Highly anisotropic slip-behavior of pyramidal I \( \langle c+a \rangle \) dislocations in hexagonal close-packed magnesium

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In hexagonal-closed-pack (HCP) metals, slip of \( \langle c+a \rangle \) dislocations on pyramidal planes is considered to be the most difficult slip mode that controls the overall plastic behavior. Nevertheless, pyramidal \( \langle c+a \rangle \) slip is a requisite for accommodation of \( c \)-axis plastic deformation. In the present study, glissile pyramidal \( \langle c+a \rangle \) dislocations with different characters gliding on type I pyramidal planes, informed by direct atomic simulations, are reproduced and studied in HCP magnesium single crystals. The Peierls stresses for these dislocations are quantitatively evaluated via molecular dynamics simulations under pure shear loading. A high anisotropy in the Peierls stress is observed for different dislocation characters, with the near-screw having the lowest Peierls stress, and the near-edge dislocations having the highest stress. Local shuffling is also found to significantly reduce the Peierls stress of near-edge dislocations. These quantifications of pyramidal \( \langle c+a \rangle \) slip provide better understanding of plastic deformation in HCP metals, and also provide necessary inputs for meso-scale dislocation models such as discrete dislocation dynamics simulations and crystal plasticity simulations.

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1. Introduction

Hexagonal-closed-pack (HCP) metals, such as magnesium (Mg) and titanium (Ti), are promising structural materials due to their light weight and unique properties. However, some intrinsic properties arising from the low symmetry of the HCP lattice structure greatly limit their wide use in different industries. Plastic deformation of metals in general is governed by lattice defects and their response to external loading. As one of the most important lattice defects in crystals, dislocations are ubiquitous in metals and play a key role in determining their mechanical properties. In HCP lattice, there are three different types of dislocations, namely \( \langle a \rangle \), \( \langle c \rangle \) and \( \langle c+a \rangle \) dislocations \cite{1}. Among these dislocations, \( \langle a \rangle \) slip on basal planes is an extremely easy mode (Peierls-stress \( \approx 0.5 \) MPa for Mg \cite{2}); while \( \langle c+a \rangle \) slip is a difficult mode (Peierls-stress \( \approx 35-80 \) MPa for Mg \cite{3}). The significant difference between the slip behavior of these dislocations leads to highly anisotropic plastic deformation, and subsequently low formability of HCP metals. Slip of \( \langle c+a \rangle \) dislocations on pyramidal planes is also a requisite for plastic deformation of HCP metals, since neither \( \langle a \rangle \) nor \( \langle c \rangle \) slip is able to accommodate the homogeneous plastic deformation along the \( c \)-axis.

Slip of \( \langle a \rangle \) dislocations on the closest-packed (0001) basal planes in HCP metals has been extensively studied and characterized using density function theory (DFT) and molecular dynamics (MD) simulations \cite{4,5}. The observed dislocation core structure and slip behavior of basal \( \langle a \rangle \) dislocations are similar to those in face-centered cubic (FCC) metals, due to the lattice similarity between HCP and FCC metals \cite{1} (i.e., both lattices consist of hexagonal closest-packed planes). In the FCC lattice, the \( \langle 111 \rangle \) hexagonal closest-packed planes are packed in an ABCABC sequence; while in the HCP lattice the basal (0001) hexagonal closest-packed planes are packed in a slightly different sequence of ABAB. Nevertheless, the local geometry of the basal slip plane in HCP, namely the relative position between \( A-B \) planes, is identical to that in FCC lattice (relative position between \( A-B \) or \( B-C \) or \( C-A \) planes).

