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Sequential transmutation of prismatic dislocations during $\{11\bar{2}2\}$ twin-slip interaction in titanium

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ABSTRACT

Atomistic simulations are performed to investigate the interaction between prismatic dislocations and $\{11\bar{2}2\}$ twin boundary in hexagonal close-packed titanium. Very unusual and interesting dislocation transmutation is observed. When a $(10\bar{1}0)\frac{1}{3}[\bar{1}2\bar{1}0]$ dislocation interacts with the twin boundary, it is first transmuted into a $(01\bar{1}2)\frac{1}{3}[2\bar{1}\bar{1}0]$ dislocation in the twin. But the $(01\bar{1}2)$ is not a common slip plane and the transmuted dislocation is unstable which is then further transmuted into a prismatic dislocation $(01\bar{1}0)\frac{1}{3}[2\bar{1}\bar{1}0]$ in the twin with a lower line energy. This behavior, along with the transmutations of other prismatic dislocations, can be understood from the perspective of lattice correspondence in deformation twinning.

Interaction between lattice dislocations and twin boundaries is crucial in the mechanical properties of structural metals and alloys [1,2], in terms of strength, ductility, strain hardening, and fatigue, etc. In plastic deformation of low-symmetry hexagonal close-packed (HCP) metals (e.g., α-Ti, Zr, Mg), dislocation slip and deformation twinning can simultaneously be activated; thus, profuse twin-slip interaction can be expected [3]. Extensive experiments and simulations have been performed to understand the interaction mechanisms [4–8]. Generally, the parent dislocation can be absorbed, dissociated at TB, or transmuted into a different dislocation in the twin. It has been realized that dislocation transmutation during twin-slip interaction should follow the principle of lattice correspondence, aka lattice transformation [9,10], which requires that the slip plane and the Burgers vector of a parent slip system should be transformed into the corresponding plane and vector in the twin. For example, a basal (or prismatic) dislocation of parent can be transmuted into a prismatic (or basal) dislocation of a $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twin, but this happens only when the Burgers vector of parent dislocation is parallel to the zone axis of the parent and twin [11]. Such inter-transmutation can be understood from the fact that the prismatic $(10\bar{1}0)$ and the basal (0002) planes are exactly the corresponding planes of the $\{10\bar{1}2\}$ twinning mode. In contrast, a basal or prismatic dislocation may be absorbed by a $\{10\bar{1}2\}$ TB when their Burgers vectors are non-parallel to the zone axis [11]. Zhou et al. [12] showed that a basal dislocation generated by dissociation of a pyramidal $\langle c+a\rangle$ dislocation can be removed by the migration of a $\{10\bar{1}2\}$ twin boundary (TB). Chen et al. [13] showed that a prismatic $(1\bar{1}00)\frac{1}{3}[\bar{1}\bar{1}20]$ dislocation could be transformed into a $(2\bar{1}\bar{1}1)[\bar{2}116]$ twin inside the primary $\{10\bar{1}1\}$ twin when the prismatic dislocation was interacting with the $\{10\bar{1}1\}$ TB. This interesting transmutation occurs because the prismatic plane and the $(11\bar{2}1)$ plane are exactly the corresponding planes of the $\{10\bar{1}1\}$ twinning mode. Thus, although dislocation transmutation during twin-slip interaction generally follows the principle of lattice correspondence, what actually happens at the TB also depends on the nature of the twinning mode and the structure of the TB.

