable calculation of kink-pair activation enthalpies, which are well described by both Kocks' law and a line-tension model.

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I. INTRODUCTION

Body-centered cubic (BCC) refractory metals (RMs) and their alloys combine high strength at elevated temperatures with generally poor tensile ductility and limited fracture toughness at low temperatures [1]. A characteristic feature of these systems is the brittle-to-ductile transition that occurs with increasing temperature [2,3]. The limited plastic deformation at low temperatures originates from the low mobility of screw dislocations ($1/2\langle 111 \rangle$), which in BCC RMs is governed by thermally activated mechanisms [4,5]. In contrast, nonscrew dislocation characters exhibit much higher mobility [6,7]. The low mobility of screw dislocations in RMs is attributed to their unique core structure; the nonplanar core introduces significant lattice resistance [8,9]. Consequently, researchers have extensively focused on understanding the connection between screw dislocation structure and plastic flow in RMs [8,10–13].

Among the available approaches, atomistic modeling has proven to be an indispensable tool for investigating the structure and energetics of screw dislocations. Density functional theory (DFT) is widely used to calculate the core structure,

Peierls barrier, and core trajectory of $1/2\langle 111 \rangle$ screw dislocations [12,14–16]. However, the high computational cost prevents its application at finite temperatures and strain rates, which motivates the use of classical molecular dynamics (MD). Although less accurate, MD offers a substantial computational speedup and can treat systems containing millions of atoms, enabling the study of dislocation interactions and finite temperature behavior. The accuracy of MD depends critically on the quality of the interatomic potentials (IAPs). Classical IAPs, including embedded atom method (EAM), modified EAM (MEAM), and angular-dependent potential (ADP) models, often predict unphysical core structures and inaccurate Peierls potentials [16–21]. For example, Gordon *et al.* showed that the Ackland-Thetford EAM potentials for V, Nb, and Ta predict double-humped Peierls energy profiles [17,22]. In a systematic assessment of 13 classical potentials for Fe, Mo, and Ta, Hale and Becker found that only three reproduced both a compact, nondegenerate core and a single-humped Peierls barrier: two EAMs for Fe and one MEAM for Mo [19]. Similarly, among the four EAM and two MEAM potentials for V examined by Wang *et al.*, only two stabilized the nondegenerate core, and both nevertheless produced double-humped Peierls profiles [21]. These limitations have motivated the development of machine-learning IAPs (ML-IAPs) specifically designed and validated for dislocation properties [21,23–26].

To date, several ML-IAPs have been proposed for BCC RMs [21,23,27–32] and for refractory high-entropy alloys (RHEAs) [25,26,33–37]. While some of the ML-IAPs were developed to model dislocation behavior, they still lack comprehensive validation against dislocation properties,

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especially those of screw dislocations. For example, the moment tensor potential (MTP) and spectral neighbor analysis potential (SNAP) were developed to investigate dislocation mobility in MoNbTaW RHEA [25,26]. However, neither SNAP nor MTP is capable of predicting the DFT Peierls barrier of screw dislocations in Nb, Mo, and W [20]. Another representative example is a family of general-purpose Gaussian approximation potentials (GAPs) constructed for V, Nb, Ta, Mo, and W (denoted here as GAP-2020) [27]. GAP-2020 has been shown to accurately reproduce a broad range of properties, including elasticity, point defects, surface energies, thermal expansion, phonons, and melting point. However, as discussed in Sec. III B, GAP-2020 does not quantitatively reproduce the Peierls potentials of the RMs considered here. This limitation highlights that good agreement with bulk and surface properties does not necessarily guarantee transferability to dislocations that are essential to simulate plastic deformation. In summary, none of the existing ML-IAPs, in their current form, are accurate enough to describe screw dislocation behavior for five elementary RMs. To address this gap, we develop atomic cluster expansion (ACE) potentials for V, Nb, Ta, Mo, and W by systematically enriching an existing DFT database. We then assess their ability to reproduce bulk, surface, and screw dislocation properties and apply the ACE models to finite temperature dislocation glide and calculations of kink-pair (KP) nucleation enthalpy barriers.

The remainder of the paper is organized as follows. Section II describes the computational methods, model parameters, and training and testing procedures. Section III A presents the validation of bulk and surface properties. The screw dislocation properties predicted by the developed models are discussed in Secs. III B and III C. Section III D examines the KP activation enthalpy barrier in Nb, Mo, and W and compares the atomistic results with theoretical models. Section IV discusses the Peierls barriers in comparison with multiple DFT references and existing IAP predictions and examines the potential impact of the lattice rescaling strategy used to construct the DFT databases. Finally, Sec. V summarizes the main conclusions of the paper.

II. METHODS

A. DFT calculations

It has been shown that systematic optimization of ML-IAPs, with respect to both the ML framework and the model hyperparameters, can significantly improve both accuracy and efficiency [24,38,39]. In this work, the GAP-2020 database developed in Ref. [27] is considered as a starting point to build an enriched DFT database. Consistent with Ref. [27], all DFT calculations for the enriched database are performed using VASP [40–43]. The Perdew-Burke-Ernzerhof generalized-gradient approximation exchange-correlation functional [44] was employed. Hard projector augmented-wave pseudopotentials were used, which are kept the same as the original database (V_sv, Nb_sv, Ta_pv, Mo_sv, and W_sv) [27]. The energy cutoff of the plane-wave expansion is set to 500 eV. The first-order Methfessel-Paxton method with 0.1 eV smearing is applied. Here, k points were sampled on Monkhorst-Pack grids with a spacing of $0.15 \text{ \AA}^{-1}$. Energy and

forces of the new configurations are included when training the new potentials.

The original GAP-2020 database includes distorted unit cells, high-temperature structures, point defects, flat and disordered surfaces, liquids, and a range of crystal structures [simple cubic (SC), BCC, face-centered cubic (FCC), hexagonal close-packed (HCP), A15, C15] [27]. The database was initially developed for W and then rescaled according to the lattice parameters of V, Nb, Ta, and Mo. GAP-2020 was developed for general purposes, focusing on radiation damage simulations, with no validation against dislocation properties. Our calculations show that GAP-2020 is unable to capture quantitatively the Peierls barrier of screw dislocations in all five RMs considered here, as discussed in Sec. III B. To improve the description of screw dislocations, we first enrich the GAP-2020 DFT database with highly distorted primitive-cell configurations, following an approach previously used for crack-related applications in BCC Fe [45]. These configurations expand the range of local atomic environments of the GAP-2020 database (see Appendix A for the principal component analysis). In total, 2963 primitive cells were generated for each element by rescaling iron primitive cells obtained via Sobol' sampling to the element-specific lattice parameters.

In addition to the primitive-cell configurations, we further enrich the database by including equations of state (EOSs) for the BCC, FCC, and HCP structures [46,47] as well as stacking fault configurations on the $\{110\}$ and $\{112\}$ planes. Finally, in preparation for future fracture-relevant applications, we also include traction-separation (T-S) data for all elements. The T-S curves were generated by separating the bulk material along the $\{100\}$ and $\{110\}$ surfaces for all elements and include both equilibrium and rattled configurations. The rattled configurations were obtained by adding random Gaussian perturbations to the atomic Cartesian coordinates. The structural categories and numbers of newly added configurations, together with the composition of the original GAP-2020 database, are summarized in Appendix B. We will discuss the motivation for selecting those configurations in Sec. III B. The complete DFT database is available in the Data Availability section.

In this work, nudged elastic band (NEB) calculations using VASP are performed to obtain the Peierls barrier of screw dislocation for five RMs [48]. A screw dislocation dipole configuration is used for the NEB calculations, and its exact geometry is described in Sec. II C. Both dislocations are moved to their next Peierls valley in the NEB final configuration. The initial and final configurations are fully relaxed before the NEB calculation. Nine intermediate replicas are generated along the NEB path by linearly interpolating between the initial and final configurations. During the NEB calculations, the force tolerance is set to $10^{-2} \text{ eV/\AA}$, and the NEB interreplica spring constant is set to the default VASP value $k = 5 \text{ eV/\AA}^2$.

B. ACE model training

In this work, we train ML-IAPs within the ACE framework. The ACE framework provides a systematically improvable polynomial basis, a linear parametrization that enables robust regularization, and high computational efficiency

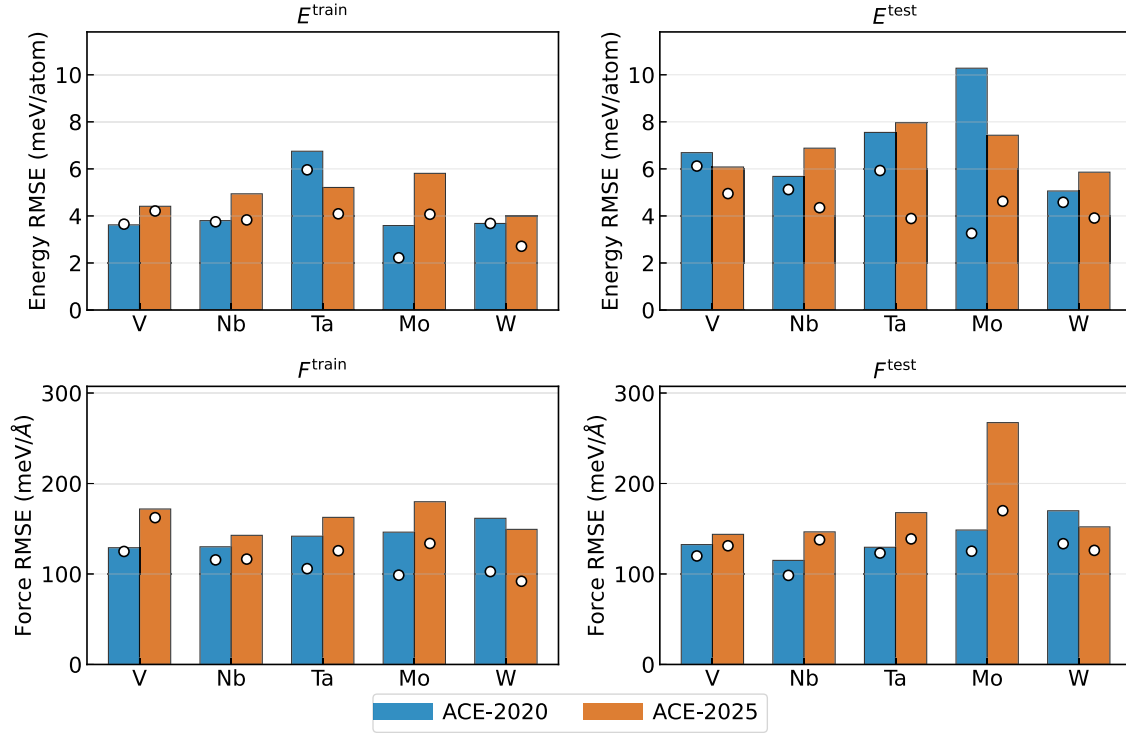


FIG. 1. Comparison of the energy and force RMSEs of the ACE-2020 and ACE-2025 potentials for V, Nb, Ta, Mo, and W. The upper panels show the training and test energy RMSEs, while the lower panels show the corresponding force RMSEs. Solid bars denote the RMSEs evaluated on the full dataset, and open circles indicate the RMSEs of datasets inside 1 eV/atom energy convex hull.

suitable for large-scale dislocation simulations [39,49]. The ACE formalism introduces a complete description of multi-body atomic interactions [49]. The energy of atom i can be expressed as a function of multiple per-atom atomic properties ψ_i^p ,

$$E_i = \mathcal{F}(\psi_i^{(1)}, \psi_i^{(2)}, \dots, \psi_i^{(P)}). \quad (1)$$

We employ complex embeddings that can lead to a more flexible description of the energy landscape at a slightly higher computational cost [50]

$$E_i = (\psi_i^{(1)})^{1/4} + (\psi_i^{(2)})^{1/2} + (\psi_i^{(3)})^{3/4} + \psi_i^{(4)} + (\psi_i^{(5)})^{5/4} + (\psi_i^{(6)})^{3/2} + (\psi_i^{(7)})^{7/4} + (\psi_i^{(8)})^2, \quad (2)$$

where atomic property $\psi_i^{(p)}$ is calculated based on the local atomic environments

$$\psi_i^{(p)} = \sum_v c_v^{(p)} \mathbf{B}_{iv}, \quad (3)$$

where $c_v^{(p)}$ are the expansion coefficients, and $\mathbf{B}_{iv}$ are the basis functions that depend on the atomic positions and species.

