Neural network for predicting Peierls barrier spectrum and its influence on dislocation motion

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\textbf{ABSTRACT}

The Peierls barrier represents the inherent lattice resistance to dislocation glide, controlling dislocation movement and dictating the resulting mechanical properties. The rise of multi-principal element alloys, with their vast compositional space and local chemical fluctuations, introduces notable challenges in efficiently computing the Peierls barriers. Here, we propose a neural network model that captures the chemistry and structure of screw dislocations. By incorporating two crucial inputs, the local atomic type and displacement, our model enables accurate and efficient prediction of the Peierls barriers in multi-component space. Using this neural network, we construct a barrier diagram across the entire ternary space of refractory Nb-Mo-Ta alloys, from which the compositions with high or low barriers can be quickly identified. We discover that the NbMo binary alloy can have a higher barrier than NbMoTa ternary system, suggesting chemical complexity may not be the predominant factor governing dislocation barrier. Subsequently, three screened compositions with different barriers are selected for studying their effects on dislocation motion. Atomistic simulations reveal that a higher mean barrier slows down dislocation mobility, while a broader distribution of barriers facilitates kink pair nucleation, altering the rate-limiting process from kink pair nucleation to kink glide and cross kinking. This study presents a general neural network model that enables rapid screening composition with the desired barrier spectrum and will impact the exploration and discovery of alloys with improved dislocation-controlled properties.

\textbf{1. Introduction}

Dislocations, line defects in crystalline materials, play a critical role in determining mechanical properties and deformation behaviors of many engineering materials [1]. For a dislocation to glide, it must overcome an energy barrier with mechanical stress, thermal activation, or a combination of both [2]. This energy barrier, known as the Peierls barrier, expresses the intrinsic lattice resistance, and is dictated by the dislocation core structure [3-5]. For pure metals, the Peierls barrier is constant and has a single value [6,7], which can be precisely computed using transition state calculations, such as the nudged elastic band method [8–10]. By contrast, multi-principal element alloys (MPEAs) are characterized by atomic-scale composition fluctuation that gives rise to a varying local chemical environment [11–13]. This results in a wide distribution of energy barriers and a hierarchical energy landscape through which dislocations must navigate [14,15]. Another complexity in studying MPEAs is their extensive compositional space. For instance, even within a single ternary system, varying the constituent element concentration by 1% could lead to a total of ~5000 distinct alloy compositions [16]. Yet only a limited number of compositions, mainly at or near the equimolar region, have been studied [17]. Given the vital role of dislocation on mechanical properties, it is of great interest to develop a methodology capable of accurately and efficiently predicting dislocation barriers across a broad compositional spectrum. However, linking the Peierls barrier to such a vast compositional space poses a grand challenge, as traditional energy barrier calculation methods are computationally expensive.

The emergence of machine learning methods has demonstrated great promise in tackling computationally complex problems in the field of material science [18–22]. For example, machine learning-derived interatomic potentials have been developed to capture complex atomic interactions in MPEAs, striking a balance between accuracy and computational efficiency [23–26]. Machine learning models have also been employed successfully in predicting activation barriers for vacancy migration [21,27]. However, the use of machine learning for the study
of dislocations and their associated energy barriers in MPEAs is currently unexplored. The main challenge lies in devising a descriptor that can effectively represent the local chemical and structural characteristics of this line defect (dislocation). Successful descriptors [28], such as atom-centered symmetry function [29] and crystal graph [30], have been developed for describing the atomic environments. However, as the number of alloying elements increases, the dimension of the descriptor can significantly grow. This escalation necessitates a more complex machine learning model and an expanded training data set.

In this study, we introduce a neural network model along with a novel representation of local chemistry and structure of screw dislocations, enabling precise and efficient prediction of Peierls barriers in ternary Nb-Mo-Ta system. The neural network simultaneously incorporates two essential features (descriptors), the local atomic type and the atomic displacement, which embody the chemical and structural characteristics of the dislocation. The model, trained on dozens of compositions, shows remarkable predictability and expandability for new (previously unseen) compositions, allowing accurate mapping of the entire ternary space. We construct a Peierls barrier diagram spanning the entire compositional space, facilitating the rapid identification of alloys with high and low barriers. We then study the effects of these barriers on dislocation mobility and motion mechanisms, which advances our understanding of the interplay between chemical complexity and dislocation motion.