Prismatic slip is the most favorable slip system during plastic deformation of HCP Ti and Zr at ambient temperature and pressure. On the other hand, $\{11\bar{2}2\}\langle 11\bar{2}\bar{3}\rangle$ twinning is the most common twinning mode when the crystals are compressed along the *c*-axis [14–18]. Therefore, it can be expected that profuse interaction between prismatic dislocations and $\{11\bar{2}2\}$ TBs can be activated during deformation and affects mechanical behavior significantly. Gong et al. [19] investigated how a type $\langle a\rangle$ prismatic dislocation interacted with a $\{11\bar{2}2\}$ twin. Their results showed that the prismatic dislocation in the parent was

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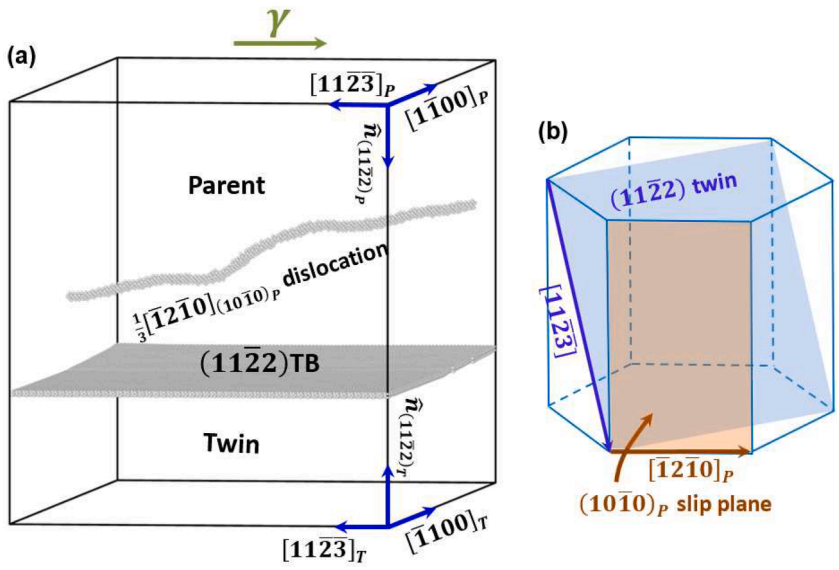

Fig. 1. (a) The initial configuration for simulating the interaction between a prismatic dislocation and a $(11\bar{2}2)$ TB in HCP titanium. Atoms in the perfect hcp lattice are hidden. (b) Schematic illustration of the orientation relationship between the prismatic slip and the TB.

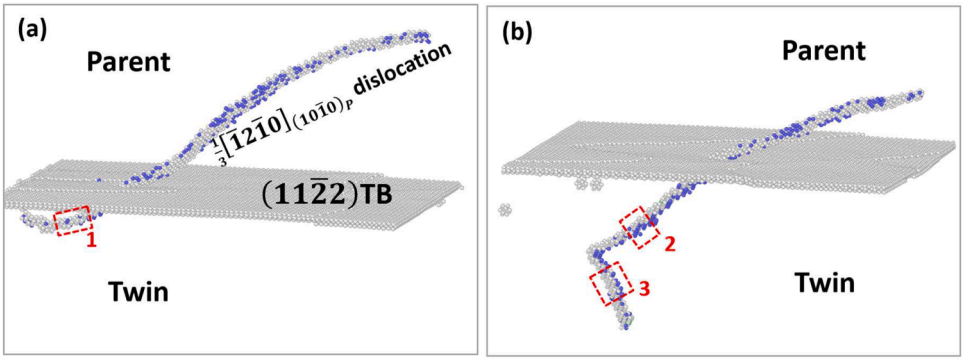

Fig. 2. (a) When the parent prismatic dislocation impinges on the $(11\bar{2}2)$ TB, it is transmuted into a dislocation in the twin. (b) As the interaction continues, the transmuted dislocation is further transmuted to a different dislocation in the twin. The boxed regions are further analyzed in Fig. 3 to determine the slip plane and Burgers vector of the selected dislocation segments.

transformed to a prismatic dislocation in the twin. There are a total of three different Burgers vectors for prismatic dislocations, thus, different modes of twin-slip interaction and transformation may occur. It is necessary to conduct a comprehensive study on all the interaction mechanisms and resolve the physics behind them.