ACE potentials are trained using PACEMAKER [39,51]. Two versions of the ACE potential, denoted ACE-2020 and ACE-2025, are constructed using the original and enriched DFT databases, respectively. Their comparison allows us to examine the effect of the additional training configurations within a fixed ACE framework. As shown in Fig. 1, all training and testing energy root mean square error (RMSE) values for ACE-2025 are below 8 meV/atom. Training on the original database is particularly challenging for Ta; therefore, we use

the optimization package XPOT to identify a parameter set that yields a reasonably low RMSE [52].

In addition to the RMSE-based validation, we also evaluate the reliability of the ACE potentials during atomistic simulations. In our previous work, we highlighted the importance of uncertainty quantification in plasticity simulations [24]. PACEMAKER implements a D-optimality criterion based on the MaxVol algorithm, which quantifies the extrapolation grade γ of new atomic environments [53,54]. Here, the extrapolation grade γ is monitored during the simulations to assess whether the sampled atomic environments remain within the interpolation regime of the training database, thereby providing an additional measure of simulation reliability beyond the training and testing RMSEs.

C. Molecular statics calculations

A dislocation dipole configuration consisting of two parallel screw dislocations with opposite Burgers vectors is used to calculate the Peierls potential, as shown in Fig. 2(a) [56]. The simulation cell contains 135 atoms. The crystal orientations along the x , y , and z directions are set to $[12\bar{1}]$, $[\bar{1}11]$, and $[101]$, respectively. The resulting Burgers vector $1/2\langle 111 \rangle$ and slip plane (101) correspond to the dominant slip system in BCC metals. Volterra dislocations, assumed to be infinitely long and perfectly straight, are introduced into an anisotropic elastic medium by imposing the displacement field obtained from anisotropic elasticity theory [57]. The dislocation dipole configuration is stable and allows a significant reduction in the simulation cell size, which makes this approach particularly useful for *ab initio* modeling of dislocations. Periodic

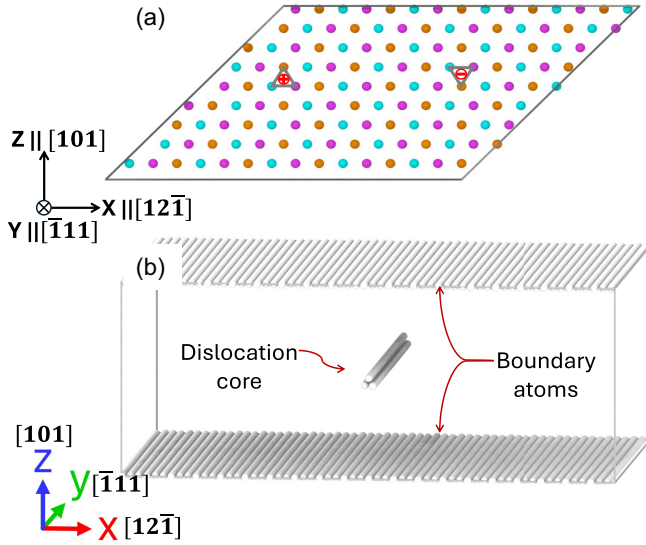


FIG. 2. Schematic representations of the screw dislocation configurations. (a) Screw dislocation dipole configuration. The dislocation core positions are indicated by $\oplus$ and $\ominus$ symbols inside the triangles, and circles represent atomic positions. Colors denote the atomic positions in the pristine BCC crystal for one periodic unit cell of length b along the dislocation-line direction y : orange atoms are used as the reference position (0), pink atoms are located at $b/3$, and cyan atoms at $2b/3$. The crystallographic directions are also indicated. (b) PAD configuration, showing the free-surface atoms and the dislocation core. The structure is analyzed using the adaptive common neighbor analysis method available in OVITO [55]. Atoms identified as BCC are removed for clarity. The crystallographic directions along x , y , and z are shown.

boundary conditions are applied in all directions. A quadrupolar periodic array of dislocation (PAD) dipoles is generated by tilting the simulation box by half a periodicity vector along the glide direction $x \parallel [12\bar{1}]$ [14]. With this modification, the dislocations have alternating Burgers vectors along both in plane directions (x - z plane), which leads to zero net stress at the dislocation centers through the nearly symmetric superposition of the elastic fields [58]. The NEB calculations of the Peierls potential are then carried out using this dipole configuration.

We make use of the Python package ATOMMAN to generate the dislocation dipole configurations [59]. The atomic simulation environment (ASE) [60] and MATSCIPY [61] were used to perform NEB calculations with the ACE, NEP, and EAM potentials. Nine intermediate replicas were generated by linear interpolation between the initial and final configurations for ACE and NEP. For the EAM and MEAM potentials, 22 intermediate images were used to resolve the more complex double-hump Peierls potential profiles. The force tolerance was set to 10^{-3} eV/Å, and the NEB spring constant between adjacent replicas was set to $k = 0.1$ eV/Å². The scripts used to generate screw dislocations, differential displacement maps (DDMs), and perform the NEB calculations are described in the Data Availability section. Atomistic configurations were visualized using OVITO [55].

For the calculation of the KP nucleation barrier under an applied shear stress, a PAD configuration was employed, as

shown in Fig. 2(b). The simulation cell has dimensions ($l_x = 60a$) $\times$ ($l_y = 40b$) $\times$ ($l_z = 40c$) and contains 96 000 atoms. Here, $a = \sqrt{2/3}a_0$ is the spacing between adjacent Peierls valleys, $b = \sqrt{3}/2 a_0$ is the magnitude of the Burgers vector, $c = \sqrt{2}/2 a_0$ is the interplanar spacing of the $\{101\}$ planes, and a_0 is the lattice parameter. Periodic boundary conditions were applied along the glide direction $[12\bar{1}]$ and the dislocation line direction $[\bar{1}11]$. All atomistic models were generated using LAMMPS (version 10 Dec 2025) [62], and the NEB calculations were also performed in LAMMPS. We use 32 replicas and the FIRE algorithm, with a force tolerance of 5×10^{-3} eV/Å, for the NEB calculations [63].

III. RESULTS

A. Bulk and surface property validations

GAP-2020 potentials were originally developed for elastic, thermal, liquid, defect, and surface properties. It has been shown that they accurately predict these properties (e.g., EOS, phonon dispersion, and melting curve) [27]. Based on ACE-2025, we predict the lattice parameter (a_0), the vacancy formation energy (E_v^f), the elastic constants (C_{11} , C_{12} , and C_{44}), and the surface energies of low-index planes (γ_{100} , γ_{110} , γ_{111} , and γ_{112}). Table I compares the ACE-2025 predictions with DFT [15,16,27,64] and experimental [65–71] reference values. The relative error is defined as $\left| \frac{p^{\text{ACE}} - p^{\text{DFT}}}{p^{\text{DFT}}} \right| \times 100\%$, where p is the property. For Mo and W, the relative errors of all considered properties remain below 5.6%, indicating an excellent level of agreement with DFT. The overall performance is further quantified using the average error index Q proposed in Ref. [24], obtaining $Q = 3.66\%$, 7.80% , 6.04% , 1.58% , and 0.86% for V, Nb, Ta, Mo, and W, respectively. These values show that the ACE-2025 models are particularly accurate for Mo and W, while the errors for V, Nb, and Ta are somewhat larger but still within a reasonable range for high-fidelity large-scale simulations.

We evaluate the generalized stacking fault energies (GSFEs) on the two primary slip planes $\{110\}$ and $\{112\}$ using the ACE-2025 IAPs for V, Nb, Ta, Mo, and W. Figure 3 compares the resulting GSFE profiles (solid lines) with DFT reference data (symbols) taken from Ref. [72]. For all five RMs and on both slip planes, the ACE-2025 potentials reproduce the characteristic shape of the GSFE curves. ACE-2025 can capture the asymmetry behavior of $\{112\}$ plane. The ACE-2025 prediction for Ta slightly deviates from the DFT results.

B. Screw dislocation core structures and migration pathways

As discussed in the Introduction (Sec. I), several ML-IAPs have been developed for RHEAs. Although some of these models have been evaluated for screw dislocation properties in elemental BCC RMs [20,25,26], the performance of others remains unclear [21,27,32,73]. Here, we first benchmark publicly available IAPs by calculating the easy core structures and Peierls energy profiles of $1/2\langle 111 \rangle$ screw dislocations in five BCC RMs: V, Nb, Ta, Mo, and W. The evaluated ML-IAPs comprise the GAP-2020 [27] and NEP-2026 [37] models for all five elements, the NbMoTaW ACE potential [73], the NbTaTiHf ACE potential for Nb and Ta [36], and

TABLE I. Lattice parameter a_0 , elastic constants C_{ij} , surface energies γ_{hkl} , and monovacancy formation energy E_v^f for V, Nb, Ta, Mo, and W. ACE-2025 predictions are compared with the DFT results by Byggmästar *et al.* [27], Dezerald *et al.* [15], and Weinberger *et al.* [16]. The monovacancy formation energies are compared with DFT results from Ref. [64]. Two sets of experimental bulk properties are included. The rows denoted “Expt. (CRC)” contain values from the CRC Handbook [65], whereas “Expt. (comp.)” denotes the experimental values compiled by Dezerald *et al.* from Refs. [66–70]. Experimental vacancy formation energies are reported as ranges [71].