2. Dislocation representation and neural network model

2.1. Structure and chemistry representation of a screw dislocation

In a crystal containing a dislocation, atoms shift from their optimal lattice sites, resulting in a distortion (displacement) in the crystalline matrix. Specifically, with screw dislocations, atoms undergo a displacement \( u \) along the dislocation line. This displacement uniformly reaches the value of \( b \) (Burgers vector) as the angle \( \theta \) increases from 0 to \( 2\pi \) around the dislocation line, as \( u = \frac{b}{2\pi} \). As shown in Fig. 1c, the atomic structure, colored by atomic displacement magnitude, illustrates this displacement field, increasing linearly from \(-0.5b\) to \(0.5b\) as the angle progresses from \(-\pi\) to \(\pi\). In a body-centered cubic (bcc) structure, the screw dislocation aligns with the \(\langle 111 \rangle\) direction, with the Burgers vector given by \( b = \frac{a}{2}(111) \), where \( a \) denotes the lattice constant. When circumnavigating a circle containing this dislocation core, a total displacement of \( b \) always accumulates. This displacement description, on top of the initial crystalline (perfect) structure, captures the fundamental structural characteristics of an embryonic dislocation. Regarding MPEAs, the second essential feature is the chemical environment surrounding a dislocation, which can possess a large chemical fluctuation. Fig. 1a depicts the local chemical environment of a screw dislocation in an equimolar NaMoTa alloy. To comprehensively represent the dislocation and link it to its properties, the associated structural and chemical attributes must be described and digitized for interpretation by the machine learning model.

We convert the atomic type and discrete atomic displacement into digital matrices using the on-lattice representation [27,31]. The conversion is performed via two steps: dividing the crystal into grid voxels with each atom located in the voxel center, and encoding the voxel by its corresponding atomic information (i.e., atom type, displacement magnitude). To ensure the minimum size of the resulting matrix (smallest feature dimension), the largest possible voxel sizes are utilized along each direction (i.e., \( a/\sqrt{6} \) along \( x = [11\overline{2}] \), \( a/\sqrt{2} \) along \( y = [1\overline{1}0] \), and \( a\sqrt{3}/6 \) along \( z = [11\overline{1}] \), for bcc structure). Fig. 1b shows the
chemical representation, where voxels are coded based on their encompassed atom type. The numbers 1, 2, and 3 denote the atom types Nb, Mo, and Ta for NbMoTa alloys, respectively, while 0 signifies an unoccupied volume resulting from the packing sequence inherent in the crystal structure. Correspondingly, the atomic displacement is encoded into a numerical matrix, in which each number is the precise atomic displacement due to the presence of dislocation (Fig. 1d). The two numerical matrices (voxel maps), signifying the atom type and displacement fields, encapsulate the chemical and structural characteristics of the dislocation. It is worth noting that this descriptor calculation is both simple and direct, requiring no additional calculations. These features are then fed into a neural network as inputs for dislocation properties prediction.

### 2.2. Peierls barrier data generation

We use the refractory Nb-Mo-Ta as a model system to demonstrate the effectiveness of the neural network model in predicting Peierls barriers. To generate the dataset required for training the machine learning model, we employ the Climbing Image Nudged Elastic Band (CI-NEB) method [9], which enables accurate computation of the Peierls barriers. We insert a short screw dislocation of 2\(b\) length into the crystal system by imposing a displacement field to atoms according to the elastic solution of a screw dislocation, followed by system relaxation through energy minimization. The resulting atomic configuration after relaxation serves as the initial state for the CI-NEB calculation. To obtain the final state, we insert a screw dislocation at the neighboring Peierls valley, followed by relaxation. This distance between the initial and final states is given by the lattice periodicity along the glide direction (i.e., \(x = [112]\)). In CI-NEB calculation, we use the inter-replica spring constant to \(k = 0.01\) eV/Å\(^2\) and the force tolerance to 0.001 eV/Å. The choice of this value that optimizes convergence of the calculations results in essentially the same energy barrier using a smaller tolerance and a large spring constant. For the model size, we gradually decrease the model dimension along the glide direction (\(x\) axis) from 40 unit cells down to 8, and the resulting barrier remains within the resolution of 0.0001 eV/\(b\). The detailed Peierls barrier calculation and model setup can be found in our previous study [14].

