Ab initio modeling of the role of local chemical short-range order on the Peierls potential of screw dislocations in body-centered cubic high-entropy alloys

Sheng Yin\textsuperscript{1,2}, Jun Ding\textsuperscript{2}, Mark Asta\textsuperscript{1,2*} and Robert O. Ritchie\textsuperscript{1,2*}

\textsuperscript{1}Department of Materials Science & Engineering, University of California, Berkeley, CA 94720, USA
\textsuperscript{2}Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA
*To whom correspondence may be addressed; email: mdasta@berkeley.edu or roritchie@lbl.gov

In traditional body-centered cubic (bcc) metals, the core properties of screw dislocations play a critical role in plastic deformation at low temperatures. Recently, much attention has been focused on refractory high-entropy alloys (RHEAs), which also possess bcc crystal structures. However, unlike face-centered cubic high-entropy alloys (HEAs), there have been far fewer investigations on bcc HEAs, specifically on the possible effects of chemical short-range order in these multiple principal element alloys on dislocation mobility. Here, using density functional theory, we investigate the distribution of dislocation core properties in MoNbTaW RHEAs alloys, and how they are influenced by local chemical short-range order (SRO). The distribution of dislocation core energies and Peierls potentials are investigated systematically and reveal a marked effect of SRO in elevating the Peierls potential of screw dislocations. The computational results thus suggest potentially important effects of SRO on dislocation morphologies and their motion.

Keywords: Refractory high-entropy alloys; screw dislocations; Peierls potential; local chemical ordering

INTRODUCTION

Previous investigation of the fundamentals of deformation in body-centered cubic (bcc) transition metals have revealed that the core properties of the \( \frac{1}{2}<111> \) screw dislocations play an
essential role in their plasticity, ¹ especially at low temperatures where the deformation is thermally activated through the kink-pair nucleation mechanism, ² and expected to be strongly temperature-dependent. The high lattice friction associated with such screw dislocation motion is a result of their nonplanar core structure ¹,³ and related to the height of the Peierls potential. ⁴

Due to their importance for plastic deformation, extensive atomistic simulation studies have been devoted to computing core structures and corresponding mobilities of screw dislocations in bcc transition metals. ³,⁵,⁶,⁷,⁸ In these studies one of the significant challenges has been the variation in properties derived from different models for the interatomic potentials. For example, early studies based on classical potential models often predicted a metastable split core structure,⁹,¹⁰,¹¹ which leads to a camel-hump shape in the Peierls potential. Later density functional theory (DFT) produced symmetric and compact dislocation cores in Mo, Ta and Fe;¹²,¹³,¹⁴,¹⁵,¹⁶ similar compact cores have also been found in other bcc transition metals, such as W, Nb and V.¹⁷,¹⁸ In DFT studies of the energy landscape of screw dislocations in bcc transition metals,¹⁸,¹⁹,²⁰ it was found that non-degenerate cores lead to a single humped curve in the Peierls potential, implying that the split core structure might not be metastable. Alloying effects on Peierls potential of W have also been explored ²¹. Recently developed machine learning based potentials ²²,²³,²⁴ and new embedded atom method (EAM) potentials that consider quantum effects on lattice vibrations ²⁵ and extra constraints ²⁶ have all led to predictions of a single humped curve in the Peierls potential. Due to the dependence of the results for screw dislocations in bcc transition metals on the model for interatomic bonding, DFT-based approaches are of interest to provide benchmarks for subsequent classical modeling.

During the past fifteen years, a new class of alloys known as high-entropy alloys (HEAs) ²⁷,²⁸ has drawn extensive research interest. These alloys involve multiple principal elements (typically
five) in nominally equimolar ratios, and were originally presumed to crystallize as a single-phase solid solution. As a new class of structural materials, some types of HEAs, in particular the CrCoNi-based alloys, have been shown to possess exceptional damage tolerance and improved strength at cryogenic temperatures.\textsuperscript{29,30} Theoretically, mechanistic, first-principles-based predictive theories for the temperature-, composition-, and strain-rate-dependence of the plastic yield strength have been developed and applied to such face-centered cubic (fcc) alloys.\textsuperscript{31,32,33} Indeed, most HEA research to date has been focused on these fcc “Cantor type” alloys,\textsuperscript{34,35} whereas a second distinct family of HEAs, comprising mostly refractory elements, has been far less studied. Such refractory high-entropy alloys (RHEAs), which are sometimes termed Senkov alloys,\textsuperscript{36,37} are invariably crystallized with bcc solid-solution phases that have been designed for elevated temperature applications.\textsuperscript{38} For example, RHEAs such as MoNbTaW in single-phase bcc crystal structure have been produced by vacuum arc melting\textsuperscript{37} or direct metal deposition\textsuperscript{39} with exceptional microhardness\textsuperscript{36} as well as excellent compression yield strength and good ductility at high temperatures.\textsuperscript{37} Transmission electron microscopy (TEM) studies on RHEAs have shown a dominant role of screw dislocations with increasing plastic strain,\textsuperscript{40,41} similar to traditional bcc metals. Additionally, strong intrinsic lattice resistance has been found in certain RHEAs.\textsuperscript{41,42} To model such behavior, molecular dynamics (MD) simulations have been used to study dislocation behavior in bcc RHEAs.\textsuperscript{43} For example, screw dislocation core structures in NbTiZr, Nb\textsubscript{1.5}TiZr\textsubscript{0.5} and Nb\textsubscript{0.5}TiZr\textsubscript{1.5} alloys were recently explored using such MD simulations and significant core structure variation was found along the dislocation line.\textsuperscript{44} Recent theory has also revealed the potential importance of edge dislocations in controlling the strength of bcc HEAs at high temperatures\textsuperscript{45} and the correlation between atomic distortions and the yield
strengths of HEAs. However, there are still only very limited studies on the deformation behavior of this new class of bcc alloys, as compared to single-phase bcc transition metals.

Another important aspect of HEAs is the presence of local chemical short-range order (SRO). Although these alloys can be described as “topologically ordered yet chemically disordered”, the local chemical environments are unlikely to be characterized by a perfectly random distribution for every atomic species. Indeed, their disordered multiple-element compositions leads to a strong possibility of SRO, e.g., the preference for certain types of bonds over the first few neighbor shells. This is not particularly rare in conventional alloys and glasses; however, it could be argued that its existence would be even more likely in multiple principal element alloys due to large number of elements and their equimolar concentrations. Recent DFT and MD simulations on the CrCoNi alloy suggest that SRO can have a profound effect on critical parameters, notably the stacking-fault energy and dislocation mobility; accordingly, such local order could be a major factor in controlling mechanical properties.