Property	Method	V	Nb	Ta	Mo	W
a_0 (Å)	DFT (Byggmästar)	2.997	3.307	3.319	3.163	3.185
	DFT (Dezerald)	3.000	3.310	3.320	3.160	3.190
	DFT (Weinberger)	2.997	3.322	3.310	3.151	3.172
	ACE-2025	3.001	3.308	3.322	3.163	3.187
	Expt. (CRC)	3.024	3.300	3.303	3.147	3.165
	Expt. (comp.)	3.030	3.290	3.300	3.140	3.160
C_{11} (GPa)	DFT (Byggmästar)	269.0	237.0	266.0	468.0	521.0
	DFT (Dezerald)	242.7	241.7	267.3	454.3	496.0
	DFT (Weinberger)	257.0	247.0	269.0	483.0	530.0
	ACE-2025	281.7	236.1	299.2	475.4	522.5
	Expt. (CRC)	232.4	252.7	266.3	450.0	532.6
	Expt. (comp.)	230.3	245.7	261.7	458.3	517.3
C_{12} (GPa)	DFT (Byggmästar)	146.0	138.0	161.0	155.0	195.0
	DFT (Dezerald)	112.7	129.7	154.3	164.3	208.0
	DFT (Weinberger)	144.0	136.0	166.0	161.0	204.0
	ACE-2025	152.7	136.9	183.1	156.6	188.6
	Expt. (CRC)	119.4	133.2	158.2	173.0	205.0
	Expt. (comp.)	120.3	132.1	155.7	168.3	203.3
C_{44} (GPa)	DFT (Byggmästar)	22.0	11.0	77.0	100.0	147.0
	DFT (Dezerald)	24.0	9.5	74.0	97.0	137.0
	DFT (Weinberger)	22.0	17.8	70.9	93.7	136.0
	ACE-2025	19.2	17.1	71.6	94.6	148.3
	Expt. (CRC)	46.0	30.8	87.4	125.0	163.1
	Expt. (comp.)	43.2	28.4	82.6	111.0	157.0
γ_{100} (J m ⁻²)	DFT (Byggmästar)	2.407	2.310	2.342	3.190	4.027
	ACE-2025	2.406	2.349	2.478	3.225	4.004
γ_{110} (J m ⁻²)	DFT (Byggmästar)	2.375	2.064	2.450	2.761	3.276
	ACE-2025	2.414	2.091	2.360	2.779	3.283
γ_{111} (J m ⁻²)	DFT (Byggmästar)	2.686	2.332	2.697	2.954	3.533
	ACE-2025	2.729	2.466	2.766	2.968	3.581
γ_{112} (J m ⁻²)	DFT (Byggmästar)	2.686	2.353	2.675	2.879	3.448
	ACE-2025	2.630	2.364	2.666	2.858	3.436
E_v^f (eV)	DFT [64]	2.49	2.77	2.95	2.83	3.36
	ACE-2025	2.63	2.89	3.21	2.74	3.39
	Expt. [71]	2.10–2.20	2.60–3.07	2.20–3.10	3.00–3.24	3.51–4.10

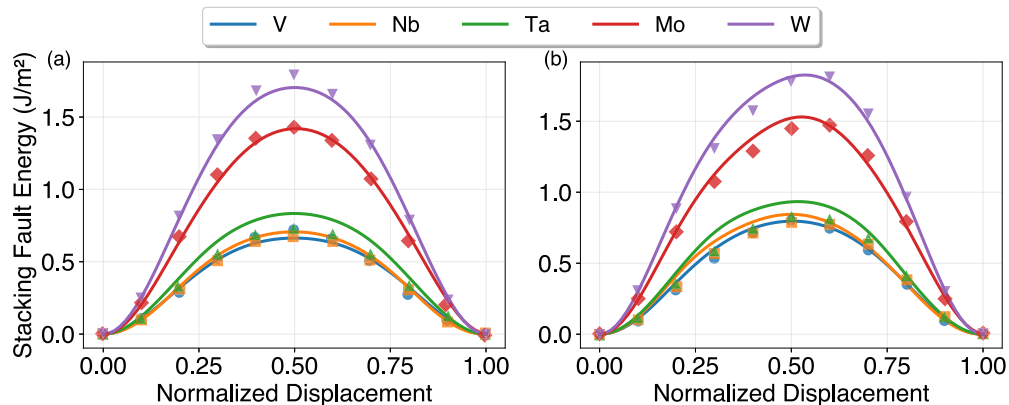


FIG. 3. GSFE curves for five BCC RMs predicted by ACE-2025 and DFT [72]. (a) $\{111\}\{110\}$ and (b) $\{111\}\{112\}$ slip system.

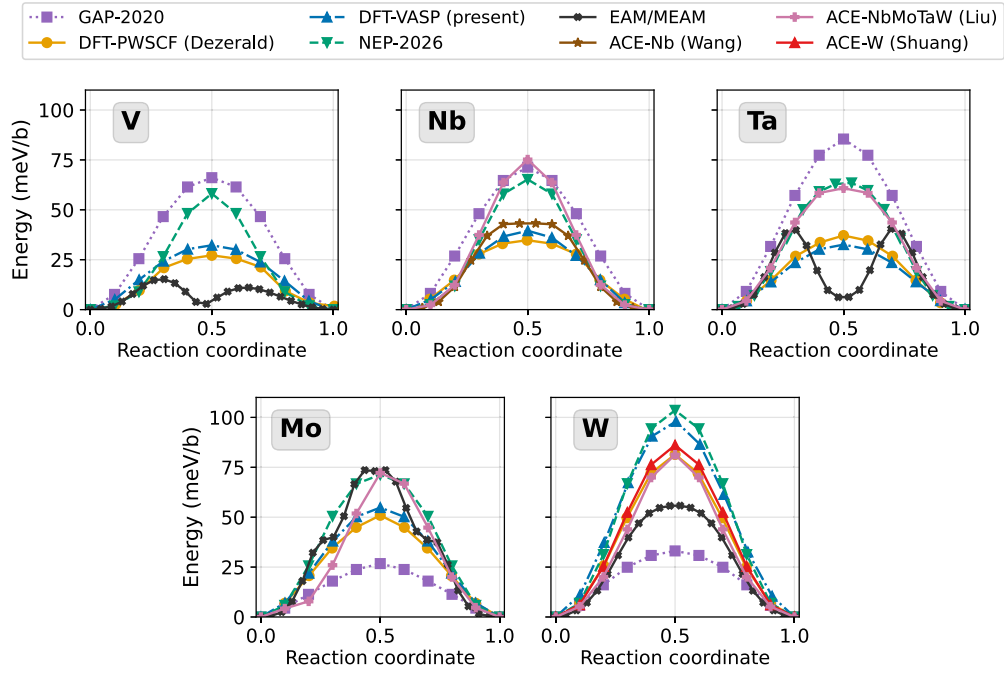


FIG. 4. Peierls energy profile of screw dislocations in V, Nb, Ta, Mo, and W. Reference DFT results obtained using PWSCF [15] and VASP are compared with GAP-2020 [27], NEP-2026 [37], ACE-NbMoTaW (Liu) [73], ACE-Nb (Wang) [36], and ACE-W (Shuang) [32]. Selected classical EAM and MEAM predictions are also shown for V [74], Ta [80], Mo [82], and W [83].

a W ACE potential [32]. We also consider selected classical IAPs for V [74,75], Nb [76,77], Ta [78,79], Mo [80–82], and W [74,83–85].

Figure 4 compares the calculated Peierls energy profiles with two sets of DFT reference data. The results taken from Ref. [15] are denoted as DFT-PWSCF, whereas DFT-VASP (present) refers to the calculations performed in this work. The differences between the two DFT datasets illustrate the sensitivity of the predicted barrier height to the DFT implementation and computational settings. All ML-IAPs examined here reproduce compact, nondegenerate core structures. In contrast, several classical IAPs predict polarized core structures, as shown in Appendix C. The Olsson potential for V [74] and the Zhou potential for Ta [80] produce double-hump Peierls potential profiles. The Marinica potential for W [83] reproduces the single-hump profile obtained from DFT but substantially underestimates the Peierls barrier. The MEAM potentials for Mo and W [82,85], however, both predict compact core structures.

GAP-2020 [27] and NEP-2026 [37] predict single-hump Peierls potential profiles for all five RMs. GAP-2020 consistently overestimates the barriers of the group 5 elements, while underestimating those of the group 6 elements. NEP-2026 overestimates the barriers for all five elements, although the magnitude of the deviation varies considerably among them. The NbMoTaW ACE potential [73] overestimates the DFT barriers for Nb, Ta, and Mo, whereas its prediction for W is closer to the DFT-PWSCF result. For Nb, the prediction of the NbTaTiHf ACE potential [36] agrees reasonably well with both DFT references. For Ta, however, the NEB calculation using the NbTaTiHf ACE potential did not converge, and no corresponding energy profile is reported. The W ACE potential [32] agrees well with both DFT results. The MEAM

potential for Mo [82] yields a stable, single-hump Peierls profile, whereas the NEB pathway predicted by the MEAM potential for W [85] is unstable and does not converge. Note that the NEP and multicomponent ACE potentials were developed to describe broad compositional spaces and chemically disordered environments. Their errors for elemental Peierls barriers should therefore be interpreted as a stringent test of dislocation-specific transferability rather than as a general assessment of their suitability for RHEA simulations.

Overall, these results demonstrate that classical IAPs often struggle to reproduce both a compact core geometry and a single-hump Peierls energy profile, whereas none of the currently available ML-IAPs consistently achieves DFT-level accuracy for the Peierls barriers of all five elements. In the remainder of this section, we examine the performance of ACE-2020 and ACE-2025 in describing screw dislocation core structures and migration properties.

Figure 5(a) shows the $\langle 111 \rangle$ -zone DDM of the relaxed dislocation core structure at $T = 0$ K and $\tau = 0$ MPa, predicted by ACE-2025. Atoms are colored according to their height along y directions in the undeformed state. Red, green, and cyan represent three different layers along $\langle 111 \rangle$ direction. DDMs reveal that ACE-2025 potentials predict nondegenerate core geometry for five elements, in agreement with DFT predictions [15].