The purpose of this work is to investigate how prismatic dislocations interact with a $\{11\bar{2}2\}\langle11\bar{2}\bar{3}\rangle$ TB by molecular dynamic (MD) simulations. All three prismatic slip systems are considered, i.e., $(\bar{1}100)\frac{1}{3}[11\bar{2}0]$, $(10\bar{1}0)\frac{1}{3}[\bar{1}2\bar{1}0]$ and $(0\bar{1}10)\frac{1}{3}[\bar{2}110]$. Very unusual and interesting interaction behavior is obtained. All the simulation results are well interpreted from the perspective of lattice correspondence in the $\{11\bar{2}2\}$ twinning mode.

In this work, MD simulations are conducted by using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [20]. The embedded atom method (EAM) for Ti-Al binary system developed by Zope and Mishin [21] is applied, which has been used extensively to investigate the deformation mechanisms and defect structures, e.g. twinning, dislocations and twin-slip interaction [19,22–24]. The software OVITO is used for visualization of the simulation results [25]. Common neighbor analysis (CNA) [26] and dislocation dynamic analysis (DXA) [27] are used to analyze interface and dislocation evolutions.

Fig. 1a shows the initial configuration for simulating the interaction between a prismatic dislocation and a $(11\bar{2}2)$ TB. The viewing direction is along the $[1\bar{1}00]_P$, i.e., the normal to the plane of shear, and the coordinate systems of the parent and twin are defined by the blue arrows. The simulation model has a dimension of $40 \times 60 \times 70$ nm^3, containing ~8.0 million atoms. To set up this simulation system, a bicrystal is first constructed to satisfy the perfect $\{11\bar{2}2\}\langle11\bar{2}\bar{3}\rangle$ twin relationship. Then, a prismatic edge dislocation on the $(10\bar{1}0)$ plane with a Burgers vector of $\frac{1}{3}[\bar{1}2\bar{1}0]$ is pre-planted in the parent lattice (Fig. S1 in Supplemental Materials). The orientation relationship between the twin and prismatic dislocation is illustrated in Fig. 1b. Free surfaces are applied to all three dimensions. The conjugate gradient algorithm is used to perform energy minimization followed by dynamic relaxation using the Nosé-Hoover thermostat. A simple shear strain is applied by moving the top surface along the direction of twinning shear to cause the TB to migrate and then interact with the dislocation. The stain rate is $\sim10^{10}$ /*s* and the timestep is 1.0 *fs*.

Fig. 2 is a 3D view showing how the $\{11\bar{2}2\}$ TB interacts with the $(10\bar{1}0)\frac{1}{3}[\bar{1}2\bar{1}0]$ prismatic dislocation. For better visualization, the atoms in the perfect hcp lattice are hidden, and only the dislocation and the TB are shown. In Fig. 2a, both the TB and the dislocation move under the applied shear strain. As the prismatic dislocation impinges on the TB, a portion of the dislocation is transmuted into the twin lattice. In Fig. 2b, the parent prismatic dislocation continues to transmute into the twin