For each alloy composition, we first introduce a screw dislocation and then randomize the types of lattice atoms according to the alloy composition. In this way, we generate 12,000 dislocations with varied surrounding chemical environments and fluctuations. After moving the dislocation to its next Peierls valley to establish the final state, we calculate the saddle point and energy barrier between the initial and adjacent Peierls valleys.

### 2.3. Determining cutoff distance and number of neighboring atoms

The Peierls barrier of dislocation in MPEAs is intimately governed by the atomic chemistry that surrounds it. As the distance from the

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**Fig. 2.** The effect of cutoff distance and number of neighboring atoms on Peierls barrier. (a) Atom concentration variation as a function of distance away from a screw dislocation. Inserted figures depict atomic configurations corresponding to different cutoff distances. (b) The total number of neighboring atoms around dislocation line with a length of 2\(b\). (c) The MAE of neural network prediction with respect to cutoff distance, suggesting that atoms located beyond a 9.6 Å distance exert a negligible influence on the dislocation barrier.
dislocation core increases, the influence of atoms presumably decays. This decay is particularly noteworthy, because when concerning a large number of neighboring atoms at an extended cutoff distance, it necessitates an increase in the neural network model size and training datasets. Therefore, it is of great importance to identify the optimal cutoff distance, which offers the best balance between prediction accuracy and model complexity.

Fig. 2a shows the variation in atomic density as a function of distance from a screw dislocation. We denote five characteristic distances away from the dislocation line core, highlighted by the dashed lines in Fig. 2a. The corresponding atomic configurations are shown in the insert, with atoms colored by the distance. For example, configuration (i), corresponding to a cutoff at the third nearest neighbor, contains 12 atomic sites. For a dislocation with a length of 2b, the total number of atomic sites as a function of cutoff distance is shown in Fig. 2b. Configuration (iii) encompasses atoms up to the tenth nearest neighbors, for a total of 96 atoms.

By taking the five different cutoff distances from Fig. 2b and converting the atomic configurations to digit maps (illustrated in Fig. 1), we train five separate neural network models for barrier prediction. Fig. 2c shows their testing performances, with the mean absolute error (MAE) between predicted and true values presented. As the cutoff distance increases, the MAE rapidly decreases, reaching a plateau near a cutoff distance of 9.6 Å (corresponding to configuration (iii)). This suggests that any further increase in the cutoff distance would contribute negligibly to the neural network model prediction, implying that the barrier is predominately influenced by the atoms within the tenth nearest neighboring shell. Configuration (iii) will hence be used for the neural network model prediction.

2.4. Neural network architecture

The neural network takes the chemistry and displacement fields of the dislocation as input parameters, and attempts to emulate atomic interactions through its hidden layers, with the goal of predicting the energy barrier. To study the effect of neural network architecture (dimension) on barrier prediction performance, we train a series of neural networks with different numbers of hidden layers (from 1 to 4) and neurons (from 32 to 256). Fig. 3a shows a direct comparison between the actual barriers and those predicted by each neural network model, providing a clear evaluation of performance. In Fig. 3b, we show the accuracy of each model by plotting its corresponding MAE.