As shown in Fig. 6, ACE-2020 can predict the Peierls barrier in W with an error of less than 10 meV/b, while the errors in Mo and Nb are less than 20 meV/b. However, the Peierls barriers for V and Ta are significantly overestimated compared with the DFT-VASP reference. Incorporating primitive cell configurations into the training database did not resolve this issue, and the revised potential still could not quantitatively capture the Peierls barriers of V, Nb, and Ta. To

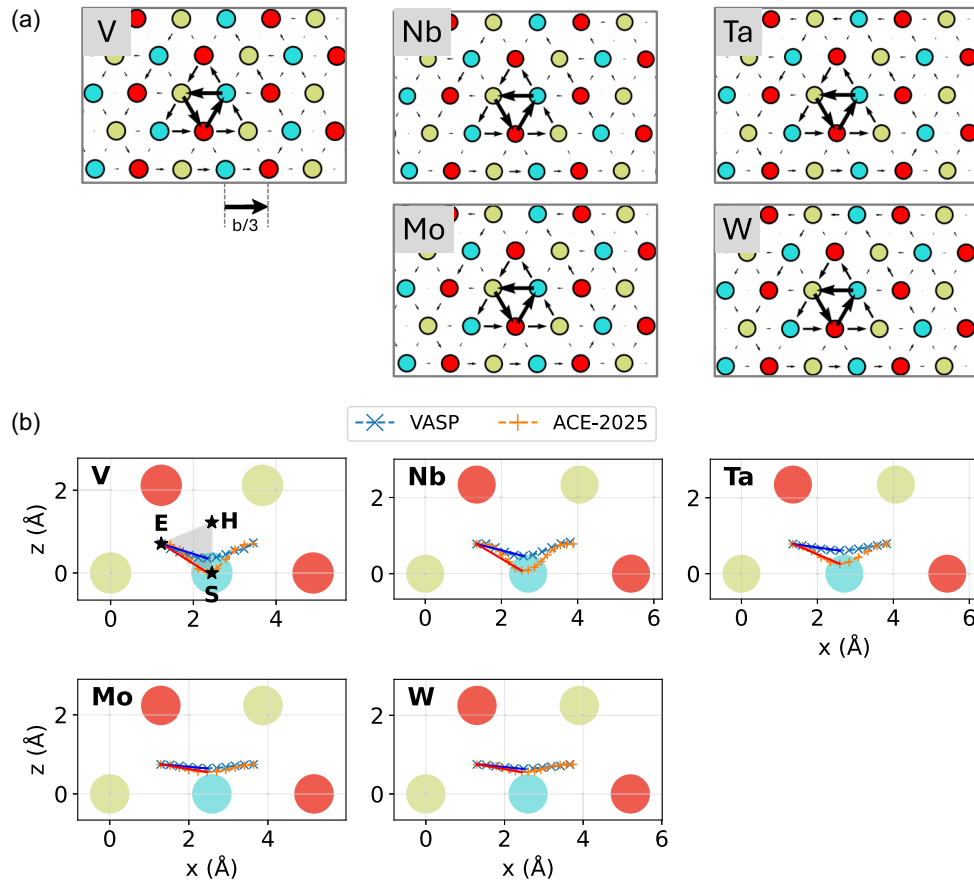


FIG. 5. (a) $\langle 111 \rangle$ -zone DDMs at the dislocation core for five elements. Atomic positions are represented by the circles. Atoms are colored by their position along out-of-the-plane (dislocation line direction y) $\langle 111 \rangle$ in the undeformed perfect state for one periodic unit cell of length b . Red atoms are used as the reference position (0), green atoms are located at $b/3$, and cyan atoms at $2b/3$. Arrows are calculated from the relative displacements before and after introducing the dislocation. The arrows are normalized by $b/3$, which is equal to the spacing of neighboring atoms. (b) Dislocation core migration trajectories along the Peierls barrier between easy-core configurations in BCC metals. The deviation angle α is defined between the blue/red solid line and the horizontal direction, where the blue/red solid line connects the lowest energy point along the trajectory to the easy-core position. The triangular region in the V panel indicates the minimum-energy paths connecting the easy core (E), hard core (H), and split core (S) configurations.

improve the description of screw dislocation core energetics, we enriched the database with more stacking fault configurations and EOSs for multiple crystal structures (BCC, FCC, and HCP) [46]. Extra screw dislocation configurations from NEB calculations are added to the database of Nb. Based on the expanded database, the ACE-2025 potentials reproduce the Peierls barriers of Nb and Ta with good accuracy, deviating from the present DFT reference by 13.7% and 7.1%, respectively, while overestimating the barrier in V by 34.7%. The remaining discrepancy for vanadium may stem from the rescaling strategy in constructing the initial database, which will be discussed in Sec. IV. The extrapolation grade distribution $\gamma < 1$ of ACE-2025 along the NEB paths indicates that the sampled configurations lie within the interpolation regime of the potential (Fig. 7).

The dislocation core trajectory along the Peierls potential pathway is highly relevant for the plastic anisotropic behavior in BCC metals, including the twinning/antitwinning (T/AT) asymmetry, deviations from Schmid's law [12], and the tendency to slip on glide planes other than $\{110\}$ with the maximum resolved shear stress. The dislocation core trajec-

tory can be evaluated via either the cost function approach or the stress method [14,15]. Here, the dislocation core trajectory is evaluated using the stress approach [12,15]. Based on the NEB results, the stress variation is measured for the replicas along the reaction pathway. The position of the dislocation is assumed to vary linearly between the initial and final configurations. The z component of the distance between two dislocation core positions (Fig. 2) is

$$\Delta z = \frac{S}{b} \left[\frac{(C_{11} - C_{12})\sigma_{xy} - C_{15}(\sigma_{xx} - \sigma_{zz})}{(C_{11} - C_{12})C_{44} - 2C_{15}^2} \right], \quad (4)$$

where S is the area of the simulation cell perpendicular to the dislocation lines, and C_{ij} is the elastic constants in Voigt notation in the crystallographic orientation of dislocation [86]. Figure 5(b) compares the screw dislocation core trajectories obtained from VASP and from the ACE-2025 potentials. The corresponding deviation angles are also reported in Table II. The three sets of DFT results differ by up to approximately 9° , illustrating the sensitivity of the predicted trajectories to the computational implementation and settings [12,87]. For

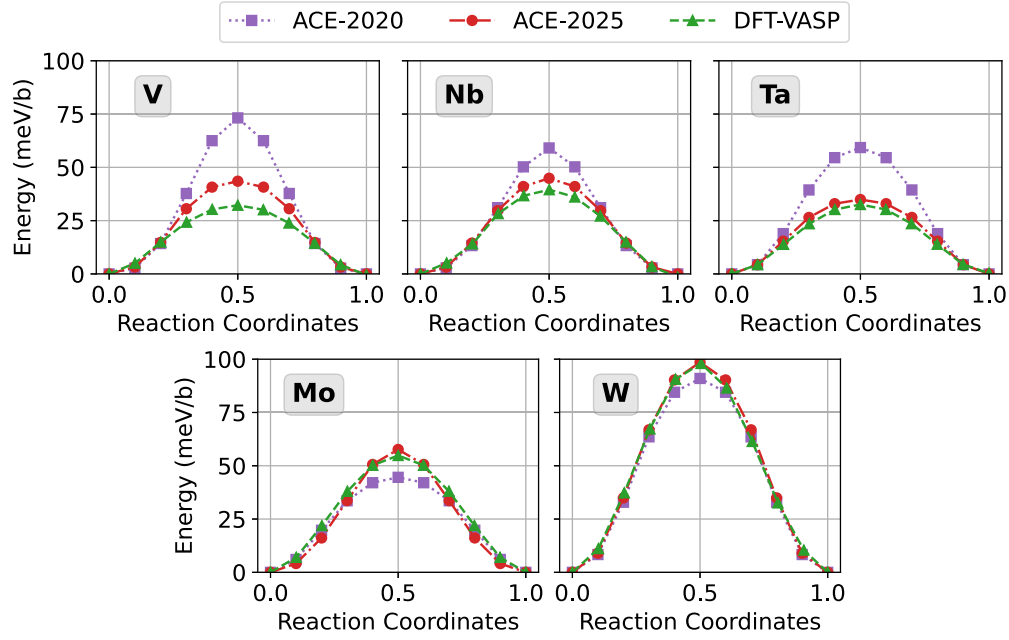


FIG. 6. Screw dislocation Peierls potential at $T = 0$ K and zero applied stress in BCC V, Nb, Ta, Mo, and W. Results obtained with the ACE-2020 and ACE-2025 IAPs are compared with our VASP calculations.

Mo and W, the ACE-2025 predictions fall within the range spanned by the DFT results and agree particularly well with Ref. [12]. For Ta, ACE-2025 is closest to Ref. [87], with a difference of approximately 4° , but deviates more substantially from the other DFT results. For Nb, ACE-2025 predicts a larger deviation-angle magnitude than all three DFT datasets, although the closest difference is approximately 7.5° . The largest discrepancy occurs for V, for which ACE-2025 consistently overestimates the deviation angle.

To further analyze these discrepancies, we compute the energy pathway from the hard to the split core (H2S) using the ACE-2025 potentials, as shown in Fig. 8. DFT prediction shows the hard-core energy (E_H) is similar to the split-core energy (E_S) for V and Nb [15]; therefore, ACE-2025 overestimates the split-core energy in V. For Ta, ACE-2025 yields E_H significantly higher than E_S , whereas DFT predicts the opposite ordering. In contrast, for W and Mo, the ACE-2025 models correctly reproduce the higher energy of E_S relative to E_H , consistent with DFT. The saddle points $\xi_{\text{H2S}}^{\text{saddle}}$ obtained

from ACE-2025 and DFT are highlighted by stars and squares, respectively, in Fig. 8. As summarized in Table II, ACE-2025 overestimates $\xi_{\text{H2S}}^{\text{saddle}}$ for all elements except Nb. This includes Mo and W, for which the correct energy hierarchy ($E_S > E_H > E_P$) is captured (see Table III for the values of different core energies). For Ta, the large discrepancy in the saddle point might be traced back to the incorrect energy hierarchy among different core structures.

To summarize, ACE-2025 shows good agreement with DFT references in describing the screw dislocation energy landscape of Nb, Mo, and W. The Peierls potentials are well captured for all five elements. The present ACE-2025 models show larger deviations from DFT for the more complex two-dimensional energy landscapes of V and Ta. These deviations may reflect the combined effects of differences in the element-specific training databases and lattice rescaling strategy. These factors are discussed further in Sec. IV B. Moreover, although the Peierls potential is often used as a key benchmark for assessing the ability of IAPs to describe dislocation properties

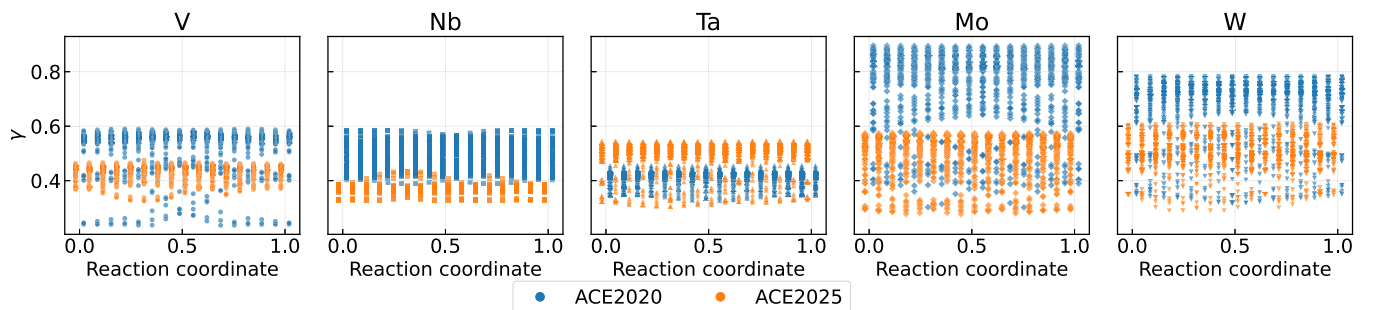


FIG. 7. Comparison of the extrapolation index (γ) distributions along the NEB reaction coordinate predicted by ACE2020 and ACE2025 for the five RMs. Each panel corresponds to one element, and the scattered points represent the γ values predicted from different replicas at each reaction coordinate. The two colors distinguish the ACE2020 and ACE2025 predictions.