On the other hand, slip of \( \langle c+a \rangle \) dislocations in HCP metals is still poorly understood either theoretically or experimentally. Firstly, there are multiple planes that a \( \langle c+a \rangle \) dislocation with Burgers vector \( b=1/3[1-21-3] \) could glide on, one prismatic \( (10-10) \) plane, two pyramidal I \((1-101) \) and \((0-111) \) planes, one pyramidal II \((1-212) \) plane the \((2-111) \) plane, and the \((1-121) \) plane. All these planes are non-closest-packed planes and have lower symmetry compared with the basal (0001) plane. Secondly, the Burgers vector of a \( \langle c+a \rangle \) dislocation, \( b=1/3(1-213) \), has a large magnitude, almost twice that of \( \langle a \rangle \) dislocations \((1/3(1-210)) \), and thus dissociation of the \( \langle c+a \rangle \) dislocation core is expected. As a result, the slip and dissociation of the \( \langle c+a \rangle \) dislocation on planes with low-symmetry can have complex scenarios \cite{6-8}, and may
lead to distinct plastic response. For example, in Mg single crystals, it was observed experimentally that \((c+a)\) screw dislocations have higher mobility than edge ones [9]. In addition, a wide range of Peierls stresses [3], as well as strong temperature and strain-rate dependences [10] for pyramidal II \((c+a)\) dislocations was reported.

In order to understand the slip behavior of pyramidal \((c+a)\) dislocations in HCP metals, atomistic-simulation based studies had been performed as early as in the 1980s to investigate their core structure and Peierls stresses, using the Lennard-Jones pair potential [11–13]. Numakura et al. introduced \((c+a)\) dislocations on pyramidal I planes [12,13], and found both planar and non-planar cores, depending on the initial configuration of the core structure introduced. They also reported the critical strain required for motion of glissile cores, but not the Peierls stress. Morris et al. introduced \((c+a)\) dislocations on pyramidal II planes [14] in HCP Zr, and obtained both planar and non-planar cores using the embedded atom method (EAM) interatomic potential. Similar results were also obtained for pyramidal II \((c+a)\) dislocations in HCP Mg [15]. Recent DFT predictions of the core structure of pyramidal II \((c+a)\) screw dislocation also showed sensitivity to the initial-configuration [16]. In these studies, the dislocation cores were artificially introduced into the simulation cells using the displacement field of either a full dislocation or using an assumed dissociation (i.e., using assumed Burgers vectors for the leading and trailing dislocations). It should be noted that, for a given interatomic potential, such sensitivity has not been observed for basal \((a)\) dislocations in HCP metals, nor for dislocations in FCC metals [17] introduced using the same displacement-field method. The existence of multiple stable core structures for \((c+a)\) dislocations might be a result of their large Burgers vector, and subsequently their large core, which has more degrees of freedom and a large number of possible configurations in configuration space. The fact that the slip behavior (sessile or glissile) of these \((c+a)\) cores is sensitive to the initial configuration and assumed dislocation dissociation strongly suggests that extra attention must be paid when artificially introducing dislocations without prior information regarding the core structure and dissociation.

In the absence of high resolution transmission electron microscopy (HRTEM) characterization, definite conclusions regarding the core structure and dissociation can hardly be made without extensive DFT/atomistic predictions. Since it is impractical to examine all possible core configurations using either DFT or atomistic methods, unlike previous studies we resort to the natural nucleation of \((c+a)\) dislocations via large scale molecular dynamics simulations. In our previous study [18], the natural nucleation process of glissile pyramidal \((c+a)\) dislocations in Mg single crystal was carefully identified, and the dislocation was found to form by sequential emission of two partials on pyramidal I planes, then transition to pyramidal II planes by cross-slip or cooperative slip. Furthermore, it was observed that the formation of a \((c+a)\) dislocation can be considered as inserting two extra basal half-planes to the lattice, one near each partial core [18]. Thus, the \((c+a)\) core has only a moderate disorder, and is planar and glissile. On the contrary, artificially introducing a full \((c+a)\) dislocation instead of two partials will result in inserting two extra basal planes at the same position. This leads to a high disorder of the lattice near the \((c+a)\) core and is the origin of the non-planar feature and sessilleness of the \((c+a)\) cores observed in previous MD studies [12–14].