In spite of extensive studies on the bcc transition metals, there are relatively few published studies of the dislocation core structures, dislocation mobility or the effect of chemical SRO for bcc RHEAs. Accordingly, the objective of the current paper is to employ DFT-based methods to compute the dislocation core structures in refractory HEAs and to explore the dislocation core energies and distribution of Peierls barriers, focusing on the MoNbTaW system. Additionally, we study how SRO can evolve in these RHEAs, and its effect on the core properties and Peierls potential of screw dislocations.

RESULTS

Dislocation core structures in RHEAs
To compute the core structures and Peierls potential for ½<111> screw dislocations in the refractory MoNbTaW HEA, we employ DFT calculations, making use of the Vienna \textit{ab initio} simulation package\cite{57,58,59}. Details of the DFT calculations are provided in the Methods section.

For screw dislocations in refractory HEAs, we employ a periodic supercell that contains 462 atoms, as illustrated in \textit{Figure 1a}. The simulation cell contains a pair of dislocations with opposite Burgers vectors, in a nearly square quadrupolar arrangement\cite{16} with triclinic periodic boundary conditions to minimize any effects of periodic boundary conditions and image stress. This dipole approach was first introduced by Bigger \textit{et al.}\cite{60} and has been widely used in DFT calculations on dislocations\cite{16,17,20,61}. The supercell adopted in current work was previously described by Weinberger\cite{17} and Li \textit{et al.}\cite{61} and was used to calculate dislocation core structures in pure \textit{bcc} transition metals. In addition, since the size of supercell is fixed for all the simulations, the short periodic length might have some influence on the dislocation dipole energy due to its effect on the nature of the SRO. In our current model, we consider an equimolar MoNbTaW \textit{bcc} RHEA\cite{37}, and doubled the periodic length along the dislocation line direction of the original 231-atom model (see Methods section for further details), to minimize as much as possible correlations in the chemical order, as described in the following section.

The initial atomic configuration was generated by creating a special quasi-random structure (SQS) on the 462-atom supercell shown in \textit{Fig. 1a}. The SQS was generated using the Alloy Theoretic Automated Toolkit (ATAT) program\cite{62}. The SQS methodology was used to minimize chemical correlations, and thus to provide a reference configuration corresponding to random substitutional disorder \textit{(i.e., minimizing chemical SRO)}. This reference configuration was used in Monte-Carlo simulations to generate supercells with varying degrees of SRO, as described below. For each of these configurations, we shifted the dislocation dipole over all the possible
sites within the simulation cell for samples with different levels of SRO, to statistically sample dislocation properties. The atomic positions in the system with the dislocation dipole were then relaxed to enable interrogation of the core structures in different lattice sites within the RHEA supercell.

Fig. 1 | Dislocation dipole model and structure of dislocation cores in an equimolar MoNbTaW bcc RHEA. a, Differential displacement map of the dislocation dipole model. b, Close-up view of the structure of a compact core. c, Close-up view of the structure of a non-compact core.

For each configuration representing a different degree of chemical SRO, we calculated 231 different structures with the dislocation dipole initiated in different local environments. We find that the screw dislocations in bcc MoNbTaW HEAs maintain a compact core structure in most of these relaxations, as illustrated by Fig. 1b, which is similar to the case in pure bcc elements. In a very few situations, the core can be extended on the (110) plane as shown in Fig. 1c. The DFT calculations thus reveal the dominant role of compact cores for dislocations in the
MoNbTaW alloy (see Supplementary Note 1 for further details); the simulation results are also consistent with the single humped Peierls potential curves, as discussed in the following sections.

**Local Chemical Short-Range Order in MoNbTaW RHEA**

It has been shown that local chemical SRO can play a critical role in influencing materials properties in *fcc* HEAs, such as the stacking-fault energy\(^5^5\) and the dislocation mobility.\(^5^6\) Previously, a cluster expansion (CE) Hamiltonian in a combination with Monte Carlo (MC) simulations have been developed to investigate the effects of SRO in MoNbTaVW and its quaternary sub-systems.\(^5^0\) The ordering in the MoNbTaW RHEA alloy has been studied by Körmann *et al.*\(^6^3,6^4,6^5\) This work revealed B2 ordering at intermediate temperatures and phase decomposition in the ground state. For the present study, we employed a different approach (which nevertheless gives results in qualitative agreement with those of Kormann *et al.*, as discussed below), chosen to enable the development of dislocation supercell models with representative degrees of chemical SRO. Our focus is specifically on the effect of SRO on the dislocation properties. Specifically, similar to previous studies in *fcc* HEAs,\(^4^7,5^5\) we applied a DFT-based lattice Monte Carlo (MC) approach to our 462-atom supercell model, with details that are described in the Methods section.

The supercell initiated with an SQS configuration was used as input for the MC simulations. The MC simulation samples swaps of atom types, following the Metropolis algorithm, and the entire simulation considers approximately 2100 such swaps, leading to the evolution of the energy shown in Fig. 2a. Due to the limited number of MC steps and the lack of sampling of atomic displacements, the final configurations may differ from the true equilibrium state of SRO at the simulation temperature, although they appear to be quite close to the state of SRO as calculated by Kostiuchenko *et al.*\(^6^5\) for high temperatures (~1200 K). However, the algorithm
does lead to appreciable lowering of the energy, as shown in Fig. 2a, and the pair-forming tendencies shown in Fig. 2b are consistent with previous work on SRO in the same system using more comprehensive methods,\textsuperscript{63,65} as discussed below. Thus, this method is used to generate representative samples with varying degrees of chemical SRO to explore the resulting effect on dislocation properties.

**Fig. 2** | Evolution of energy and local chemical SRO in the MoNbTaW RHEA. 

**a,** Potential energy change vs. SRO parameter during the MC relaxation. Three states (s1, s2, s3) with different levels of SRO as indicated by red arrows were chosen for calculations of the dislocation cores and Peierls potentials. 

**b,** The detailed values of $\Delta\delta_{ij}$ for all atom pairs. The red lines and dots represent state s3 with SRO and the dashed lines represent the ideal random solid solution case.