As the number of layers increases from 1 to 4, there is a significant drop in MAE, leading to a saturation point. A similar trend can be seen when the number of neurons is increased from 32 to 256. This convergence with 256 neurons is meaningful, as the input data size (chemistry and displacement) has a dimension of 192 (excluding the zero values), enabling the neurons to explicitly process the individual atomic information specifically. The ultimate model, with 4 layers and 256 neurons in each layer, achieves a high prediction accuracy, with an MAE of 0.0137 eV. While it is expected that further increasing the hidden layers and neurons could enhance accuracy, the complexity of the model would necessitate larger training datasets and extended training times. Additionally, an overly complex model might risk overfitting, potentially making it too specialized for the training data.

2.5. Number of compositions required for harnessing the ternary space

Accurate prediction of machine learning models in unseen space often hinges on the choice of diverse and representative training datasets. To explore the minimum number of compositions necessary to harness the entire ternary Nb-Mo-Ta system, we train neural networks using different composition subsets. Fig. 4a shows the 44 compositions, uniformly spread across the ternary compositional diagram. For each composition, we compute 12,000 Peierls barriers using CI-NEB calculations. From these datasets, we select subsets containing 3, 5, 10, 25, 33, 39, and 44 compositions, to train the neural network model. Fig. 4b shows the MAE for the new compositions (i.e., blue dots in Fig. 4a), plotted against the number of compositions used in training. It can be seen that the prediction error decreases significantly as the number of compositions expands from 3 to 25, after which the increase in accuracy starts to converge, and the MAE reaches a prediction error of 0.012 eV. These results demonstrate that the neural network, cultivated on dozens of compositions, effectively captures the ternary space and establishes the relationship between composition and dislocation barrier.

3. Peierls barriers in the entire composition space

3.1. Peierls barriers for dilute and concentrated solutions

We calculate the Peierls barriers in dilute and concentrated solid solutions, illustrating the prediction ability of the neural network in new compositions. Using the optimized network (4 hidden layers and 256 neurons), we evaluate the testing performance on nine previously
unseen alloy compositions (not included in the training). These alloys span both the concentrated and dilute regions in the composition diagram. Fig. 5 presents their barrier distributions from prediction and direct CI-NEB calculation. For all the alloys, the predicted and true barriers exhibit essentially the same distributions, with the tiny error on the mean barrier falling within 0.0008 eV. As to the MAE, it varies from 0.007 eV (dilute alloy Nb$_2$Mo$_3$Ta$_9$) to 0.0158 eV (concentrated alloy Nb$_{27.5}$Mo$_{45}$Ta$_{27.5}$). These results demonstrate that our model, trained using sparse composition data, possesses the capability to capture the full compositional space of the ternary system, highlighting the generalization ability the neural network in learning multi-composition space.

The revealed barrier spectrum provides direct insight into the roughness of the dislocation glide energy landscape. In the case of dilute alloys, as shown in Fig. 5a, there is a narrow barrier distribution associated with a sharp peak. This indicates that introducing small amounts of solute elements to a primary element marginally alters the energy...
barrier, giving rise to a slightly distorted energy landscape. In contrast, the distribution of dislocation barriers in concentrated alloys is markedly wider. The broad spread of barriers and the significant variance in their values suggest that the dislocation glide energy landscape in concentrated solid solutions undergoes substantial modifications. This leads to more complex and highly rugged structures, exhibiting characteristics like hierarchical features [14].

3.2. The impact of chemical short-range order on Peierls barriers

In concentrated alloys, chemical short-range order (SRO), a salient feature pertaining to this class of materials, emerges from enthalpic interactions among the constituent elements. To test the capability of our trained model, we examine its performance on alloys with various degrees of SRO. Utilizing a Monte Carlo (MC) swap method coupled with MD simulation [32], we prepare SRO in an equimolar NbMoTa alloy. By manipulating the swap steps, we create two distinct levels of SRO, in addition to a random solid solution, as shown in Fig. 6a.

For each level of SRO, we prepare 10,000 dislocations, and then their barriers are predicted by the neural network and calculated using the CI-MD simulation [32]. We observe that the prediction error slightly increases as the degree of SRO grows, as shown in Fig. 6b,c. This increase in prediction error may be due to the enhanced elastic interactions in a chemically ordered environment, which suggests a larger cutoff distance for better performance.