The existence of pyramidal I \((c+a)\) dislocations actually is in agreement with geometrisic analysis of the HCP lattice [18], DFT calculations of the generalized stacking fault energy surface [15], as well as HRTEM observations [19]. Therefore, it is reasonable to consider pyramidal I and II \((c+a)\) slip as co-existing in Mg. Thus, in this study, we investigate the slip behavior of pyramidal I \((c+a)\) dislocations having different characters, along with their corresponding Peierls stresses. Pyramidal I \((c+a)\) dislocation cores were introduced into the simulation cell by computing the anisotropic displacement field [20] of both the leading and trailing partials (the corresponding Burgers vectors are \(b_{l}=1/9\ [−3−25−6]\) and \(b_{l}=1/9[10−11−3]\), respectively, for \(b_{l}=(c+a)=1/3 [−1−12−3]\) as indicated in Ref. [18]) having an initial separation of 2 nm followed by energy minimization. In order to practically avoid artifacts during the introduction of dislocation cores, the initial configurations were manually adjusted according to those naturally nucleated in direct MD simulations [18] whenever available. For cores not available from direct MD simulations, the initial configurations were extensively adjusted to obtain smoothly-gliding planar cores. The obtained cores can be divided into two categories: sessile and glissile cores. For sessile cores, multiple configurations exist, depending on the incorrectly introduced initial configurations. For glissile cores, despite the differences in the trial initial configurations, only one stable configuration was found. Although not all possible configurations were examined, which is also impossible, and other glissile cores cannot be completely excluded, it is still reasonable to assume that the obtained smoothly-gliding planar cores are sufficiently representative for a given interatomic potential.

2. Un-shuffled and Shuffled Pyramidal I \((c+a)\) dislocation core structures

From our previous direct MD simulations showing \((c+a)\) dislocation nucleation [18], two types of pyramidal I \((c+a)\) full dislocations were identified, as shown in Figs. 1a and 2a. The structure of the first core shown in Fig. 1a is more planar, while the second core, which is shown in Fig. 2a, exhibits a multi-layer feature. Detailed analysis of the slip processes via a tracer method [18] shows that a local shuffing process occurs during the formation of the second \((c+a)\) dislocation core as shown in Fig. 2a. On the other hand, no shuffling process is observed for the first core shown in Fig. 1a. Fig. 1b shows a portion of the lattice behind the \((c+a)\) dislocation core in the already-slipped area. Atoms below and above the slip plane are denoted by large and small spheres, respectively. Tracers consisting of six atoms in the lower and upper pyramidal I \((0−111)\) planes are highlighted as white and green spheres, respectively. By backtracking these tracers to the un-deformed initial configuration, the relative atomic movement during the formation of a \((c+a)\) dislocation is identified, as shown by the black and red hexagons in Fig. 1b and c. Clearly, a mechanical shear with a displacement vector of \(b_{l}=(c+a)=1/3[1−21−3]\) is evident. Applying the same tracer method to the \((c+a)\) core shown in Fig. 2a clearly reveals the occurrence of shuffling, as shown in Fig. 2b and c. A-type (cyan spheres) and B-type (pink spheres) atoms in the same \((0−111)\) plane follow the slip paths of 1/6[0−22−3] (red arrows in Fig. 2c) and 1/6[2−20−3] (black arrows in Fig. 2c), respectively, completing the translation symmetry by replacing each other. Above the shuffled single layer, the same mechanical shear with a displacement vector of \(b_{l}=(c+a)=1/3[1−21−3]\) is evident again, as shown in Fig. 2d and e. Thus, shuffling is observed to take place only for one single layer.