Similar to the conventional Warren–Cowley description\textsuperscript{66} and the previous study for fcc HEAs\textsuperscript{55}, we characterize the state of SRO using the so-called nonproportional number of local atomic pairs, $\Delta\delta_{ij}$, as described in more detail in the Methods section. Based on our calculations, the evolution of total potential energy and the overall chemical SRO ($\sum_{i,j} |\Delta\delta_{ij}|$) in the sample during the MC relaxations are plotted in **Fig. 2a.** With respect to axes, the abscissa is the total potential energy change of the system and the ordinate is the overall chemical SRO of the system. As the MC simulation proceeds, the potential energy of system decreases monotonically while the chemical SRO parameter increases at the same time. This clear trend indicates that chemical
SRO is naturally occurring in the system with the MC simulations. To quantify the effect of SRO on dislocations, three different samples from the simulation (s1, s2, s3) were chosen for further calculation of Peierls potentials, indicated by the red arrows in Fig. 2a. State s1 represents the nearly random solid solution configuration with lowest magnitudes of the SRO parameter; s2 represents the intermediate configuration with a medium level of SRO, and s3 represents the configuration with highest SRO.

Figure 2b shows the detailed values of $\Delta \delta_{ij}$ between all the species in the MoNbTaW alloy, the red dots show that the local SRO in state s3 clearly deviates from the random solid solution case. Preferred atomic pairings between Mo-Ta, Mo-Nb and Ta-W were observed as the $\Delta \delta_{ij}$ values are 0.308, 0.196 and 0.112, while unfavorable pairings between Mo-W and Ta-Nb were also apparent as the $\Delta \delta_{ij}$ values are -0.392 and -0.294. This result confirms the existence of SRO in MoNbTaW alloys; moreover, the tendency to form SRO that we see here is consistent with previous studies using other methods that have shown the Mo-Ta pairs are the most dominant SRO contributors to the SRO, followed by Ta-W and Mo-Nb pairs.

**Distribution of dislocation core energies in bcc RHEAs**

After the introduction of SRO through MC relaxations, the dislocation dipole described in Fig. 1a was then created in samples s1, s2 and s3. To sample over the distribution of local chemical environments for dislocation cores, the dislocation dipole was shifted over all the possible sites within the simulation cell leading to 231 different configurations for each of the three states of SRO. All the configurations with the dislocation dipole were then minimized, following the procedures described in the Methods section.

Figure 3 shows histograms of the dislocation dipole energies (determined by subtracting the energy of the perfect crystal configuration from the total potential energy with the dislocation
dipoles) of all the configurations minimized at different SRO states. The histograms, especially $s1$ and $s2$, fit well with the normal distributions (the fitted lines are also shown in Fig. 3). The green dash-dot line represents the energy distribution of the nearly random solid-solution sample $s1$. The blue dash line represents the sample $s2$ with a medium degree of SRO and the red solid line represents the sample $s3$ with highest degree of SRO. The mean values of the supercell dipole energies for the two samples with SRO differ by 4.16 eV ($s2$) and 9.0 eV ($s3$) from that for the most disordered sample ($s1$). The histograms of total potentials energies are also plotted in Supplementary Figure 2. We can observe the decreases in average total potential energies with increasing SRO, which is expected; this is also consistent with the trend in the MC simulation which contains no dislocation cores. Despite the change in mean potential energy, the most significant feature of Fig. 3 and Supplementary Fig. 2 is that the increase in SRO also leads to an increase in the standard deviation (variance) of dislocation dipole energy. The standard deviation of the supercell dipole energy in $s1$ is 0.81 eV, which increases to 1.05 eV in $s2$ and to 1.87 eV in $s3$, i.e., with higher degrees of SRO, this effect becomes more significant.

Previous studies have shown that the energies of the types of supercells used in this study can be affected by the residual stress in the simulation box.$^{67,68,69}$ In Supplementary Figure 3, we plot the distribution of this residual stress on all the simulation cells. The data rule out the correlation between the increase in variance in the dislocation energies cited above and the residual stresses. Another potential origin of the variance in energies of the supercells is associated with the cut plane between the two dislocation cores - when SRO is present this cut plane leads to a contribution to the energy of the supercell arising due to the shift of adjacent planes, which disrupts the state of SRO. The energy associated with the cut plane between the dislocation core is dependent on the levels of chemical ordering and can be quantified through the so-called
diffuse antiphase boundary (DAPB) energy ($\gamma_{DAPB}$). According to our calculations, for the state $s1$ which represents the random solid solution, $\gamma_{DAPB}$ is $\sim 3$ mJ/m$^2$, i.e., essentially zero within the accuracy of our statistical sampling. With increasing SRO, $\gamma_{DAPB}$ increases to 29 mJ/m$^2$ in state $s2$ and 59 mJ/m$^2$ in state $s3$ with the highest degree of SRO. Based on the calculated values of $\gamma_{DAPB}$, we can quantify that the cut plane gives rise to a maximum contribution to the energy of the supercell of 0.1 eV/b, and the variation in this energy due to the shift of the cut plane as the positions of the dislocation cores are shifted is much smaller, as discussed in further detail Supplementary Note 2. We thus conclude that the dominant contribution to the variance in supercell energy shown in Figure 3 arises from the variations in dislocation core energies, and the results thus demonstrate the important role of SRO in broadening their distribution.
Fig. 3 | Histograms of dislocation dipole energies at different levels of SRO in MoNbTaW. Histograms of supercell dislocation dipole energies with dislocation cores in different sites over the sample for three different states (s1, s2, s3) of SRO, fitted with a Gaussian distribution. The normalized dipole energy is the supercell dipole energy divided by the total Burgers vector length in the supercell. Note that state s1 represents the random solid-solution state with minimum SRO, s2 has a medium level of SRO, and state s3 has the highest level of SRO.
**Fig. 4 | Contours of Peierls valleys and the difference in the Peierls valley energy at three levels of SRO in the MoNbTaW supercell (no barriers data included).** a, random solid solution state $s1$ with minimum SRO. b, state $s2$ with a medium level of SRO. c, state $s3$ with the highest level of SRO. Grid-$x$ and grid-$y$ represent the relative position of the dislocation dipole as shown by the black dots on the right column figures. The contours were plotted by interpolating data points on grids through bivariate spline.

To further illustrate the spatial effect of SRO on the distribution of dislocation core energies, we plot the 3D contours of the dislocation dipole energies and energy differences in our supercell in Figure 4 (a 2D projection of these contours is shown in Supplementary Figure 4). For simplicity, each dislocation dipole was treated as a single point; they are plotted on an $x$-$y$ grid based on their relative positions. The dipole energies normalized by the total length of the dislocation lines, which can be regarded as the Peierls valleys, were shifted to make the minimum value equal to zero. Based on these data, the left column of Figs. 4a-c shows contours of the Peierls valleys at different SRO states from $s1$-$s3$, respectively. Note that this is not a minimum energy path (MEP) contour, since no transition-state data were included.