As the SRO increases, the Peierls barrier shifts to a higher value (Fig. 6b,c). This SRO-enhanced barrier arises from the generation of a diffuse anti-phase boundary (APB) [25,33,34] associated with dislocation glide. As the dislocation moves from one Peierls valley to the adjacent one, it disrupts the chemical order on the glided plane. This APB generation, resulting in an energy penalty, raises the dislocation barrier. The raised barrier could influence the critical stress [35] at which the barrier vanishes, and hence the system-level yielding stress [36].

3.3. Peierls barrier diagram

The precise and efficient prediction of dislocation barriers using neural network enables the study of Peierls barriers for the entire ternary space. Fig. 7a,b shows the Peierls barrier for the Nb-Mo-Ta system in random solid solutions, where both average value and standard deviation are shown. It is worth noting that the binary NbMoTa, exhibits the highest barrier in the whole compositional space. This implies that chemical complexity (configurational entropy) is not the predominant factor in influencing the dislocation glide resistance. The standard deviation of the barrier, shown in Fig. 7b, suggests that the concentrated alloys can possess a more rugged glide landscape compared to their dilute counterparts. Intriguingly, the region with the highest standard deviation is closer to a binary Ta-Mo alloy, rather than the equimolar central region. To elucidate the variation of energy barrier with solute concentration, we choose two representative alloys, the binary Nb,Mo and the ternary (NbMo)Ta, and further analyze them.

Fig. 8a shows how the Peierls barrier varies in response to varying Mo concentration, x, in Nb,Mo. With increasing Mo concentration from pure Nb, the barrier exhibits a nearly linear growth. However, starting from approximately 25 %, the trend bends and flattens out. The similar behavior can be seen at the other end of the diagram, when the Nb concentration is increased from pure Mo (i.e., from the right end of the curve towards the center); the trend changes in behavior at around ~33 % Nb. The variation of dislocation barrier with solute concentration suggests two distinct strengthening regimes associated with both dilute and concentrated alloys. The composition that results in the highest barrier does not occur exactly at the equimolar concentration, but rather at a slightly deviated ratio, specifically NbMo.

For the (NbMo)Ta system, the Peierls barrier as a function of NbMo concentration (x) is shown in Fig. 8a. With increasing NbMo from 0 % to 100 % (i.e., decreasing Ta from 100 % to 0 %), the variation of barrier shows two regimes, corresponding to the dilute system (with Ta >70 %) and the concentrated one. It is noted that, in the concentrated regime, the NbMo alloy (right end of the curve) exhibits the highest barrier, surpassing the equimolar ternary NbMoTa alloys. This observation again indicates that MPEAs with a larger number of constituent components do not necessarily exhibit a larger lattice distortion and higher energy barrier.

The Peierls barrier diagram, efficiently constructed here by the neural networks, reveals the relationship between alloy composition and the fundamental dislocation property in a wide compositional space. With the diagram, compositions with high or low barriers can be quickly screened for detailed study. In the following section, we will study the effects of the Peierls barrier spectrum on dislocation mobility and motion mechanisms.

4. Peierls barrier spectrum and dislocation motion

4.1. Mean barrier and dislocation mobility

To understand the impact of the Peierls barrier on dislocation mobility, we conduct molecular dynamics (MD) simulations in three representative compositions, including a dilute alloy of NbMo, the equimolar NbMoTa, and the binary NbMo. They have distinct

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Fig. 6. Peierls barrier spectra of NbMoTa alloy with varying degrees of chemical SRO. (a) The SRO parameters of RSS (orange curve) and two SRO (blue and green curves) systems. (b-c) The model prediction and Peierls barrier spectra for NbMoTa with low and high degrees of SRO, respectively. The number of atomic swaps involved in the hybrid MC-MD simulation to generate SRO is labeled.
average barriers, as shown in Fig. 9a. Among them, the Nb_{10}Mo_{10}Ta_{80} dilute alloy possesses the lowest mean barrier of 0.018 eV, while NbMo carries the highest barrier of 0.023 eV.