3. Simulation method

Pyramidal I \((c+a)\) dislocations having near-edge, near-screw, and pure screw characters are studied. The line directions, \(I\), and Burgers vector, \(b\), for the near-edge \((I=[2−1−10])\), near-screw \((I=[10−12])\) and pure screw \((I=[1−21−3])\) dislocations are shown in Fig. 3a. Pure edge dislocations were not considered since no periodicity exists along the edge line direction. Fig. 3b shows the schematic of the simulation cell with dimensions \(L_{x}×L_{y}×L_{z}\) equal to 60 nm × 30 nm × 60 nm, where the z-axis is normal to the
pyramidal I plane, the \( y \)-axis is along the dislocation line direction, \( l \), and periodic boundary conditions (PBCs) were applied along \( l \). The actual atomic configuration of a near-edge dislocation is shown in Fig. 3c, where only non-HCP atoms are shown.

Simulations of pure shear loading were performed using the MD code LAMMPS [21]. Two different EAM interatomic potentials for Mg developed by Liu et al. [22] and Sun et al. [23] were utilized to cross-check the potential dependence. It should be noted that, the generalized stacking fault energy curve for the pyramidal I \( \langle c+a \rangle \) slip system \( 1/3 \langle 1–21–3 \rangle \{0–111\} \) was calculated for both potentials and no significant difference was found [18]. The Common Neighbor Analysis (CNA) [24] was used for defect (i.e., non-HCP atoms) detection and VMD [25] tool was used for visualization.

In the present study, pyramidal I \( \langle c+a \rangle \) dislocations with both un-shuffled and shuffled cores are considered. The shuffled cores with \( b=\langle c+a \rangle=1/3]\langle 1–21–3 \rangle \) are introduced by the following procedure: (1) select a single \( \{0–111\} \) layer of atoms, then divide it into two halves by a specified dislocation line; (2) displace A-type and B-type atoms in half of the single \( \{0–111\} \) layer by \( 1/8 \{6–4–2–3 \} \) and \( 1/18\{0–44–3 \} \), respectively; (3) introduce the leading partial \( b_l=1/9\{3–52–6 \} \) in a plane just above the shuffled layer near the specified dislocation line; (4) introduce the trailing partial \( b_t=1/9\{0–11–3 \} \) in a plane just below the shuffled layer at a position 2 nm away (on the shuffled side) from the specified dislocation line.

The shear stress is applied along the \( x \)-axis for near-edge simulations, and along the \( y \)-axis for near-screw and screw simulations, using two different loading methods. In the first loading method, an increasing homogeneous shear stress at a constant rate of 1 MPa per picosecond is applied on a 1.5 nm thick layer at the top surface, while fixing a 1.5 nm thick layer at the bottom surface. Fig. 4a shows the variation in the global shear stress, which is averaged over the whole sample containing a shuffled near-edge core, as a function of time. The shear stress profile, i.e., stress distribution along the \( z \) direction, at \( t=20 \) ps and \( t=40 \) ps. The position where the dislocation core stays (\( z=0 \)) is indicated by a dashed line and an inverse “T” symbol. At \( t=20 \) ps, a linear distribution of shear stress from 0 to 20 MPa is observed, indicating that the shear stress distribution is still non-uniform. At \( t=40 \) ps, the shear stress is almost uniform along the \( z \) direction, indicating that at this stage a homogeneous shear stress state has been reached. After observing the first motion of the dislocation core, the shear stress
was kept constant at a series of values in the neighborhood of the shear stress at which the first motion commenced, and the Peierls stress was determined as the lowest constant stress at which the dislocation core starts gliding while maintaining a steady motion.

In the second loading method, a constant force was applied instantaneously to the top layer (shock loading), which generates a square-shaped single shear wave that travels along the z direction. The dislocation was intentionally positioned at one forth the height of the simulation cell (z=0) from the top surface in the z direction. This allows the dislocation to experience a simple stress state for a longer period before the reflected wave meets the incident wave, which subsequently induces a more complex stress.