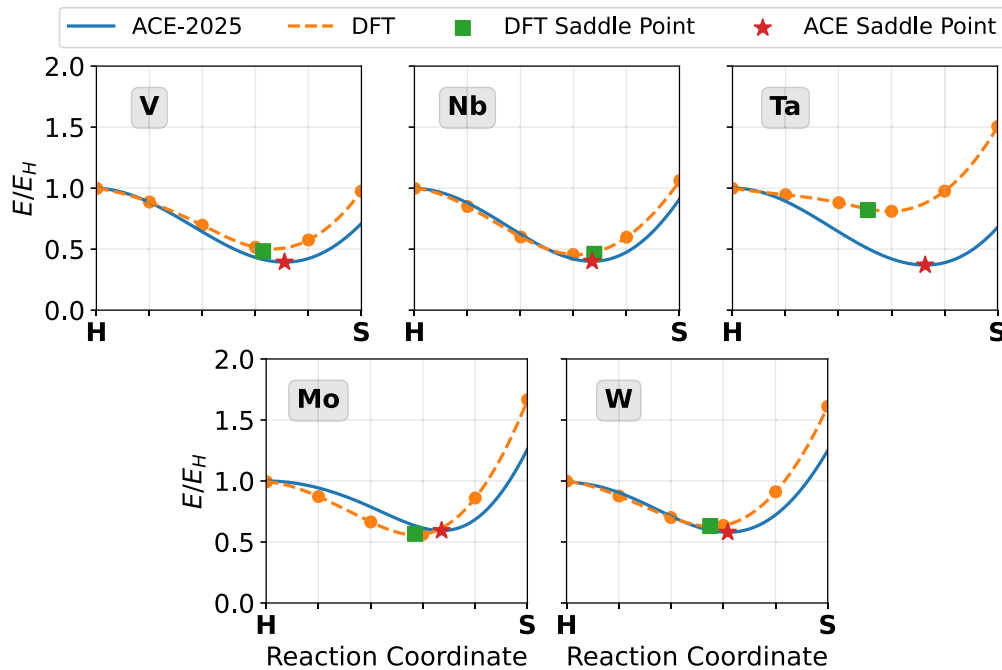


FIG. 8. Energy variation between the hard and split cores of screw dislocation for five RMs. The energies are normalized by the hard-core energy (E_H). The square and star symbols correspond to the saddle point along pathway predicted by DFT [15] and ACE-2025, respectively.

in BCC RMs [13,23,88], an accurate Peierls barrier alone does not guarantee a faithful description of the relative energies of different screw dislocation core geometries, nor correct glide behavior, as will be discussed next.

C. Dislocation glide behavior in Nb, Mo, and W

The analysis of the screw dislocation two-dimensional Peierls potential and the corresponding core trajectories indicates that the ACE-2025 potentials for Nb, Mo, and W can faithfully reproduce the DFT-predicted core energetics and migration paths. The preceding validations concern an infinitely long, perfectly straight dislocation. At finite temperatures in the thermally activated regime, screw dislocation glide proceeds through KP nucleation followed by lateral migration of the kinks. Reproducing the core energetics and migration path of a straight dislocation therefore does not, by itself, establish that the potential captures this finite length

glide mechanism. Moreover, because an NEB calculation requires the migration pathway and slip plane to be specified in advance, we first perform finite temperature MD simulations to identify the glide plane selected spontaneously by the screw dislocation in Nb, Mo, and W. We subsequently construct KP migration pathways on the identified slip plane and use NEB calculations to determine the stress-dependent activation enthalpy.

To investigate the finite temperature glide mechanism, we use a simulation cell of dimensions ($l_x = 60a$) $\times$ ($l_y = 52b$) $\times$ ($l_z = 30c$), containing $N = 93\,600$ atoms. Shear stress is applied to the top and bottom boundary atoms in opposite directions (details of the force application are given in the next section). The system is first equilibrated for 20 ps in the NPT ensemble at $T = 200$ K. An initial shear stress of $\tau_{\text{init}} = 0.5\tau_P$ for W and Mo and $\tau_{\text{init}} = 0.4\tau_P$ for Nb is then applied, followed by an additional 200 ps of equilibration in the NVT ensemble. This step confirms that the dislocation remains immobile under τ_{init} . After equilibration, the applied

TABLE II. Deviation angle α ($^\circ$) of the screw dislocation trajectory along the Peierls potential and relative saddle-point position $\xi_{\text{H2S}}^{\text{saddle}}$ along the H2S migration pathway in BCC V, Nb, Ta, Mo, and W. ACE-2025 results are compared with previous and present DFT calculations.

	Method	V	Nb	Ta	Mo	W
α ($^\circ$)	DFT [12]	-10.6	-21.7	-7.1	-9.9	-10.9
	DFT [87]	-14.4	-17.4	-16.2	-13.9	-14.4
	DFT-present	-17.58	-14.42	-8.01	-4.88	-5.50
	ACE-2025	-31.82	-29.17	-20.45	-9.24	-9.13
$\xi_{\text{H2S}}^{\text{saddle}}$	DFT [15]	0.63	0.68	0.51	0.57	0.55
	ACE-2025	0.71	0.67	0.73	0.67	0.62

TABLE III. Split-core (E_S) and hard-core (E_H) energies relative to the easy core. The DFT reference values are taken from Ref. [15], and the ACE-2025 values are calculated in this work. All energies are given in meV/b.

Element	E_S		E_H	
	DFT	ACE-2025	DFT	ACE-2025
V	51.3	80.6	52.5	112.4
Nb	81.8	105.6	76.3	115.5
Ta	67.0	66.5	44.0	96.7
Mo	147.6	128.9	88.2	103.7
W	208.5	218.9	128.6	174.1

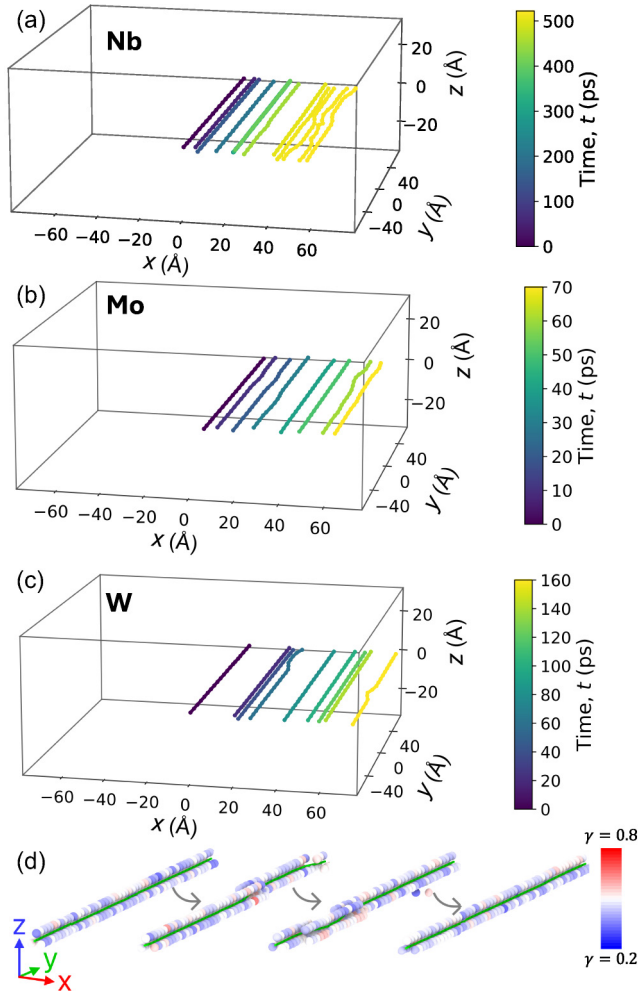


FIG. 9. Screw dislocation glide in (a) Nb, (b) Mo, and (c) W obtained from MD simulations. Each line represents the dislocation configuration at a different time. The line color indicates the elapsed simulation time, with $t = 0$ defined as the instant at which the dislocation begins to move, corresponding to the leftmost configuration in each panel. The applied shear stresses are $\tau_{\text{app}} = 0.6, 1.2$, and 2.05 GPa for Nb, Mo, and W, respectively. All simulations were performed at $T = 200$ K. The dislocation lines were identified using the dislocation extraction algorithm (DXA) implemented in OVITO. (d) KP nucleation and migration process in Nb. Atoms are colored according to the extrapolation grade γ .

shear stress is increased stepwise until dislocation motion is observed, using increments of 50 MPa every 200 ps. This corresponds to a loading rate of 2.5×10^8 GPa s^{-1} .

Figures 9(a)–9(c) show the dislocation core trajectories of Nb, Mo, and W obtained from MD simulations at $T = 200$ K. Each line represents the dislocation configuration at a different simulation time, and the color scale indicates the elapsed time after the onset of glide. The displacement of the lines along the glide direction reveals steady motion in Mo and W, whereas the Nb dislocation exhibits more pronounced spatial fluctuations and line curvature at $t = 500$ ps. In all three metals, the screw dislocations glide predominantly on the $\{110\}$ plane, consistent with DFT-based predictions [89,90]. The trajectory fluctuations further indicate a strong tendency

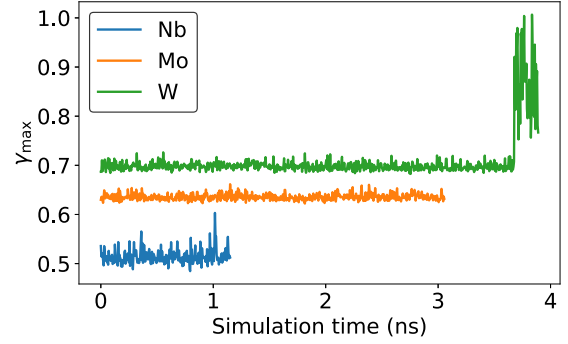


FIG. 10. Maximum extrapolation grade γ_{max} as a function of simulation time for Nb, Mo, and W during shear loading at $T = 200$ K, using ACE2025. The γ_{max} is the maximum extrapolation grade among all atoms at each timestep.

for cross-slip in Nb, which is not observed in Mo or W. This behavior is consistent with the large deviation angle predicted for Nb (Table II). Previous calculations have also shown that screw dislocations can cross-slip onto different $\{110\}$ slip planes [13,91].

The dislocation trajectories in Figs. 9(a)–9(c) show that some dislocation lines become curved through the formation of kinks at $T = 200$ K. Figure 9(d) further illustrates the atomistic mechanism of screw dislocation glide, consisting of KP nucleation followed by the lateral migration of the two kinks along the dislocation line. The atoms are colored according to the extrapolation grade γ predicted by ACE-2025. Although fluctuations in γ are observed during the simulation, the values remain below 1, indicating that the sampled configurations remain within the interpolation regime of the potential (see Fig. 10).