For a pure element metal, the contour in Figure 4 would be a flat surface since the depth of the Peierls valley has a constant value. However, due to variations in local environment within the RHEA, the dislocation dipole energy in these alloys follows a normal distribution, as shown in Fig. 3, which leads to rugged Peierls valleys contours, as shown in Fig. 4. The variation in the Peierls valleys ranges from 0 to 1.125 eV/b in the near-random $s1$ state; with increasing SRO, this increases to 1.2 eV/b in $s2$ and to 2.25 eV/b in $s3$. It is clearly shown in Figs. 4a-c that the contours become more and more rugged as the SRO increases. The changes in the contour of energy with glide of the dislocations in the $[\bar{1}12]$ direction by each unit of the Peierls valley spacing were determined and are plotted in the right column of Fig. 4. Here, standard analyses of transitions in various complex systems are consistent with the basic trend that the energy difference between the final and initial states is associated with the change in the energy barrier.
In the contours of valley energy differences in Fig. 4, the values range from -0.45 to 0.56 eV/b in the s1 state; these increase to -1.25 to 1.0 eV/b in state s2 and to -2.5 to 2.0 eV/b in the state s3. The fraction of these energies with relatively high values increases with the degree of SRO. Similar to Fig. 3, histograms of the differences in valley energy at different SRO states are shown in Supplementary Figure 5. As expected, the valley energy differences also fit with a Gaussian distribution but contain higher variance as the energies of the Peierls valleys themselves follow a Gaussian distribution (demonstrated in Fig. 3). These results, along with the change of distribution of dipole energies in Fig. 3, demonstrate that the presence of SRO serves to broaden the distribution of dislocation core energies and increase the spatial heterogeneity of dislocation core energies in the system. The more rugged energy landscape and high variance in core energies is anticipated to have a profound effect on the distribution of Peierls barriers, as explored further below.

**Peierls potentials of screw dislocations in bcc RHEAs with local chemical order**

After minimizing all the configurations with dislocation dipoles, the Peierls barriers for \( \frac{1}{2}\langle 111 \rangle \) dislocations were computed from the energy pathway between two samples, in which the dislocation dipole was uniformly translated along the [\( \bar{1} \bar{1} 2 \)] direction on the \{110\} plane to the nearest neighboring site. The full transition pathways and saddle points were calculated using the reaction coordinate method (also termed the “drag method”), which has been successfully applied to different pure bcc transition metals in previous studies.\(^{17,20}\) The reaction coordinate vector is the relative displacement between the initial configuration and the final configuration with the shifted dislocation dipole. Comparing with other widely used energy pathway calculation methods, such as the “nudged-elastic-band (NEB) method”,\(^{71}\) the Peierls barriers calculated by these two methods are very close in transition metals, as shown in previous
However, in a system with a complex energy surface, such as the RHEA considered here, the simplified interpolation of states between the initial and final configurations serves to force the reaction pathway along the $[\overline{1}12]$ direction on a $(1\overline{1}0)$ plane. As such, it is expected that this will lead to an overestimation of the actual energy barriers. Although the detailed barrier values that we obtained here using the drag method may be somewhat overestimated, the subsequent conclusions are consistent with the analysis based on the dislocation dipole energy alone, as described above. The advantage of the drag method is that it is more computationally efficient and each job can be run as an individual simulation rather than requiring multiple images to run in parallel. This was of critical importance to the current study as with HEAs since, due to the variation in local atomic environments, it is imperative to sample over a large number of configurations to understand the distribution of the dislocation core energies and Peierls potentials.

Different from pure element metals, the equilibrium energies of the dislocation dipoles are not constant due to the different local environments of the dislocation cores. Thus, the potential energy of the initial configuration (where the reaction coordinate is 0), is generally not equal to that of the final configuration (reaction coordinate of 1). To remove any bias due to the asymmetry of energies of the initial and final configurations, we only consider the dislocation dipole to glide in one direction ($[\overline{1}12]$ direction), which is consistent with the picture of a screw dislocation gliding in a preferred direction due to the effect of external loading.

As will be discussed in the context of the distributions of Peierls barriers below, the values can be divided into two distinct classes that we will refer to as Type-1 and Type-2. Representative results are shown in Fig. 5. Depending on the relative energy difference between the initial and final configurations, Fig. 5 shows two types of barrier curves calculated
using the drag method in the MoNbTaW RHEA. When the potential energy difference between the initial and final configurations is less than \( \sim 1 \) eV, or when the energy of the final configuration is smaller than that of the initial configuration, the barrier curves are usually of Type-1, illustrated by the curves in Fig. 5a. This condition is satisfied by 98.3% of the cases in the random solid solution sample s1, as indicated by the green dash-dot line in Fig. 3, which displays a relatively narrow distribution of dislocation core energies. However, with progressively increasing SRO in samples s2 and s3, the distribution of core energies broadens, as shown by the blue and red histograms in Fig. 3. The higher variance of the core energies leads to another scenario during the calculation of the dislocation Peierls potentials, in which the final configuration has a much higher potential energy than that of the initial configuration (\( > \sim 1.5 \) eV). The typical barrier curves under this condition are shown in Fig. 5b and are referred as Type-2 barriers, in which the Peierls barrier is dominated by the difference in potential energy between the initial and final configurations. As the variance or standard deviation of the core energies is enlarged due to the progressively increasing degree of SRO, there is a higher probability for the second condition to be satisfied and the barrier curves fall into the second type.

According to the calculations based on the drag method, a single humped Peierls potential curve is obtained in all cases examined in detail, with the peak of the curve always close the middle of the reaction coordinate, irrespective of whether the barriers are Type-1 or Type-2. Accordingly, in the interest of enabling a more thorough sampling with finite computer time, most of the Peierls barriers were determined using only one configuration in the middle of the energy path in the results that follow.
Fig. 5 | Two types of Peierls barrier obtained in the MoNbTaW RHEA. a, Several examples of Type-1 barrier curves, which are often observed when the energy of final configuration is lower, or no larger than, ~1.0 eV of the initial configuration. b, Several examples of Type-2 barrier curves, which are controlled by the energy difference between initial and final configurations; these are often observed when the final configuration has a much higher energy than that of the initial configuration.