Fig. 2. (a) Top view of a shuffled pyramidal \( \langle c+a \rangle \) dislocation. (b) Close-up top view of a slipped area behind the shuffled pyramidal \( \langle c+a \rangle \) dislocation. Only one lower (1st layer) and one upper layer (2nd layer) are shown. (c) Top view of a pyramidal \( \langle c \rangle \) slip plane before deformation. (d) The same view in (b) showing only the 1st layer and the 3rd layer. (e) The same view in (c) showing only the 1st layer and the 3rd layer. The tracers in lower, upper layer and the layer one layer above the upper layer are marked as white, green and purple spheres, respectively. The simulation cell is 20 nm \( \times \) 50 nm \( \times \) 63 nm, and the strain rate is \( 5 \times 10^8/s \) in c-axis compression using the Liu et al. potential [22]. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
state. Fig. 5a shows the variation of the global shear stress, which is averaged over the whole sample containing the shuffled near-edge core, as a function of time for a shock loading of 350 MPa. The near-edge core starts moving at \( t = 7 \) ps and exits the simulation cell at \( t = 24 \) ps. At \( t = 27 \) ps the average shear stress in the simulation cell reaches 500 MPa due to wave interactions. Fig. 5b shows the shear stress profiles at \( t = 20 \) and 40 ps. The dislocation is positioned at \( z = 0 \) and is shown for reference as an inverse “T” symbol.

In all simulations the initial temperature was 0 K and the NVE ensemble was used during loading. The temperature rise is \(< 4\) K for 530 MPa shock loading, and \(< 2\) K for 320 MPa shock loading. For homogeneous shear, the temperature rise is about 0.1 K when the shear stress reaches 500 MPa. Thus, the Peierls stress can be considered to be athermal. In some cases, very high shear stresses were initially applied to drive the dislocation some distance to enable the core to self-correct, then the core was relaxed to its equilibrium configuration and re-loaded to compute the Peierls stress appropriately.

4. Results and discussion

4.1. Glissile core structures of pyramidal \( \langle c+a \rangle \) dislocations

Peierls stresses under shock loading, the shear stress was averaged in a 2 nm thick slab containing the dislocation core, and the Peierls stress was taken as the lowest averaged shear stress at the moment the dislocation core starts gliding and can maintain a steady motion in a short period thereafter.

In all simulations the initial temperature was 0 K and the NVE ensemble was used during loading. The temperature rise is \(< 4\) K for 530 MPa shock loading, and \(< 2\) K for 320 MPa shock loading. For homogeneous shear, the temperature rise is about 0.1 K when the shear stress reaches 500 MPa. Thus, the Peierls stress can be considered to be athermal. In some cases, very high shear stresses were initially applied to drive the dislocation some distance to enable the core to self-correct, then the core was relaxed to its equilibrium configuration and re-loaded to compute the Peierls stress appropriately.

Fig. 6 shows the equilibrium configurations of the glissile pyramidal \( \langle c+a \rangle \) near-edge, near-screw and pure screw dislocations, as well as their smoothly-gliding configurations under positive (causing \( c \)-axis tension) and negative (causing \( c \)-axis compression) shear stresses, using the Liu et al. EAM potential [22]. The spacing between the equilibrium configuration (center core) and its corresponding...
configuration under shear loading (in the left or right directions) represents the actual distance the core has moved. It is clear that all the glissile cores obtained are relatively planar and can glide in a smooth manner.

When using the Sun et al. EAM potential [23] glissile cores that can smoothly glide on their original slip planes were also obtained for all the three dislocation orientations, except for the un-shuffled near-edge core subject to negative shear, as shown in Fig. 7. This core is glissile when subject to a positive shear, but decomposes into a (c) and a basal (a) dislocation when subject to negative shear as shown in Fig. 7a. These (c) and (a) dislocations all have non-zero Schmid factors in pure shear, and thus are able to glide. Although various initial trial configurations were tested, no glissile un-shuffled near-edge core was found using the Sun et al. potential.