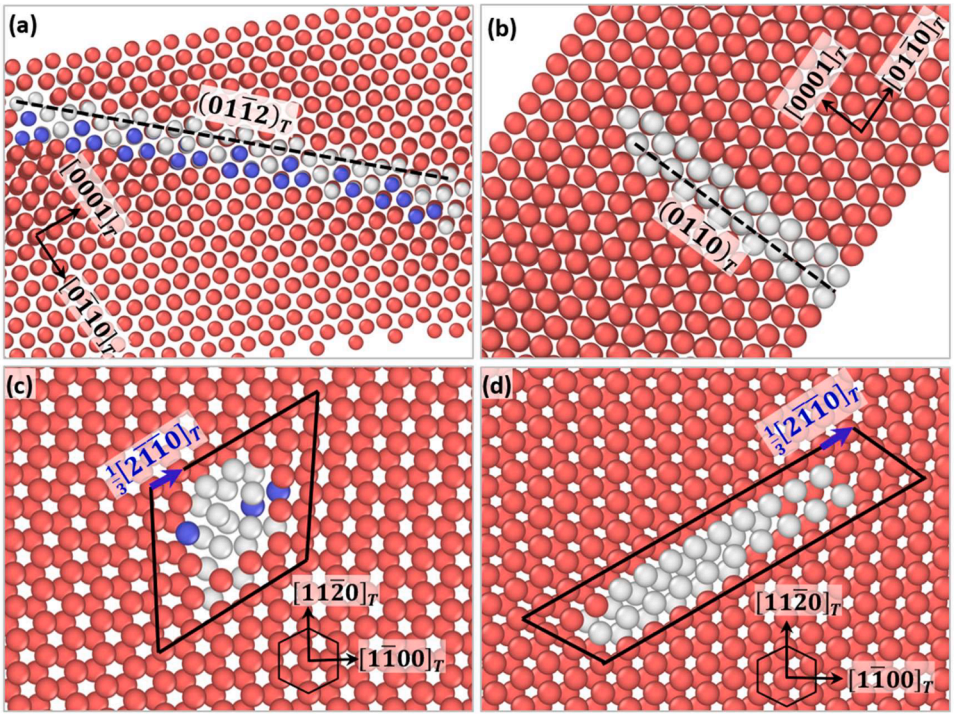

Fig. 3. (a) Edge-on view of the selected dislocation (box 2 in Fig. 2) showing that the parent prismatic dislocation is transmuted to a dislocation that lies on the $(01\bar{1}2)_T$ plane in the twin. (b) Edge-on view of the selected dislocation (box 3 in Fig. 2) showing that the slip plane is the $(01\bar{1}0)_T$. (c) The Burgers vector of the intermediate dislocation in (a) is determined as $\frac{1}{3}[2\bar{1}\bar{1}0]_T$. (d) The Burgers vector of the $(01\bar{1}0)_T$ prismatic dislocation in (b) is also $\frac{1}{3}[2\bar{1}\bar{1}0]_T$, indicating that the Burgers vector remains unchanged.

during twin-slip interaction. Very interestingly, as the transmutation continues, a portion of the transmuted dislocation line appears to have changed its characteristics. It can be seen that the transmuted dislocation becomes kinked. The evolution of the characteristics of the transmuted dislocation in terms of slip plane, Burgers vector and elastic energy is analyzed by taking out three segments of the transmuted dislocation as indicated by the three red boxes 1, 2 and 3.

First, we carefully examine the slip plane and the Burgers vector of the dislocation segments in box 2 and 3 and the results are shown in Fig. 3a–d. To determine the slip plane of the selected dislocation line segment in box 2, we tilt the slip plane such that it is right at edge-on view. To our surprise, the slip plane is identified as the $(01\bar{1}2)_T$ of the twin. However, it is well known that the $(01\bar{1}2)_T$ is not a slip plane in common hcp metals. To confirm this result, we further analyze the transmuted dislocation in box 1 of Fig. 2a. Again, the slip plane is indeed $(01\bar{1}2)_T$ (Fig. S2). Fig. 3b is the edge-on view of the dislocation in box 3, which clearly shows that the slip plane resides on the $(01\bar{1}0)_T$ now. Next, we analyze the Burgers vector of the transmuted dislocations and the results are shown in Fig. 3c-d. It can be seen that both Burgers vectors are $\frac{1}{3}[2\bar{1}\bar{1}0]_T$ and have zero $\langle c\rangle$ component. This indicates that the Burgers vector remains unchanged while the slip plane has changed from the $(01\bar{1}2)_T$ to the $(01\bar{1}0)_T$. This analysis indicates that, during twin-slip interaction, the parent $(10\bar{1}0)\frac{1}{3}[\bar{1}2\bar{1}0]$ prismatic dislocation is first transmuted to a dislocation with the slip plane of $(01\bar{1}2)_T$ in the twin, and then further transmuted to the $(01\bar{1}0)_T$ plane in the twin, which is a common slip plane. The whole twin-slip interaction process can be described as:

$$(10\bar{1}0)\frac{1}{3}[\bar{1}2\bar{1}0]_P \rightarrow (01\bar{1}2)\frac{1}{3}[2\bar{1}\bar{1}0]_T \rightarrow (01\bar{1}0)\frac{1}{3}[2\bar{1}\bar{1}0]_T$$