We calculated the dislocation Peierls barriers (defined as the energy difference between the saddle-point and initial state shown in Fig. 5) sampled over all the possible sites within the simulation cell along the [112] direction in three configurations (s1, s2, s3) with different degrees of SRO; the resulting distributions of the Peierls barrier for the bcc MoNbTaW RHEA are shown in Fig. 6. Note that the energy barriers are the barriers for moving both dislocations in the dipole at the same time; the barriers presented here are divided by the total dislocation line length and is thus reported as energy per Burgers vector. Figure 6a shows a histogram of Peierls barriers in the nearly random solid-solution sample s1 with minimal SRO. Most cases (98.3%) in the s1 sample show the Type-1 barriers described in Fig. 5a; as such, the calculated Peierls barriers fit well with a normal distribution, with an average value of the normalized barriers of 387 meV/b. Figure 6b shows the corresponding histogram of Peierls barriers in sample s2 with a medium level of SRO. Again, the major peak in Fig. 6b corresponds to a Type-1 barrier (Fig. 5a), i.e., it is the same as for sample s1 in Fig. 6a, although next to the Gaussian peak, we can observe
some large barriers on the right side of the histogram; these conversely correspond to Type-2 barriers (Fig. 5b), where the core energy difference between the initial and final states dominates. In the current study, 21% of the calculated cases for sample s2 comprised Type-2 barriers. As the SRO is further increased in sample s3, the proportion of Type-2 barriers becomes increasingly more significant, with 34% of the calculated cases falling into this category. Figure 6c shows the histogram of Peierls barriers in sample s3 with highest degree of SRO. The major peak of the histogram in Fig. 6c still coincides with that in samples s1 and s2; however, there are many more barriers on the right (higher) side of the peak that result from the difference in core energies. This is consistent with the observation in Fig. 3 that local short-range order increases the variance of core energies distributed in the sample and leads to more Type-2 barriers.

Although the transition from Type-1 to Type-2 barriers is not rigorously defined, it is highly dependent on the relative energy difference between the initial and final dislocation configurations. Due to the nature of RHEAs, the core energy for two neighboring positions of the dislocations might have very distinct energies, as shown in Figure 4, and if the final configuration has a much higher core energy, this will lead to a Type-2 barrier. Here, we assume that for our alloy with a certain level of SRO, the dislocation dipole energy will follow a normal distribution: $\text{Normal}(\mu, \sigma^2)$ (similar to Fig. 3), as shown in Figure 7a. If we assume that there are two random independent neighboring dipoles, dipole-1 and dipole-2, dipole-2 represents the initial configuration and will have a preference to glide to its final configuration dipole-1. The energy of these two dipoles are written as $E_{d1}$ and $E_{d2}$. For the transition from a Type-1 to a Type-2 barrier, we postulate that there exists a critical energy difference $E_{\text{critical}}$ that when $E_{d1} - E_{d2} > E_{\text{critical}}$, the Peierls barrier will become a Type-2. Based on our assumptions for the distribution in dipole energies in Figure 7a, the energy of dipole-1 and dipole-2 are:
\[ E_{d1} \sim \text{Normal}(\mu, \sigma^2), E_{d2} \sim \text{Normal}(\mu, \sigma^2) \]. The energy difference between the two dipoles is \[ E_{d1} - E_{d2} \sim \text{Normal}(0, 2\sigma^2) \]. Thus, the probability of observing a Type-2 barrier for this condition can be written as:

\[
P_{\text{type2}} = P(E_{d1} - E_{d2} > E_{\text{critical}}) = 1 - P(E_{d1} - E_{d2} \leq E_{\text{critical}}) = 1 - \Phi\left(\frac{E_{\text{critical}}}{\sqrt{2}\sigma}\right) \tag{1}
\]

where \( \Phi \) is the standard Normal cumulative distribution function.

Based on this equation, the probability of a Type-2 barrier is a function of \( E_{\text{critical}} \) and the standard deviation \( \sigma \) (or variance) of the dipole energy distribution. In Figure 7b, we plot \( P_{\text{type2}} \) as a function of \( \sigma \) for three different values of \( E_{\text{critical}} \). These curves clearly demonstrate that the probability of a Type-2 barrier will increase monotonically with the standard deviation \( \sigma \), which is highly correlated with the state of SRO; this is shown in Figure 3. In addition, in Figure 7b, we have also plotted the \( P_{\text{type2}} \) and \( \sigma \) for the three SRO states \( s1-s3 \) based on our DFT data shown in Figures 3-6. Although we cannot accurately fit the \( E_{\text{critical}} \) due to the limited amount of DFT data, the trend in the values of \( P_{\text{type2}} \) and \( \sigma \) in our DFT calculations is consistent with the analytical results. For a single screw dislocation, rather than the dislocation dipole geometry considered in this study, we can obtain similar results as \( P_{\text{type2}} = 1 - \Phi\left(\frac{E_{\text{critical}}}{\sigma}\right) \); as discussed in further detail in Supplementary Note 3). This analysis explains the origin of the Type-2 Peierls barrier and its correlation with the state of SRO in the RHEAs.

The Peierls barriers for pure \( bcc \) elements, such as W, Mo, Ta and Nb, were also calculated using the same drag-method. The values that we obtained (Fig. 6d) are consistent with previous calculations.\(^\text{17}\) Although possibly not an ideal way to present these data, the average Peierls barriers of the RHEA in the three different states of SRO are plotted and compared with the corresponding values for pure \( bcc \) metals in Figure 6d. Due to lattice mismatch and resulting distortion, the Peierls barrier of the \( bcc \) RHEAs is much larger than that of pure \( bcc \) metals.
Although the drag method may not provide precise accuracy in such complex material system, we can conclude that in simple terms, the increase of SRO in the RHEA serves to increase the range of dislocation core energies, which further enhances the probability of observing Peierls barriers of Type-2, which will finally influence the dislocation morphologies and their motion.

Fig. 6 | Distributions of Peierls barriers in the MoNbTaW RHEA as compared to pure metal systems. a, Peierls barriers in the random solid-solution sample s1 with minimal SRO. b, Peierls barriers in sample s2 with a medium level of SRO. c, Peierls barriers in sample s3 with highest level of SRO. d, Average Peierls barriers in samples s1, s2 and s3 are compared with Peierls barriers calculated for pure W, Mo, Ta and Nb.
Fig. 7 | Probability of a Type-2 barrier dependent on the standard deviation of the dipole energy. a, Schematic figure of the distribution of dipole energy and two random neighboring dipoles. b, Probability of a Type-2 barrier as a function of the standard deviation of the dipole energy.