Moreover, the T/AT asymmetry associated with glide on the $\{112\}$ plane is a characteristic feature of plastic anisotropy in BCC metals and is closely linked to non-Schmid effects [12]. Capturing this asymmetry is therefore essential for IAPs intended for large-scale simulations of plastic flow. Here, we evaluate screw dislocation glide on the $\{112\}$ plane in both the twinning and antitwining directions at $T = 0$ K.

Table IV summarizes the critical resolved shear stress (CRSS) for glide in the two directions. For all three RMs, τ_c^{AT} is higher than τ_c^{T} , confirming the expected T/AT asymmetry. To quantify this effect, we define the asymmetry factor $\chi = (\tau_c^{\text{AT}} - \tau_c^{\text{T}}) / \tau_c^{\text{T}}$ and compare the ACE-2025 predictions with the DFT-based estimates reported in Ref. [12]. Mo and W exhibit only modest asymmetry ($\chi < 0.4$), whereas Nb shows much stronger asymmetry ($\chi > 1.2$). ACE-2025 reproduces this element-dependent trend well, as shown in Table IV.

TABLE IV. CRSS on the $\{112\}$ slip plane in the twinning (T) and antitwining (AT) directions for Nb, Mo, and W.

Element	τ_c (GPa)		χ	
	T	AT	ACE-2025	DFT estimate
Nb	1.25	3.75	2	>1.2
Mo	1.6	2.2	0.38	0.21
W	3.35	4.3	0.28	0.24

TABLE V. KP formation enthalpy at zero applied stress $\Delta H^*(0)$ and Peierls stress τ_p for Nb, Mo, and W. ACE-2025 predictions are compared with values obtained from experimental fits, LT models parameterized using DFT Peierls potentials, and previous DFT calculations. The Peierls stresses reported for ACE-2025 were obtained from direct molecular statics simulations at $T = 0$ K.

	Method	Nb	Mo	W
$\Delta H^*(0)$ (eV)	Expt.	0.62 [94]	1.19 [95]	2.05 [96]
	LT based on DFT [90]	1.28	1.05	1.54
	ACE-2025	0.72	1.07	1.49
τ_p (GPa)	Expt.	0.45 [94]	0.87 [95]	0.9 [96]
	DFT [15] (Disregistry)	0.86	—	1.8
	DFT [16]	0.74	1.6	2.4
	DFT [87]	0.79	1.4	2.36
	ACE-2025	1.375	1.525	2.875

In summary, ACE-2025 predicts screw dislocation glide on the $\{110\}$ plane in Nb, Mo, and W at $T = 200$ K, while maintaining bounded extrapolation grades throughout the simulations. It also reproduces the DFT trend in T/AT asymmetry on the $\{112\}$ plane. In the next section, we use ACE-2025 to evaluate the KP nucleation enthalpy.

D. KP nucleation enthalpy

Screw dislocation motion is governed by a thermally activated process of KP formation and migration. Here, the KP nucleation enthalpy as a function of the applied shear stress is evaluated via NEB calculations and compared with theoretical models. The rate associated with a thermally activated process is a key component in determining a dislocation mobility law. The KP nucleation and propagation process can be described by transition state theory, i.e.,

$$R \propto \exp\left(-\frac{\Delta H}{k_b T}\right), \quad (5)$$

where R is the KP nucleation rate, ΔH is the activation enthalpy, k_b is the Boltzmann constant, and T is the absolute temperature. The activation enthalpy $\Delta H(\tau, T)$ is a function of the applied stress τ and temperature. Within the harmonic approximation, the temperature dependence is neglected [92], and we therefore approximate the activation enthalpy only as a function of the applied stress, i.e., $\Delta H(\tau)$.

We first compute the enthalpy as a function of applied stress from the NEB calculation. To perform the NEB calculations, we used a PAD configuration [Fig. 2(b)]. Shear stress τ is applied to both the top and bottom boundary atoms in opposite directions during the NEB optimization. The stress is applied by adding forces to boundary atoms with a thickness of $6c$. The force $\mathbf{f}$, corresponding to applied stress τ , is computed as $\mathbf{f}(\tau) = \tau l_x l_y / N_{\text{atoms}}$. Note that $\mathbf{f}(\tau)$ is the force exerted on each atom, where N_{atoms} is the total number of atoms in the top or bottom slab where forces are being applied.

The enthalpy of replica i , with the reaction coordinate ξ^i , is computed as

$$H(\tau, \xi^i) = E_p(\tau, \xi^i) - W^{\text{ext}}(\tau, \xi^i), \quad (6)$$

where $E_p(\tau, \xi^i)$ is the potential energy of replica i . In the atomistic calculations, $W^{\text{ext}}(\tau, \xi^i)$ is the work done by the

applied force $\mathbf{f}(\tau)$ on the boundary atoms

$$W^{\text{ext}}(\tau, \xi^i) = \sum_{j \in \partial\Omega} \mathbf{f}_j(\tau) \cdot \mathbf{u}_j(\xi^i). \quad (7)$$

Here, j indicates the boundary atoms on which external forces are applied, and $\mathbf{u}_j(\xi^i)$ is the displacement vector of boundary atom j in replica i . Note that both top and bottom boundary atoms need to be considered in this calculation, as shown in Fig. 2. The work can already be subtracted in LAMMPS by combining `fix addforce` and `fix_modify energy` commands. Example scripts are provided in the Data Availability section.

Symbols in Fig. 11 show the enthalpy barrier for screw dislocation motion as a function of applied stress in Nb, Mo, and W. At a given applied stress, the activation enthalpy follows the trend $W > \text{Mo} > \text{Nb}$. Table V reports the KP nucleation enthalpy at $T = 0$ K and zero applied stress. ACE-2025 predictions are compared with values obtained from experimental fits [94–97] and from a line-tension (LT) model parameterized using DFT Peierls potentials [90]. For Nb, ACE-2025 agrees well with the experimental value. For Mo and W, ACE-2025 is in better agreement with the DFT-parameterized LT model.

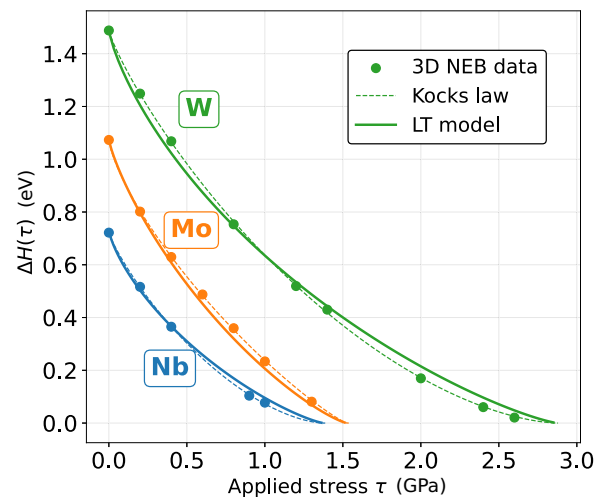


FIG. 11. Activation enthalpy barriers for W (green), Mo (orange), and Nb (blue) as a function of applied stress. Symbols represent NEB data, solid lines show predictions from the LT model of Dorn and Rajnak [93], and dashed lines correspond to fits based on Kocks' law.

TABLE VI. Fitted parameters of Kocks' law (p and q) and of the LT model (α) for Nb, Mo, and W.

	Parameter	Nb	Mo	W
Kocks' law	p	0.865	0.742	0.854
	q	1.613	1.149	1.633
LT model	α	-1.114	-0.203	-0.631

The overall trend across the three RMs is also consistent with that reported previously for other BCC RMs [10,11,97–99].

Table V also lists the Peierls stress at $T = 0$ K obtained from direct molecular statics (MS) simulations using the ACE-2025 potential, together with experimental measurements and DFT predictions. Note that the Peierls stress is derived from the Peierls potential according to $\tau_p = \max[(1/b)dE/dx]$, where E is the Peierls potential and b is the magnitude of the Burgers vector. ACE-2025 agrees well with the DFT results of Ref. [16] for Mo and W but overestimates τ_p for Nb. Compared with experiment, ACE-2025 correctly predicts the ordering of the Peierls stress among the three elements, namely, $W > Mo > Nb$. However, this discrepancy should not be viewed as a limitation specific to the present ACE-2025 model but rather as a broader challenge in quantitatively predicting experimental Peierls stresses from atomistic calculations. This difficulty is associated with effects such as zero-point vibrations at low temperatures and nonglide stresses [12,93,99–101].

We next fit the simulation data using Kocks' phenomenological expression. This phenomenological model, originally proposed by Kocks [102], has been widely applied to thermally activated dislocation motion and takes the general form

$$\Delta H^*(\tau) = \Delta H^*(0) \left[1 - \left(\frac{\tau}{\tau_p} \right)^p \right]^q. \quad (8)$$

Here, $\Delta H^*(0)$ and τ_p denote the activation enthalpy at zero stress and the Peierls stress, respectively, both of which can be obtained directly from atomistic simulations. The parameters p and q are determined by fitting. Using the ACE-2025 values of $\Delta H^*(0)$ and τ_p reported in Table V, we fit Eq. (8) for Nb, Mo, and W. The fitted curves closely reproduce the simulation data, indicating that screw dislocation motion in all three RMs follows Kocks' law. The resulting fitting parameters p and q are listed in Table VI. For W, the fitted parameters are in very good agreement with those obtained previously using an EAM potential ($p = 0.86$, $q = 1.69$) [83,103].

Finally, we consider theoretical models for KP nucleation in screw dislocations. To this end, we briefly review and apply the LT model of Dorn and Rajnak [93]. In this model, the dislocation is represented as a flexible line moving in the Peierls potential $V_P(x)$ under an applied stress. Changes in shape away from a straight dislocation are countered by the line energy Γ_0 . The resulting energy functional describes the enthalpy of the dislocation as a function of its shape, and its saddle-point solution yields the critical KP configuration and the corresponding enthalpy barrier, written as

$$\Delta H(\tau) = 2 \int_{x_0}^{x_c} \{ [\Gamma_0 + V_P(x)]^2 - [\tau b(x - x_0) + \Gamma_0 + V_P(x_0)]^2 \}^{\frac{1}{2}} dx, \quad (9)$$

where x_0 represents the equilibrium configuration of the straight screw dislocation at the applied stress τ , which can be obtained via

$$\tau b = \frac{\partial V_P(x)}{\partial x} \Big|_{x=x_0}. \quad (10)$$

Here, x_c is the extremum position of the kink bulge in the critical configuration at the applied stress τ , and it can be

TABLE VII. Peierls barriers (meV/b) of 1/2(111) screw dislocations in V, Nb, Ta, Mo, and W predicted by DFT and different IAPs. The superscript dh denotes a double-humped Peierls potential. Dashes indicate unavailable results.