There are three prismatic slip systems in an HCP unit cell, and Figs. 2 and 3 only show a very special scenario of twin-slip interaction. We also simulate the interaction between the other two prismatic dislocations with a $\{11\bar{2}2\}$ TB. Our results and analyses show that, for the $(01\bar{1}0)$ $\frac{1}{3}[\bar{2}110]_P$ dislocation, a similar scenario also occurs, and the dislocation transmutation can be described as: $(0\bar{1}10)\frac{1}{3}[\bar{2}110]_P \rightarrow (10\bar{1}2)\frac{1}{3}[\bar{1}2\bar{1}0]_T \rightarrow (10\bar{1}0)\frac{1}{3}[\bar{1}2\bar{1}0]_T$ (Fig. S3); but for the $(10\bar{1}0)\frac{1}{3}[\bar{1}\bar{1}20]_P$ dislocation, the slip plane and the Burgers vector remain identical before and after transmutation, and the transmutation can be described as: $(1\bar{1}00)\frac{1}{3}[11\bar{2}0]_P \rightarrow (1\bar{1}00)\frac{1}{3}[11\bar{2}0]_T$ (Fig. S4).

Our results reveal very unusual, unexpected dislocation transmutation during $\{11\bar{2}2\}$ twin-slip interaction in which a mobile prismatic dislocation in the parent is transmuted into an intermediate, unstable dislocation on the $\{10\bar{1}2\}$ of the twin. This plane is not a slip plane but the most common theoretical twinning plane in HCP metals. The unstable dislocation is then further transmuted into a mobile prismatic dislocation. Such behavior has not been reported before. In the following, we analyze and discuss why such an unusual dislocation transmutation occurs during twin-slip interaction, from the perspective of lattice correspondence in deformation twinning.

In classical twinning theory, there exists a one-to-one lattice correspondence for any crystallographic plane and vector between the parent and twin lattice [9]. In other words, an atomic plane of the parent must be transformed into the corresponding plane of the twin. For any twinning mode, if a homogeneous shear on the twinning plane is assumed, then such a lattice correspondence can be calculated mathematically [9,10]. This important principle allows one to determine the corresponding planes of any slip system in a crystal because the slip plane of the parent must be transformed into its corresponding plane of the twin. According to Christian [9], a vector of parent V_M can be associated with the corresponding vector of twin V_T by a lattice correspondence matrix C by: $V_T = CV_M$. Using atomistic simulations, Chen et al. [11,13] confirmed the existence of lattice correspondence and analyzed dislocation transmutations during twin-slip interaction in $\{10\bar{1}2\}$ and $\{10\bar{1}1\}$ twinning mode. Following the concept of lattice correspondence, Niewczas [10] calculated the corresponding slip systems of the four major twinning modes in HCP metals. Specifically for the $\{11\bar{2}2\}\langle 11\bar{2}3\rangle$ twinning mode, the corresponding slip systems were calculated by assuming the $\{11\bar{2}4\}$ was the K_2 or the second invariant plane [9,28,29]. This K_2 is controversial because most atomistic simulations show that the (0002) is the K_2 plane [23,30], irrespective of the interatomic potentials [21,31–33]. Recent transmission electron

Table 1
The lattice correspondences of prismatic slip modes in $\{11\bar{2}2\}\langle 11\bar{2}3\rangle$ twinning obtained by MD simulations and crystallography-based calculations [35].