DISCUSSION

Using first principles calculations of dislocation energies and Peierls barriers in bcc RHEAs, our results reveal fundamental differences between behavior in the multiple principal element alloys and a pure metal or dilute solution. The complex local environments within the RHEAs lead to a distribution of dislocation core energies for different dislocation segments; moreover, the characteristics of this core energy distribution are significantly influenced by the presence of local short-range order. In contrast, all the local environments are constant in pure metals and would be expected to show much smaller distributions for dilute solutions. With our present DFT calculations, although we have doubled the thickness of the sample, the dimension of out-of-plane direction is still limited to only two Burgers vectors. The calculated core energies and Peierls potentials thus represent the local characteristics of a small straight segment of dislocation line. When considering a long dislocation line gliding in the RHEA, due to the
Gaussian distribution of local energies of dislocation segments, described in Figure 3, the dislocation line will prefer to form a wavy shape to reduce the total potential energy. For alloys with multiple principal elements in equal molar ratios, statistically the composition fluctuation always exists even for a random solid solution. However, our results have shown that the presence of short-range order will significantly broaden the distribution of energies of dislocation segments as shown in Figure 3, thereby increasing the heterogeneities of the system (shown in Fig. 4) to further facilitate the formation of wavy dislocation morphologies.

The Peierls potential plays a crucial role in governing dislocation motion. Here, we have identified two types of Peierls barriers in the bcc RHEA which depend critically on the energy distribution of the dislocation segments. Considering a long dislocation motion associated with kink-pair theory, it is extremely difficult for some segments gliding through the path of the Type-2 barriers due to its high magnitude. Under these circumstances, these segments can become pinned or are forced to glide on alternative planes or in different directions. This will serve to facilitate cross slip, dislocation multiplication and the formation of wavy dislocation lines, all of which will eventually enhance the strength and ductility of the material at the macroscale due to homogenization of plastic strains. Indeed, such a form of wavy slip and enhanced mechanical properties has been reported for a bcc TiZrNbHf RHEA with short-range ordered (O,Ti,Zr)-complexes. Recently, a theory developed for screw dislocation strengthening in RHEAs has been presented based on the assumption that screw dislocations will naturally adopt a kinked configuration. Along with the MD simulations of the NbTaV alloy, our DFT data, as shown in Figures 3-4, strongly supports the idea that dislocation lines in this and related RHEAs would tend to form a kinked structure.
In summary, we have systematically studied the Peierls potential of screw dislocations in a bcc MoNbTaW refractory high-entropy alloy using ab initio modeling, considering the effects of chemical short-range order. Similar to the pure bcc transition metals, compact cores were found to dominate in screw dislocations in the bcc MoNbTaW RHEA. The dislocation core energies were found to follow a Gaussian distribution with the increasing degree of SRO resulting in a progressively higher variance of the distribution of core energies. Resulting from the intrinsic fluctuation of core energies in HEAs, two types of Peierls barriers were discovered, which depend on the difference in core energies between initial and final configurations. By comparison with pure bcc transition metals, the Peierls barrier of screw dislocations in bcc RHEAs is much higher in samples with SRO, further increasing the overall value of the Peierls potentials due the formation of Type-2 Peierls barriers. The findings from the present work highlight the major role of short-range order in influencing dislocation Peierls potentials and the consequent effects on dislocation morphology and activity, all of which can have a significant impact on the mechanical properties of refractory high-entropy alloys.

METHODS

Lattice constant determination and simulation cell with dislocation dipole

The lattice constant of the equimolar MoNbTaW HEA was determined by relaxing the 64-atoms quaternary quasi-random structure (SQS)\textsuperscript{75} provided by Gao et al.\textsuperscript{76} The calculated lattice constant was 3.230Å and was adopted in all simulations. For the simulation cell with dislocation dipole, we first defined $e_1 = a_0[\overline{1}12], e_2 = a_0[\overline{1}10], e_3 = a_0/2[111]$. Then, the supercell with a dislocation dipole was built with three edges’ $h_1 = 7e_1, h_2 = 3.5e_1+5.5e_2+0.5e_3, h_3 = 2e_3$, to contain 462 atoms. The periodic length along the dislocation line direction, $h_3$, was twice the magnitude of the Burgers vector.
DFT-based Monte Carlo simulations

For the Monte Carlo (MC) simulations, the sample was generated as an SQS for the initial starting point. The temperature employed in the MC simulations was 500 K. Energy calculations were performed using the Projector Augmented Wave (PAW) method, as implemented in the Vienna ab initio simulation package. A plane wave cut-off energy of 400 eV was employed, and the Brillouin zone integrations were performed using Monkhorst–Pack meshes with a $3 \times 1 \times 1$ grid, where the first index corresponds to the direction along the dislocation line. Projector augmented wave potentials were employed with the Perdew–Burke–Ernzerhof generalized-gradient approximation for the exchange-correlation function. Lattice MC simulations were then conducted similar to the methods utilized by Tamm et al. and Ding et al., which included swaps of atom types with the acceptance probability based on the Metropolis–Hastings algorithm. In the current MC simulations, a total of 2094 swaps were conducted and 471 swaps were accepted. For the choice of PAW potentials, 6 valence electrons were used for Mo and W, 5 valence electrons for Ta, and 11 valence electrons for Nb.

Core structure and barrier calculation-Drag method

Following the MC simulations, the dislocation dipole was introduced into the sample at all possible sites. All configurations with the dislocation dipole were then relaxed through a conjugate-gradient algorithm with a denser k-point mesh of $7 \times 1 \times 1$. Atomic positions were relaxed with a convergence criterion on forces of $10^{-2}$ eV/Å. For each relaxed sample selected as the initial configuration, we chose the sample with a nearest dislocation dipole on the same {110} plane and displaced in the $\bar{1}\bar{1}2$ direction as the final configuration; further details are given in Supplementary Figure 6. The Peierls barrier was computed from the energy pathway between these two samples. The reaction coordinate vector was taken as the relative displacement.
between the initial configuration and the final configuration of the shifted dislocation dipole. The drag method was adopted here due to its much lower cost and numerical stability for applications where complex alloy systems are considered. However, this method can lead to a reduction in accuracy compared to other chain-of-states methods such as NEB, especially for asymmetric cases, since an unbiased straight-line interpolation is assumed for the reaction coordinate, which can be expected to lead to some degree of overestimation of the true energy barriers.