	Method	V	Nb	Ta	Mo	W
DFT	PWSCF [15]	25.7	35.2	36.6	50.5	81.8
	VASP [16]	24.3	28.6	38.0	61.0	94.0
	VASP [87]	27	26	33	54	89
	VASP (present)	32.2	39.5	32.6	54.8	98.0
	GAP-2020 [27]	66.1	71.4	85.5	26.8	33.1
	NEP-2026 [37]	58.1	65.2	63.5	71.3	103.6
ML-IAP	ACE-2025 (present)	43.5	44.9	34.9	57.6	98.6
	ACE-NbTaTiHf [36]	—	43.2	—	—	—
	ACE-W [32]	—	—	—	—	86.1
	ACE-NbMoTaW [73]	—	75.2	60.8	72.1	81.3
	MTP [20,25]	—	79.5	—	54.0	59.0
	SNAP [20,26]	—	75.5	—	151.5	126.0
	Linear MLP [108]	—	—	—	—	86.0
	ADP [20]	—	54.5 ^{dh}	—	46.0 ^{dh}	94.0 ^{dh}
Classical IAP	ADP21 [88]	—	25.0	—	—	—
	EAM [74,80,83]	15.3 ^{dh}	—	40.4 ^{dh}	—	55.8
	MEAM [82]	—	—	—	73.6	—

obtained by solving

$$\Delta H^*(0) = 2\Gamma_0 \int_{-a/2}^{a/2} \sqrt{\left(\frac{\Gamma_0 + V_P(x)}{\Gamma_0}\right)^2 - 1} dx, \quad (11)$$

where $\Delta H^*(0)$ is the KP nucleation energy obtained by atomistic simulations. The Peierls potential is fitted to the following form:

$$V_P(x) = \frac{\Delta E_P}{2} \left[1 + \frac{\alpha}{4} + \cos\left(\frac{2\pi x}{a}\right) - \frac{\alpha}{4} \cos\left(\frac{4\pi x}{a}\right) \right]. \quad (12)$$

Here, α is chosen to match the Peierls stress from atomistic simulation results

$$\tau_P = \frac{1}{b} \max_{\{x \in [-a/2, a/2]\}} \left[\frac{d}{dx} V_P(x) \right]. \quad (13)$$

Following this procedure, we apply the LT model for Nb, Mo, and W, and the resulting parameters are listed in Table VI. The fitting uses the values of $\Delta H^*(0)$ and τ_P predicted by the ACE-2025 potential (Table V). As shown by the solid lines in Fig. 11, the LT model reproduces both the NEB data and the fitted Kocks' law very well. This result indicates that the enthalpy barrier as a function of applied stress can be described accurately using only the zero-stress activation enthalpy and the Peierls stress, thereby significantly reducing the computational cost [104,105].

IV. DISCUSSION

A. Peierls potential in BCC RMs

Accurately predicting screw dislocation behavior at the atomic scale has remained a longstanding challenge in BCC RMs. Classical IAPs often predict degenerate core structures and double-humped Peierls potentials [20,99,100,106]. More recently, ML-IAPs have been developed and benchmarked against screw dislocation properties, especially for W [23,38]. However, comparable models for other BCC RMs remain scarce, and comprehensive validation across multiple RMs is still missing. As shown in Fig. 4, even recent ML-IAPs cannot consistently reproduce DFT Peierls barriers across the BCC RMs considered here [37]. In this work, we developed a family of ACE-2025 potentials for BCC RMs and validated them against elastic and surface properties as well as screw dislocation behavior. In the remainder of this subsection, we discuss the DFT database design required to reproduce the Peierls potential and its implications for predicting the more complex energetics of screw dislocations in BCC RMs.

To obtain accurate Peierls potentials, we follow an iterative, task-oriented database construction procedure rather than a controlled strategy in which identical configuration categories are added for each element. We enrich the databases of V and Nb with stacking fault configurations and EOSs, whereas additional screw dislocation configurations are required for Nb to recover the DFT barrier. This observation suggests that the transferability of the potential to screw dislocation properties depends not only on the configuration types represented in the training database but also on the element specific energy landscape.

Earlier work on W based on GAP showed that including vacancy-containing γ surfaces can worsen the description of the Peierls barrier, whereas adding screw dislocation quadrupole cells restores quantitative agreement with DFT [38]. In that study, it was further demonstrated that a database composed only of screw dislocation configurations can quantitatively reproduce the screw dislocation structure, dislocation-vacancy binding energies, and the Peierls barrier. By contrast, within the present ACE framework, adding γ -surface configurations is sufficient to recover the screw dislocation energy landscape of V with the selected DFT reference, without explicitly including screw dislocation configurations. This difference may arise from how the respective models represent and fit the relevant local atomic environments [107].

The comparisons among the present models provide further insight into these effects. Comparing ACE-2020 with ACE-2025 demonstrates the influence of database enrichment within a fixed ACE framework, whereas comparing GAP-2020 with ACE-2020 indicates that model representation and optimization also affect transferability when the underlying DFT database is unchanged. Nevertheless, because GAP and ACE differ in their representations, fitting procedures, regularization, and hyperparameters, the contribution of each factor cannot be isolated. Decoupling the effects of database composition, element-specific energetics, and model formulation would require a controlled study using consistent configuration categories and sampling strategies for all elements, which lies beyond the scope of the present work.

Figure 12 compares selected Peierls barriers predicted by DFT and different IAPs, while a more comprehensive compilation is provided in Table VII. The DFT results consistently show that the Peierls barrier increases from group 5 to group 6 RMs, with W exhibiting the highest barrier [15,16,87]. Nevertheless, appreciable quantitative scatter exists among the DFT datasets. The predicted barriers differ by approximately 5–16 meV/b, with the largest absolute spread for W and the largest relative spread for Nb. These discrepancies reflect differences in the DFT code implementation, pseudopotentials, and numerical parameters. The present DFT calculations therefore agree with previous DFT studies at the level of the overall elemental trend. ACE-2025 reproduces the overall trend across the five RMs and yields values that are broadly comparable with the DFT reference data. In contrast, larger discrepancies are observed for several previously reported ML and classical IAPs. SNAP strongly overestimates the Peierls barrier for Mo and W, whereas ADP predicts a doubly humped barrier for Nb, Mo, and W, indicating the presence of an intermediate metastable configuration [20]. These comparisons show that, among the available IAPs for BCC RMs, only ACE-2025 achieves quantitative agreement with DFT across multiple elements.

Although ACE-2025 accurately reproduces the Peierls barrier along the minimum energy path of screw dislocations, a faithful description of the more complex two-dimensional energy landscape, including the energetics of the hard and split cores, remains challenging for V and Ta. This limitation is reflected in the less accurate prediction of the deviation angle along the core trajectory in V and Ta (Table II) as well as in the difficulty of reproducing the correct energy hierarchy of the hard and split cores in Ta. These results indicate that

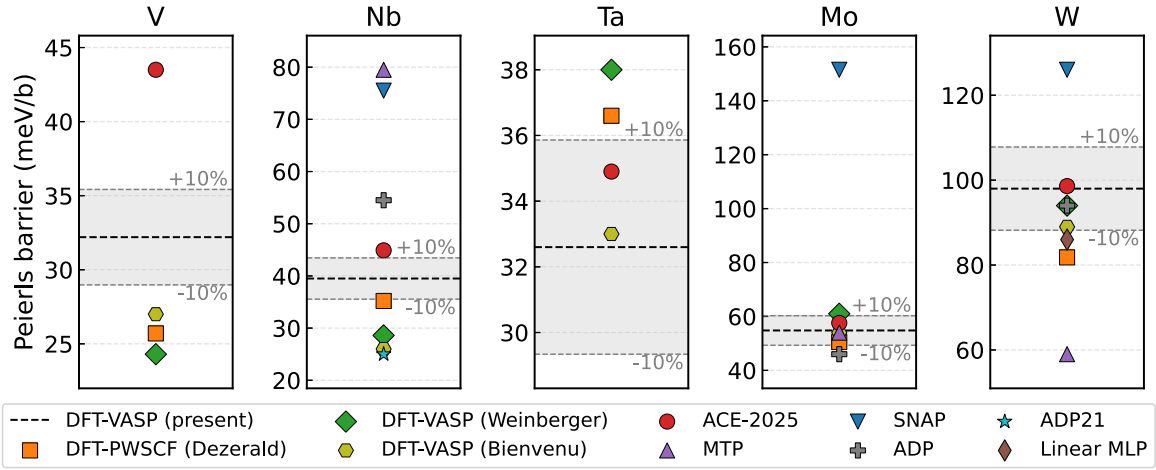


FIG. 12. Comparison of the Peierls barriers of $1/2\langle 111 \rangle$ screw dislocations in V, Nb, Ta, Mo, and W predicted by ACE-2025 and selected IAPs. The black dashed lines denote the present DFT-VASP results, and the shaded regions indicate deviations of $\pm 10\%$. Literature DFT results obtained using PWSCF [15] and VASP [16,87] are included for comparison. The MTP [25], SNAP [26], and ADP results are taken from Ref. [20]; the ADP21 results are taken from Ref. [88]; and the linear MLP result for W is taken from Ref. [108]. The ADP barriers are doubly humped, with an intermediate local minimum corresponding to a metastable core configuration.

ACE-2025 still requires further refinement for V and Ta, while also demonstrating that the Peierls barrier alone is an incomplete metric for validating IAPs in BCC RMs. For example, ADP21 reproduces a single-hump Peierls potential but nevertheless fails to predict screw dislocation glide on the $\{110\}$ plane at $T = 240$ K [13,88]. A reliable potential should reproduce the correct energetic hierarchy of the three core structures (easy, hard, and split) before being applied in large-scale dislocation simulations. Ideally, validating the dislocation properties of elementary BCC RMs should be regarded as a necessary step before extending the IAPs to multielement systems, such as RHEAs.

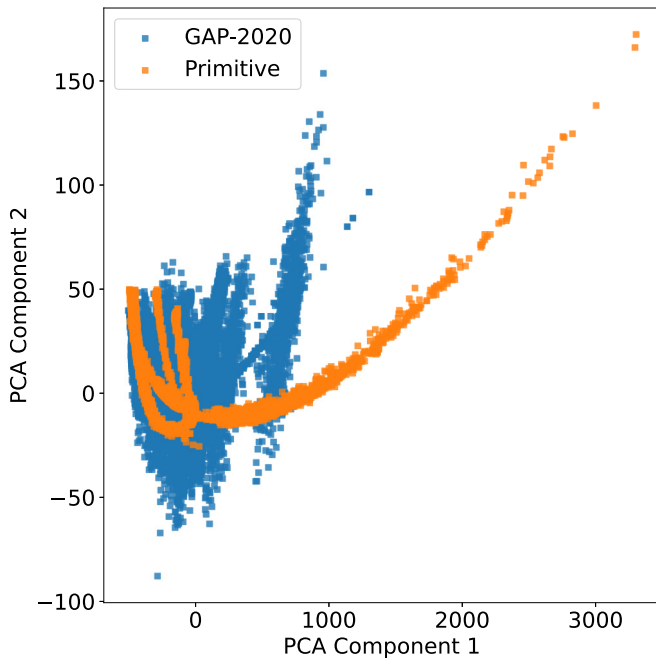


FIG. 13. Principal component analysis projection of the tungsten database in the ACE B-basis descriptor space.