Slip systems of parent	Corresponding slip systems of twin	
	Simulation results	Calculation results
$(10\bar{1}0)[\bar{1}2\bar{1}0]$	$(01\bar{1}2)[2\bar{1}\bar{1}0]$	$(01\bar{1}2)[2\bar{1}\bar{1}0]$
$(0\bar{1}10)[2\bar{1}\bar{1}0]$	$(\bar{1}01\bar{2})[\bar{1}2\bar{1}0]$	$(\bar{1}01\bar{2})[\bar{1}2\bar{1}0]$
$(\bar{1}100)[\bar{1}\bar{1}20]$	$(1\bar{1}00)[\bar{1}\bar{1}20]$	$(1\bar{1}00)[\bar{1}\bar{1}20]$

microscopy (TEM) observations and atomistic simulations revealed that the K_2 plane is indeed the (0002) rather than $\{11\bar{2}4\}$ [23,34]. He [34] studied $\{11\bar{2}2\}\langle 11\bar{2}3\rangle$ twinning in rhenium (*Re*) using in-situ atomic resolution TEM and unambiguously showed that the K_2 plane was the (0002) rather than the widely accepted $\{11\bar{2}4\}$. Although the (0002) K_2 plane seemingly gives a magnitude of twinning shear 1.26 for Ti which is greater than 1.0 and impractically large, Li et al. [23] revealed that half of the atomic displacement involved in twinning came from shuffling which made no contribution to the overall twinning shear. Thus, the actual magnitude of twinning is only half of 1.26. If the K_2 plane were $\{11\bar{2}4\}$, the corresponding slip system in the twin would be $\{\bar{1}2\bar{1}4\}\langle 5\bar{4}\bar{1}3\rangle$ [10], and both the slip plane and slip direction are of high index.

Zhou et al. [35] recalculated the corresponding slip systems for the $\{11\bar{2}2\}$ mode, using the (0002) as the K_2 plane. They also conducted atomistic simulations to track the lattice transformation during $\{11\bar{2}2\}$ TB migration. Their calculations perfectly agreed with the simulation results. For clarity, the lattice correspondence for three prismatic slip systems from their results are shown in Table 1. Note that the coordinate system of Table 1 is consistent with the one used in this work, thus a direct comparison can be made. From Table 1, It can be seen that the $(10\bar{1}0)[\bar{1}2\bar{1}0]$ of parent is transformed to $(01\bar{1}2)[2\bar{1}\bar{1}0]$ of twin. Therefore, when a parent $(10\bar{1}0)[\bar{1}2\bar{1}0]_P$ prismatic dislocation interacts with a $\{11\bar{2}2\}$ TB, it would be transformed into the $(01\bar{1}2)[2\bar{1}\bar{1}0]_T$ dislocation in the twin. This is exactly what is revealed in our simulations (Figs. 2 and 3). For a parent $(0\bar{1}10)[2\bar{1}\bar{1}0]_P$ prismatic dislocation, it would be transformed to the $(10\bar{1}2)[\bar{1}2\bar{1}0]_T$ in the twin; and for a parent $(1\bar{1}00)[11\bar{2}0]_P$ prismatic dislocation, it would be transformed to the $(1\bar{1}00)[11\bar{2}0]_T$ in the twin. Previous works by Chen et al. [11,13] revealed similar lattice correspondence during twin-slip interaction in the $\{10\bar{1}1\}$ and $\{10\bar{1}2\}$ mode.