**Local chemical short-range order parameter**

Similar to the definition described by Ding *et al.*\(^{55}\), which was modified from the Warren–Cowley parameter,\(^ {66}\) we defined the nonproportional number of local atomic pairs, \(\Delta \delta_{ij}\), to quantify the chemical ordering around an atomic species for the combined first and second nearest-neighbor shells in the \(bcc\) structure, for which the corresponding coordination numbers are \(N = 14\). The value of \(\Delta \delta_{ij}\) was then calculated as:

\[
\Delta \delta_{ij} = N(p_{ij} - p_{ij}^{ideal}) ,
\]

where \(N = 14\) is the coordination number of first and second nearest-neighbor shells in the \(bcc\) structure, \(p_{ij}\) is the actual probability of bonds between atoms of type \(j\) and type \(i\) in the sample, \(p_{ij}^{ideal}\) is the ideal probability of bonds between atoms of type \(j\) and type \(i\) for the random solid solution case based on the species concentrations. \(\Delta \delta_{ij} = 0\) for the case of a random solution. The overall SRO is represented by the sum of all the \(|\Delta \delta_{ij}|\) for all species (\(SRO = \sum_{i,j} |\Delta \delta_{ij}|\)).

**DATA AVAILABILITY**

The data that support the findings of this study are available from Dr. Sheng Yin (email: shengyin@berkeley.edu) upon reasonable request.

**CODE AVAILABILITY**
The DFT calculations were performed with the Vienna ab initio simulation package. All the other codes that support the findings of this study are available from Dr. Sheng Yin (email: shengyin@berkeley.edu) upon reasonable request.

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AUTHOR CONTRIBUTIONS

S.Y. and R.O.R. conceived the research, S.Y. and J.D. performed the numerical simulations and analyzed the results, and M.A. and R.O.R. supervised the research. S.Y. and R.O.R. wrote the manuscript with assistance of all co-authors.

COMPETING INTERESTS

The authors declare no competing interests.

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Supporting Information

*Ab initio* modeling of the role of local chemical short-range order on the Peierls potential of screw dislocations in body-centered cubic high-entropy alloys

Sheng Yin\textsuperscript{1,2}, Jun Ding\textsuperscript{2}, Mark Asta\textsuperscript{1,2*} and Robert O. Ritchie\textsuperscript{1,2*}

\textsuperscript{1}Department of Materials Science & Engineering, University of California, Berkeley, CA 94720, USA
\textsuperscript{2}Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

*To whom correspondence may be addressed; email: mdasta@berkeley.edu or roritchie@lbl.gov
Supplementary Figure 1 | Definition of compact cores and non-compact cores in differential displacement maps. The upper panel represents a typical compact core, and the lower two are examples of non-compact cores, as described further in Supplementary Note 1.

Supplementary Note 1: Compact vs. non-contact dislocation cores

In the compact cores shown in Supplementary Figure 1, the differential displacement map is similar to the displacement of an ideal screw dislocation obtained by the Volterra construction, with the red arrow and blue arrow forming an equilateral triangle. Around the dislocation cores, the length of red arrows is written as \( l_{ri} \) and the length of blue arrows is written as \( l_{bi} \), where \( I = \)
1, 2, 3. Ideally, in a perfect Volterra construction, $l_{ri} = constant_1$, $l_{bi} = constant_2$ for $I = 1, 2, 3$ and $l_{ri} = 2l_{bi}$. In the RHEA, due to the complexity of numerous chemical species, local atomic environments and lattice distortions, $l_{ri}$ and $l_{bi}$ are not expected to be constant. Here, we define the ratio $r = \min(l_{ri})/\max(l_{bi})$, according to the observations that if $r < 1.10$, the dislocation core can be classified as a non-compact core. Supplementary Figure 1 shows two more examples of non-compact cores. However, among all the dislocation cores examined, compact cores are the most dominant, with the fraction of non-compact cores being around ~1%.

Supplementary Figure 2 | Histograms of system energies with dislocation dipole at different levels of SRO in MoNbTaW. Histograms of system energies with dislocation cores placed in different sites in samples with three different states of SRO, each fit with Gaussian distributions. The energy distribution is essentially equivalent to the core energy distribution with a constant reference energy difference. The green dash-dot line represents the nearly random solid solution state $s1$ with minimum SRO. The blue dash line represents the state $s2$ with a medium level of SRO. The red solid line represents the state $s3$ with the highest level of SRO.
Supplementary Figure 3 | Distribution of pressure and shear stresses on the simulation cells. a, Histograms of residual stress in the simulation cells with dislocation cores in different sites in the samples with three different states of SRO, each fit with a Gaussian distribution. a, Histogram of the pressure (from the trace of the stress tensor), b-d, Histograms of residual shear stress. The green dash-dot line represents the nearly random solid solution state s1 with minimum SRO. The blue dash line represents the state s2 with a medium level of SRO. The red solid line represents the state s3 with the highest level of SRO. The standard deviation of the residual pressure shows small changes in magnitude going from s1 to s3. The magnitude of the residual shear stresses is much smaller than the residual pressure; the standard deviations do not show monotonic relationships with the degree of SRO. If we assume the bulk modulus $K \approx 175$ GPa, the strain energy due to the current external pressure on the supercell is in the order of $0.05 \text{ eV}$; similarly, if we assume the shear modulus has a value of $100$ GPa then the contribution of shear stress to the strain energy has a value on the order of $0.01 \text{ eV}$. These values are much smaller than the variations in core energies obtained in the calculations, which further verifies that the variance in core energies is not induced by the stress fluctuations in the supercells.
Supplementary Figure 4 | 2D contours of the Peierls valleys and the differences in the Peierls valley energy at three levels of SRO in the MoNbTaW supercells (no energy barrier data included). Shown are 2D projection of contours from Fig. 4. a, random solid solution state $s_1$ with minimum SRO. b, state $s_2$ with a medium level of SRO. c, state $s_3$ with the highest level of SRO. Grid-$x$ and grid-$y$ represent the relative position of the dislocation dipole as shown by the black dots on the right column figures. The contours were plotted by interpolating data points on grids through bivariate spline.
Supplementary Figure 5 | Histograms of the differences in Peierls valley energy shown in Fig. 4 at different levels of SRO in MoNbTaW. Fits with Gaussian distributions are superimposed. The green dash-dot line represents the nearly random solid solution state $s1$ with minimum SRO. The blue dash line represents the state $s2$ with a medium level of SRO. The red solid line represents the state $s3$ with the highest level of SRO.
Supplementary Figure 6 | Initial and final configurations of the dislocation dipole for barrier calculations. 

a, Initial configuration. b, Final configuration. Both configurations are plotted using differential displacement maps, and the compact dislocation core position is represented by the red arrows. For each relaxed sample selected as the initial configuration, as shown in a, we chose the sample with a nearest dislocation dipole on the same {110} plane and in the [112] direction as the final configuration.
Supplementary Note 2: Calculation of diffuse antiphase boundary energies

**Supplementary Figure 7 | Calculation of diffuse antiphase boundary (DAPB) energy.** a, Initial configuration without the dislocation dipole, the blue dashed lines represent two diffuse antiphase boundaries. b, Side view of the original supercell. c, Side view of the supercell with DAPBs. Six layers of atoms were shifted along [111] direction by 1 Burgers vector to create two APBs.