Instead of testing all possible initial configurations, which is impossible, an alternative approach was utilized to address whether a glissile un-shuffled near-edge core exists using the Sun et al. potential. As shown in Fig. 8a, an un-shuffled mixed pyramidal l (c+a) dislocation (l=[−5140], b=1/3[1−12−3]) was introduced into a finite rectangular sample, and uniaxial compression was applied along the c-axis. The edge component remains sessile while the screw component of the core can glide easily until it gets absorbed by the free surface, leading to only a near-edge dislocation (l=[−2110]) remaining in the simulation cell, as shown in Fig. 8b. The sessile un-shuffled near-edge dislocation will then decompose into an (a) and a (c) dislocation, as shown in Fig. 8c, similar to that observed during pure shear as shown in Fig. 7a. However, these (c) and (a) dislocations will not move due to their zero Schmid factors during c-axis loading. As the applied stress increases, the decomposed un-shuffled core re-combines and transforms to a shuff glissile core by climb, leaving interstitials behind, as seen in Fig. 8c and d.

In the above simulation, the sessile near-edge core results from the motion of a glissile mixed core, thus artifacts during core introduction have been greatly eliminated. The remaining sessile near-edge un-shuffled core indicates that this un-shuffled core might be intrinsically sessile and the transformation into shuffled cores might be more favorable for the Sun et al. potential. For the Liu et al. potential, although glissile un-shuffled near-edge cores exist, as shown in Fig. 8a, transition to shuffled cores by climb was also observed at high stress levels, indicating that shuffled cores are also more favorable [18]. It is worth noting that all these
dislocations can be subsequently used as sound trial configurations for future extensive DFT studies of (c+a) dislocation core structures.

4.2. Sessile core structures of pyramidal I (c+a) dislocations

Due to the large Burgers vector of pyramidal I (c+a) dislocations, it is common to obtain unrealistic sessile cores in atomistic simulations when introducing dislocations artificially. Thus, in the following all the sessile cores obtained from this study are discussed to provide guidelines on how to avoid incorrectly introducing such sessile cores in future atomistic simulations. This would also be helpful for studies of (c+a) slip in other HCP metals such as Ti [26,27], in which pyramidal I slip is operative. Some of the sessile cores obtained in this study are shown in Fig. 9.

For near-edge dislocations, only one equilibrium configuration exists for the un-shuffled core when using the Liu et al. [22] potential. This core is glissile only when the shear stress is applied by shock. Upon homogeneous shear loading, the glissile core becomes sessile due to the huge difference in the Peierls stresses for the two partials. The trailing partial with the smaller Burgers vector can glide only at a much higher stress (~480 MPa). Thus, the trailing partial pushes the leading partial to extend onto other planes before the shear stress reaches 480 MPa, producing a non-planar sessile dislocation core, as shown in Fig. 9a. On the other hand, most introduced near-edge shuffled cores relax to the glissile core, except one which becomes sessile at low stress levels by extending onto a prismatic plane, as shown in Fig. 9b. However, this core will subsequently transform to the same glissile core shown in Fig. 6a at high stress levels, exhibiting self-correction of the core. When using the Sun et al. potential [23], there are multiple relaxed un-shuffled near-edge cores. All these cores are sessile in compression and will decompose into an (a) and a (c) dislocation. As shown in Fig. 8, when subject to c-axis compression loading, these dislocations re-combine and transform to a shuffled glissile core by climb. By examining the shuffled core structure, it was possible to reproduce a similar glissile shuffled near-edge dislocation core using the Sun et al. potential as shown in the lower row of Fig. 7a.