Finally, we explain why the $(01\bar{1}2)\frac{1}{3}[2\bar{1}\bar{1}0]_T$ intermediate dislocation in the twin further evolves into a $(01\bar{1}0)\frac{1}{3}[\bar{2}110]_T$ prismatic dislocation during twin-slip interaction. Presumably, the intermediate dislocation that lies in the $(01\bar{1}2)$ plane of the twin is energetically unfavorable, because the interplanar spacing of this plane is very small (~1.73 Å). In crystalline metals, dislocation slip preferably occurs on those atomic planes with large interplanar spacings along the directions with short slip distances, or more accurately, along the directions with the lowest energy barriers. For HCP metals, these planes are the basal and prismatic planes. To explain the transition from the unstable dislocation to the stable configuration observed in this work, we compute the energies of these two dislocations. We first select the atoms in box 2 and 3 in Fig 2b, then we track the evolution of potential energy of these atoms throughout the simulation. This approach has been used to compute the energy evolution of selected crystalline defects [22,36,37]. The results are shown in Fig. 4a. The black curve represents the energy evolution of box 2. Before the twin-slip interaction, these atoms reside in the perfect hcp lattice, and the average energy fluctuates around −4.835 eV/atom which is slightly higher than the equilibrium lattice energy. When the selected region is occupied by the $(01\bar{1}2)\frac{1}{3}[2\bar{1}\bar{1}0]_T$ intermediate dislocation, the potential energy spikes up, and the peak represents the energy of the intermediate dislocation. Similarly, the energy evolution of the atoms in box 3 is displayed as the red curve, and the energy peak represents the energy of the $(01\bar{1}0)\frac{1}{3}[\bar{2}110]_T$ prismatic dislocation in the twin, which is about 19.2 meV/atom lower than the energy of the intermediate structure. Hence, after the parent prismatic dislocation interacts with the TB and is transmuted into the intermediate dislocation on the $(01\bar{1}2)$ plane in the twin, energetically, it will further transmute into a lower energy configuration which lies on the $(01\bar{1}0)$ plane. The geometrical relationship between these two slip planes is illustrated in Fig. 4b.

To summarize, we simulate the interaction between prismatic dislocations with a $\{11\bar{2}2\}$ TB in Ti. Our simulation results reveal sequential dislocation transmutations. A prismatic dislocation is first transmuted into an intermediate, unstable dislocation which lies in a $\{10\bar{1}2\}$ plane of the twin, and then the intermediate dislocation is further transmuted into an energetically favorable, stable prismatic dislocation in the twin. For all the transmutation modes, whether an intermediate structure is formed or not, they can be perfectly explained from the perspective of lattice correspondence in deformation twinning. These findings provide fresh insight on twin-slip interaction in HCP metals.

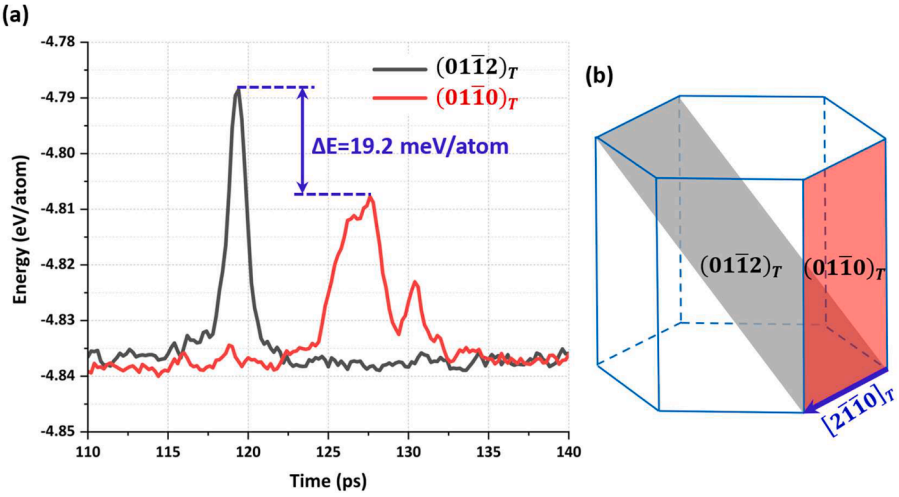

Fig. 4. (a) Comparison of the potential energy between the intermediate dislocation on the $(01\bar{1}2)_T$ plane and the $(01\bar{1}0)_T$ prismatic dislocation in the twin. The prismatic dislocation has a lower line energy and hence is energetically favorable. (b) Schematic illustrations of the orientation relationships between the two slip planes, i.e., the $(01\bar{1}2)_T$ and $(01\bar{1}0)_T$, which have an identical Burgers vector.

Declaration of Competing Interest

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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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.scriptamat.2023.115678.

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