To obtain statistically meaningful results on dislocation motion and ensure the dislocation is exposed to varied chemical environments, we set up ten independent configurations for each composition. The model has a dimension of approximately 48 nm along $x = [112]$, 29.2 nm along $y = [110]$, and 0.56 nm along $z = [110]$, for a total of 46,848 atoms. A screw dislocation with 2b length is inserted into the system. To study dislocation motion, we apply a constant shear stress by exerting a constant force on both the upper and lower boundary layers. The dislocation location is tracked as a function of time, allowing extraction of its velocity from the linear slope of the displacement-time curve.

Fig. 9c shows the dislocation velocity across a range of applied stress, from 0.5 GPa up to 1.3 GPa, at a constant temperature of 300 K. At the same stress levels, Nb_{10}Mo_{10}Ta_{80}, which has the lowest Peierls barrier, shows the highest dislocation mobility. NbMo, having the highest barrier, manifests the most limited mobility, with the equimolar NbMoTa holding an intermediate position. The data reveal the average Peierls barrier significantly governs dislocation mobility at high stresses. This barrier-motion relationship demonstrates the potential of the neural network-predicted barrier diagram in rapidly screening alloys with specific dislocation mobilities and their controlling mechanical behaviors.

4.2. Barrier variation and dislocation glide mechanisms

The standard deviation of the barrier distribution (barrier fluctuation) reflects the ruggedness of the dislocation glide energy landscape. To understand its influence on dislocation motion mechanisms, we perform MD simulations of a long dislocation of 70b in pure Nb, its dilute alloy Nb_{59}Mo_{50}Ta_{5}, and its concentrated alloy NbMoTa. Note that pure Nb has a constant barrier, with a standard deviation $\sigma = 0$. The Nb_{59}Mo_{50}Ta_{5} has a $\sigma = 0.068$, and NbMoTa has a higher value $\sigma = 0.088$, representing the most rugged landscape among the three. For each composition, we constructed five independent configurations to obtain statistically meaningful results.

Analyzing dislocation motion, we examine its atomic structure and reveal six different structures, characterized as (i) a single kink pair, (ii) two kinks pairs located in one Peierls valley, (iii) two kinks across two adjacent valleys, (iv) multiple kink pairs across two adjacent valleys, (v) multiple kinks spanning three consecutive valleys, and (vi) multiple kinks covering four valleys (Fig. 10a). The frequency of these configurations indicates the relative importance of kink pair formation versus kink glide on mediating dislocation glide. For example, Nb shows the single kink pair is predominated (top panel of Fig. 10b), implying dislocation moves primarily due to a single kink pair event and the subsequent kink glide. For dilute alloy Nb_{59}Mo_{50}Ta_{5} (middle panel of Fig. 10b), dislocation structures manifest a decrease in the frequency of single kink pair configurations but an increase in kink pairs. This suggests that kink pair nucleation is promoted in the alloy. This trend in enhancing kink pairing events is more evident for NbMoTa concentrated solid solutions, in which local chemical fluctuation presumably facilitates the formation of kink pairs. The dislocation line experiences significant roughness under stress, with the dislocation line even occupying multiple Peierls valleys (structures v and vi in Fig. 10a).

It is worth noting the effect of Peierls barrier distribution (spectrum) on the dislocation motion mechanism is probed by MD simulations. Due to the timescale limitation inherent in MD method, a high-stress level of 0.7 GPa is used (the high stress could be relevant to high strain rate deformation under dynamic loading). When decreasing the applied stress, there are fewer kink pair nucleations, leading to dislocations that are less rugged and irregular. We speculate that the physical insight inferred from the simulation, i.e., a broader distribution of barriers facilitates kink pair nucleation, likely remains valid because of the low-barrier tail in the spectrum that promotes kink pair events.