In the dislocation dipole model, there is a cut plane between two dislocation cores, which will induce extra energy when SRO is present in the sample. The energy associated with the cut plane between dislocation core varies depends on the levels of chemical ordering and can be quantified through the diffuse antiphase boundary (DAPB) energy. Here, we calculate the DAPB energy in our system for the s1-s3 states and based on the calculated DAPB energy, we quantify the contribution of the cut plane to the energy of the dislocation dipole supercell. **Supplementary Figure 7** illustrated how the DAPB energies were computed. **Supplementary Fig. 7a** shows the supercell without dislocation dipole, in which six layers of atoms in the supercell are shifted by
one Burgers vector in the [111] direction, as shown in Supplementary Figs. 7b-c; accordingly, two DAPBs indicated by the blue dashed lines are created. The DAPBs are also shifted in the [1̅1̅0] direction, which leads to 11 different configurations for each SRO states. All the configurations with DAPBs are then relaxed in the same way as described in the Method section and the average DAPB energies are calculated; values are shown in Supplementary Table 1. For the state $s1$ close to the random solid solution sample, $\gamma_{DAPB}$ is around $3 \text{ mJ/m}^2$, i.e., essentially zero within the precision of the statistical sampling. With increasing SRO, the diffuse antiphase boundary energies increase; specifically, $\gamma_{DAPB}$ increases to $29 \text{ mJ/m}^2$ in $s2$ and $59 \text{ mJ/m}^2$ in $s3$.

**Supplementary Table 1 | Diffuse antiphase boundary energy.** Averaged DAPB energy for different SRO states.

| SRO state | DAPB energy $\gamma_{DAPB}$ ($\text{ mJ/m}^2$) | Standard error $\sigma_{\gamma_{DAPB}} / \sqrt{\# \text{ of samples}}$ ($\text{ mJ/m}^2$) |
|-----------|-----------------------------------|-----------------------------------------------|
| $s1$      | 3                                 | 2.2                                           |
| $s2$      | 29                                | 2.8                                           |
| $s3$      | 59                                | 2.7                                           |

**Supplementary Figure 8 | Schematic of two neighboring dislocation dipoles.** Triangles represent the dislocation cores in the dipole; the black lines represent the cut planes (DAPBs).
The distance between the two cores within the dislocation dipole supercell is around $l_c = 2\, nm$ and the thickness of the sample is 2 Burgers vectors; thus, the total energy induced by the cut plane can be estimated as $E_{cut} = 2blc\gamma_{DAPB} \approx 0.4\, eV$ ($0.1\, eV/b$ if normalized by total Burgers vector) for $s3$, which only constitutes 2% of the excess energy due to the dipole (Fig. 3).

When we consider the energy difference between two neighboring dipoles, the contribution of the cut plane is expected to be much smaller since the total area of the cut plane is preserved. Specifically, assume there are two neighboring dipoles as shown in Supplementary Figure 8. $c1 = c2 = 0.2nm$ is the distance between two neighboring dipoles. Considering the effect of cut during the glide of a dipole, the majority of the cut remains the same and only two small segments need to be analyzed. The energy difference between the two configurations ($\Delta E$), shown in Supplementary Figure 8, contains two parts: the energy difference between dislocation cores ($E_{cores1} - E_{cores2}$) plus the energy difference between two segments of cuts $c1$ and $c2$ ($E_{c1} - E_{c2}$):

$$\Delta E = E_{cores1} - E_{cores2} + E_{c1} - E_{c2}.$$ 

Considering the $s3$ state, for the effect of cut plane:

$$E_{c1} - E_{c2} \leq |E_{c1} - E_{c2}| \leq |E_{c1}| + |E_{c2}| \approx \gamma_{DAPB}(l_{c1} + l_{c2})2b \approx 0.08\, eV.$$ 

However, as we shown in the Figure 4, $|\Delta E|$ can be very large at some positions ($2\sim2.5\, eV/b$ if normalized by total Burgers vector or 8~10 $eV$ for the supercell), and in this case the contribution for the change in position of the cut plane is only on the order of 1% to the $|\Delta E|$. Thus, the energy of the dislocation cores is much higher than that of the segments of cuts: $E_{cores1} - E_{cores2} \gg E_{c1} - E_{c2}$. The same conclusion also holds for the $s1$ and $s2$ states. The effect of SRO on the dislocation core energies is thus much more significant compared to that associated with the DAPB energies on the cut plane between the cores. The high variance of the
dipole energy, shown in Figure 3, is then due to the effect of the local atomic environment of the dislocation core structure.

**Supplementary Note 3: Analysis of Type-2 barrier for a single screw dislocation**

Assuming that the dislocation dipole energy follows a normal distribution: $\text{Normal}(\mu,\sigma^2)$, as shown in Figure 7a, we consider two dislocations in one dipole, termed $c1$ and $c2$, with their core energies are written as $E_{c1}$ and $E_{c2}$:

$$E_{c1} + E_{c2} \sim \text{Normal}(\mu,\sigma^2).$$

If these two dislocations are independent and their energy also follows the same normal distribution, we can state that:

$$E_{c1} \sim \text{Normal}(\mu/2,\sigma^2/2), E_{c2} \sim \text{Normal}(\mu/2,\sigma^2/2).$$

Thus, a single dislocation follows the normal distribution: $\text{Normal}(\mu/2,\sigma^2/2)$.

Now if we consider two independent neighboring dislocations $w1$ and $w2$, their core energies can be written as $E_{w1}$ and $E_{w2}$:

$$E_{w1} \sim \text{Normal}(\mu/2,\sigma^2/2), E_{w2} \sim \text{Normal}(\mu/2,\sigma^2/2),$$

and

$$E_{w1} - E_{w2} \sim \text{Normal}(0,\sigma^2).$$

The criterion for a type-2 barrier is written as: $E_{w1} - E_{w2} > e_{\text{critical}}$, then we can write the probability of a Type-2 barrier as:

$$P_{\text{type2}} = P(E_{w1} - E_{w2} > e_{\text{critical}}) = 1 - P(E_{w1} - E_{w2} \leq e_{\text{critical}}) = 1 - \Phi\left(\frac{e_{\text{critical}}}{\sigma}\right),$$

where $\Phi$ is the standard Normal cumulative distribution function.