B. Scaling strategy for constructing DFT database

The differences in the accuracy of different elements motivate a closer examination of the strategy for constructing the underlying DFT database. Across all validation tests, we found a consistent trend: ACE-2025 predictions are in good agreement with the spread of available DFT values for the group 6 elements, Mo and W, whereas its performance becomes less accurate for the group 5 elements (V, Nb, Ta). For Mo and W, ACE-2025 reproduces bulk properties such as elastic constants, surface energies, and vacancy formation energies while also capturing more subtle features, including the Peierls barrier and the full screw dislocation energy landscape.

The strong dependence on the chemical group may be partly associated with the construction of the underlying DFT database. The original training set was designed for W and then transferred to the other elements by a simple rescaling of the lattice parameter. For V, Nb, Ta, and Mo, DFT energies and forces were generated by performing only self-consistent electronic structure calculations at these rescaled geometries, without relaxing either the ionic positions or the simulation cell. As a consequence, a substantial fraction of the database for these elements may correspond to nonequilibrium configurations and may not adequately sample the relevant local minima and transition states on the true potential energy surface. This problem is particularly important for elements outside the group 6 column, where bonding characteristics and equilibrium structures differ significantly from those of W, even though all elements share the same BCC crystal structure. Our results therefore suggest a limitation of the lattice-rescaling procedure used to construct the GAP-2020 database. Rescaling a database constructed for W works well for Mo, which belongs to the same chemical group, but fails to provide equally accurate models for V, Nb, and Ta.

These findings highlight an important limitation of constructing multielement DFT databases by straightforward lattice parameter rescaling, even when the materials have identical crystal symmetry [37,109,110]. While such a

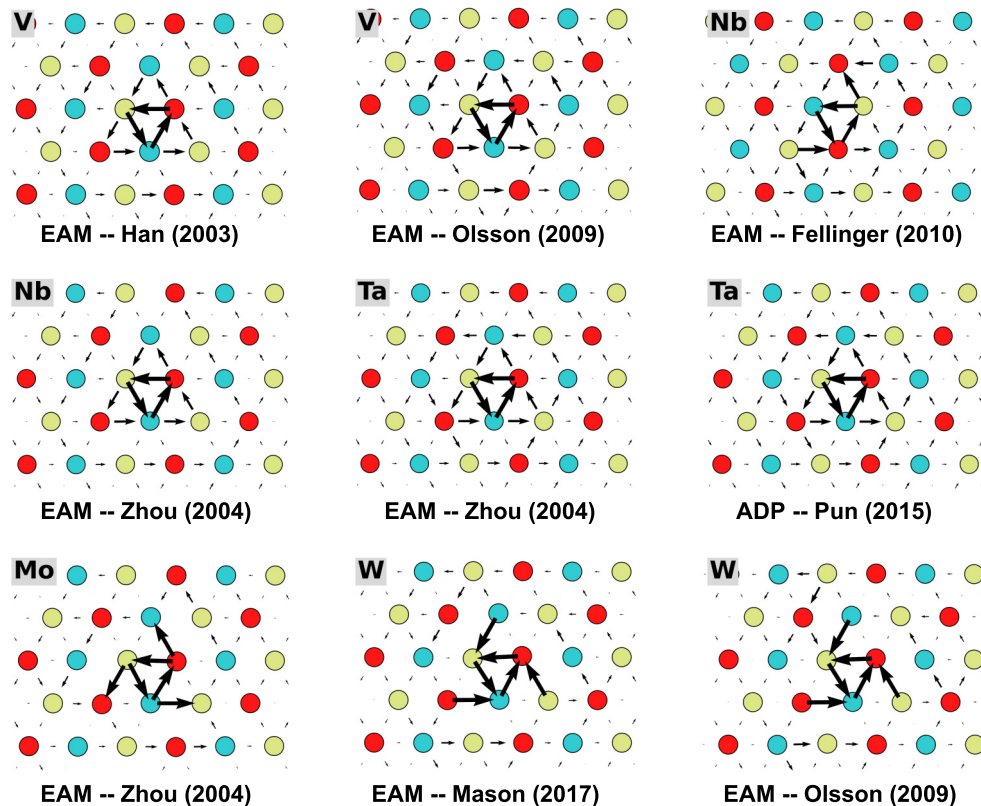


FIG. 14. DDMs of relaxed $1/2\langle 111 \rangle$ screw dislocation cores predicted by EAM and ADP models. From left to right, the top row shows V described by the Han [75] and Olsson [74] EAM potentials and Nb described by the Fellingner EAM potential [76]; the middle row shows Nb and Ta described by the Zhou EAM potential [80] and Ta described by the Pun ADP potential [78]; and the bottom row shows Mo described by the Zhou EAM potential, and W described by the Mason [84] and Olsson EAM potentials. Colored circles distinguish the three successive atomic layers along the $\langle 111 \rangle$ dislocation-line direction. Arrows indicate the relative $\langle 111 \rangle$ displacements between neighboring atomic columns, with their lengths and widths proportional to the displacement magnitude. Each panel is centered on one dislocation core.

strategy is convenient for database construction and ensures consistent structural categories across different elements, it can introduce systematic biases into the training data and, in turn, into the learned IAPs, especially for complex defect configurations such as dislocation cores. Our results emphasize the need for element-specific, fully relaxed DFT configurations or active learning strategies when high fidelity is required to capture the detailed atomistic energy landscape of complex defects.

V. CONCLUSIONS

In this work, we developed ACE-2025 potentials for five BCC RMs and benchmarked a broad range of screw dislocation properties. The main conclusions are as follows:

(1) None of the existing ML-IAPs can provide a consistently accurate description of screw dislocation Peierls barriers across V, Nb, Ta, Mo, and W. By extending a publicly available DFT database and training within the ACE framework, we obtained ACE-2025 potentials that significantly improve the description of screw dislocation properties.

(2) The transferability of ML-IAPs to screw dislocation properties depends sensitively on both the composition of the training database and the specific element considered. The present results show that the Peierls barrier alone is not a

sufficient validation metric. A reliable validation should also include the two-dimensional energy landscape of the screw dislocation.

(3) For Nb, Mo, and W, the ACE-2025 potentials enable reliable calculations of KP activation enthalpies under applied stress. The atomistic results are well described by both Kocks' law and a LT model, providing an efficient route to connect atomistic screw dislocation energetics with dislocation mobility models in BCC RMs.

(4) The present results also reveal an important limitation of the lattice rescaling strategy used to construct the original multielement DFT database. While this approach works reasonably well for Mo and W, it is less effective for V, Nb, and Ta, indicating that more element-specific relaxed configurations are needed when high-fidelity descriptions of complex defect energetics are required.

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L.Z. and F.M. designed the research together. L.Z. performed all the DFT, MS, and MD calculations. All authors analyzed the data, discussed the results, wrote the manuscript together, and contributed to the discussions and revisions of the paper.

The authors declare no competing interests.

DATA AVAILABILITY

LAMMPS and VASP inputs, DFT databases, and ACE potential files are available on our Github page [111]. Python scripts for the LT model and screw dislocation analysis, including Peierls potential and trajectories, are available on the same Github page [111].

APPENDIX A: PRINCIPAL COMPONENT ANALYSIS OF THE DFT DATABASE

Figure 13 compares the extended primitive cell configurations with the original GAP training database, showing how the newly generated configurations are distributed relative to the reference dataset in descriptor space. The primitive cells were generated by rescaling primitive cell configurations previously constructed for iron [45]. These cells were subjected to large strains in the six independent strain components ε_{ij}

TABLE VIII. Summary of the enriched DFT database for each RM.

Element	Configuration	Number of structures	Number of local atomic environments (LAEs)
V	Primitive	2963	2963
	Traction-separation	276	6624
	Stacking fault {110}	314	6280
	Stacking fault {112}	380	11 400
	EOS of FCC	80	80
	EOS of BCC	80	80
	EOS of HCP	180	360
	Primitive	2963	2963
Nb	Traction-separation	276	6624
	Stacking fault {110}	826	16 520
	Stacking fault {112}	450	13 500
	EOS of FCC	80	80
	EOS of BCC	80	80
	EOS of HCP	180	360
	Screw dislocation	29	3915
	Primitive	2963	2963
Ta	Traction-separation	276	6624
	EOS of FCC	30	30
	EOS of BCC	30	30
	EOS of HCP	30	60
	Primitive	2963	2963
Mo	Traction-separation	276	6624
	Primitive	2963	2963
W	Traction-separation	276	6624
	Primitive	2963	2963

TABLE IX. Configuration types included in the original GAP-2020 DFT database for W. The same configuration types are used for the other RMs [27].

Configuration	Number of structures	Number of local atomic environments (LAEs)
A15	100	800
BCC distorted	500	1000
C15	100	600
Di-SIA	15	2350
Divacancy	10	1180
Diamond	100	200
Dimer	13	26
FCC	100	100
γ surface	178	2136
HCP	100	200
Isolated atom	1	1
Liquid	45	5760
Phonon	20	1080
SC	100	100
Short range	90	4860
SIA	32	3872
Slice sample	1996	1996
Surf liquid	24	3264
Surface (100)	45	540
Surface (110)	45	540
Surface (111)	43	516
Surface (112)	45	540
Trivacancy	15	1755
Vacancy	210	11 130
Total	3927	44 546

ranging from -0.22 to 0.3 , with the strain space sampled using a Sobol' sequence [112].

APPENDIX B: COMPOSITION OF THE DFT DATABASES

Table VIII lists the additions to the original GAP-2020 DFT database and the corresponding numbers of structures and local atomic environments (LAEs) for each refractory metal. These include distorted primitive-cell and traction-separation configurations for all five elements, stacking-fault configurations for V and Nb, equation-of-state configurations for V, Nb, and Ta, and screw-dislocation configurations for Nb. Table IX lists the configuration types and the corresponding numbers of structures and LAEs in the original GAP-2020 database for W [27]. The same configuration types are used for the other refractory metals.

APPENDIX C: DDMs PREDICTED BY CLASSICAL IAPs

Figure 14 shows the DDMs predicted by the classical interatomic potentials considered here. DDMs were obtained by comparing the displacement along the dislocation line direction y before and after introducing the screw dislocation. For V, both the Han [75] and Olsson [74] EAM potentials predict compact, nondegenerate cores. The Olsson potential was subsequently used to calculate the Peierls barrier shown in Fig. 4.

For Nb, the Fellingner potential [76] predicts a polarized core, whereas the Zhou potential [80] produces a compact core. However, the NEB calculations did not converge for either Nb potential, and their Peierls barriers are therefore not reported. For Ta, both the Zhou EAM potential [80] and the Pun ADP potential [78] predict compact cores, although their Peierls energy profiles exhibit pronounced double-hump features. The Zhou EAM potential predicts a polarized core in Mo. For W, the Mason [84] and Olsson [74] potentials also produce

polarized cores. By contrast, the Marinica EAM potential [83] predicts a compact core and a single-hump Peierls-energy profile, as shown in Fig. 4. These results demonstrate that an EAM potential can be parametrized to reproduce both the correct screw dislocation core structure and the qualitative shape of the Peierls barrier. Nevertheless, even when these qualitative features are captured, the predicted barrier height can remain quantitatively inaccurate (see Fig. 4 and Table VII).

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