Fig. 11a presents typical glide displacement-time curves for the three material systems. Dislocation motion exhibits a discontinuous and jerky pattern, characterized by the dislocation advancement in distance, followed by retardation. We analyze the dislocation structure and extract the mechanism responsible for the pinning. Fig. 11b shows the frequency of each individual mechanism, which hinders dislocation motion. In pure Nb (depicted by the orange column in Fig. 11b), we find all pinning (immobile) stages are associated with kink pair nucleation, emphasizing the dominant role of kink pair mechanism as the rate-limiting mechanisms in pure bcc metals. For the dilute alloy Nb_{59}Mo_{50}Ta_{5}, there is an increase in the frequency of kink glide and cross-kink events associated with the pinning, implying their role as the rate-limiting process. This behavior becomes more pronounced for NbMoTa, where kink glide and cross-kink mechanisms predominantly retard dislocation motion. For example, the prolonged stationary duration, surpassing 400 ps in Fig. 11a (the purple line), originates from the formation of one cross kink. This occurs when two kinks gliding laterally on two different slip planes collide, generating a cross kink and subsequently leading to dislocation self-pinning. The extended waiting time required for dislocations unpinning from cross-kink breaking underscores its strong self-pinning effect. The chemical fluctuation, especially in concentrated alloys, promotes kink pair nucleation and hence facilitates cross-kink formation. This can be understood from the
perspective of the Peierls barrier spectrum: an alloy with a broader distribution and large variation of Peierls barrier provides many potential locations along the dislocation line at which the barrier can be small or even vanish under mechanical stress, leading to a spontaneous kink pair event.

5. Discussion and conclusions

The chemical complexity of MPEAs introduces a vast and unexplored compositional space, rendering the traditional experimental tests and computational calculations impractical for exploring the entire space. The neural network model introduced in this study and trained on tens of compositions demonstrates an efficient and accurate approach to probing the entire compositional space and connecting it with the dislocation Peierls barrier. One notable feature of the model is the direct on-lattice representation of the chemistry and displacement fields of dislocations, which can be simply calculated from continuum theory. This avoids the need for dislocation relaxation for barrier prediction, because the local chemical environment, captured by the model, fully determines the dislocation barrier. This on-lattice feature representation used to transfer discrete atomic information to digital neurons (descriptor) has a small size, which simplifies the process of machine learning model training. By efficiently sampling the entire ternary space of the Nb-Mo-Ta system, the Peierls barrier diagram is constructed and studied. It is found that the barrier spectrum plays a vital role in determining dislocation mobility and its glide mechanisms. The uncovered connection underscores the potential of utilizing a predicted barrier diagram for screening alloys with desired dislocation behaviors. The efficient barrier prediction is expected to influence mesoscale simulations [15], including methods like kinetic Monte Carlo and phase field dislocation dynamics (PFDD) [37], enabling dislocation modeling over diffusive timescale and larger length scale.

In summary, our study introduces a neural network model that accurately predicts Peierls barriers for screw dislocations, and we
demonstrate its accuracy within the ternary Nb-Mo-Ta system. This model harnesses local atomic types and atomic displacement fields as input, captures the local chemical and structural features of dislocations, and efficiently predicts the corresponding barriers. Through efficient model prediction, a barrier diagram spanning the entire compositional space is built, which enables the identification of alloy compositions with particularly high and low energy barriers. The screened compositions with different barriers are selected for studying their effects on dislocation motion. Dislocation motion simulations indicate that a higher mean barrier leads to lower dislocation mobility, while a larger variation of barrier promotes kink pair nucleation and cross-kink formation, thereby altering the rate-limiting process of dislocation motion. This work, introducing a machine learning model for exploring the large compositional dimensions that MPEAs inherently hold, will facilitate the discovery of alloys with compositionally tunable dislocation behavior and its controlling mechanical properties.

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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representing dislocation.

**Data and Code availability**

All source codes of neural network model are publicly available at: https://github.com/UCICaoLab/Dislocation-neural-network.

All the raw data and supporting information can be obtained from Zenodo (https://doi.org/10.5281/zenodo.10463585).

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