The near-screw dislocation core is always glissile and is not sensitive to the initial-configuration. Only one shuffled or un-shuffled core exists for a given potential, making it the best candidate dislocation for building a dislocation network when studying the evolution/interactions of dislocations in atomistic simulations. On the other hand, for the pure screw dislocation, the partial having the larger Burgers vector can easily extend to another pyramidal I plane when using the Liu et al. potential, and to an un-defined plane when using the Sun potential, as shown in Fig. 9c and d. As a result, these non-planar un-shuffled and shuffled (c+a) screw dislocation cores become sessile. In order to obtain glissile cores as identified in direct MD simulations [18], the atomic arrangement near the core is manually modified to suppress out-of-plane extension of the larger partial. After modification, these cores exhibit planar feature and are glissile, as shown in Figs. 6c and 7c.

4.3. Peierls stresses for glissile pyramidal I (c+a) dislocations

Table 1 summarizes the calculated Peierls stresses for all the glissile cores shown in Figs. 6 and 7 using the Liu et al. [22] and Sun et al. [23] EAM potentials, respectively. The un-shuffled near-edge core using the Sun et al. potential was the only case that a
The symmetry of the pyramidal I slip plane.

Liu potential, and 295 MPa versus 30 MPa for the Sun potential) for energy curves [18]. Nevertheless, both predictions show high Sun potential, as demonstrated by the generalized stacking fault which is a result of the higher lattice resistance predicted by the potential is slightly higher than that by the Liu et al. potential, other. In general, the Peierls stress predicted by the Sun et al. two potentials are qualitatively in good agreement with each

Three main conclusions can be drawn from Table 1. First, the pure screw and near-screw dislocations have much lower Peierls stresses than the near-edge orientation, resulting in a high anisotropy, similar to that experimentally reported for pyramidal II \((c+a)\) dislocations [9]. In addition, the near-screw dislocation has the lowest Peierls stress. Since easy slip of near-screw and screw dislocations will result in the formation of near-edge dislocations, which are much more difficult to slip, the complicated slip behavior of near-edge dislocations is speculated to contribute to the complicated pyramidal slip behavior, such as strong temperature and strain-rate dependences, as well as the anomalous thermal-hardening observed in Mg [10]. In BCC metals, a high anisotropy also exists for \(1/2\{111\}\) edge and screw dislocations [28], but arises mainly from their different core structures, namely extended edge cores versus compact screw cores, not the low symmetry of the \(110\) or \(112\) slip planes. Here all pyramidal \((c+a)\) dislocation cores are extended and no significant difference is observed in their core size, as shown in the center column of Figs. 6 and 7. Thus, such a high anisotropy could only be attributed to the low symmetry of the pyramidal I planes. Generally speaking, the relationship between the Peierls stress of a dislocation and its character (the angle between the dislocation line direction and the Burgers vector) could depend on many factors. A simple and important factor is speculated to be the line density of the atoms along the dislocation line direction. Higher line density will lead to higher lattice resistance per unit length and subsequently a higher Peierls stress. For pyramidal I plane, the near-edge dislocation indeed has the highest line density and Peierls stress. However, the line densities of the near-screw and pure screw cannot be simply compared to each other. One has to resort to the Peierls-Nabarro model [29,30] or the line-on-substrate (LOS) model [28] to fully understand the character dependence of Peierls stress in HCP metals.

### Table 1

<table>
<thead>
<tr>
<th>Character</th>
<th>Liu et al. potential [22]</th>
<th>Sun et al. potential [23]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Near-edge</td>
<td>480°</td>
<td>270</td>
</tr>
<tr>
<td>Near-screw</td>
<td>35</td>
<td>30</td>
</tr>
<tr>
<td>Screw</td>
<td>72°</td>
<td>72°</td>
</tr>
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*° Shock loading.

The second conclusion that can be made based on the results in Table 1 is that the shuffled cores of near-edge dislocations have significantly lower Peierls stresses than un-shuffled cores. As discussed earlier, the un-shuffled near-edge core can transform to a shuffled core by climb at high stress levels using both potentials [18]. The lower Peierls stress for shuffled near-edge cores actually confirms that shuffling can be a mediating mechanism for slip and that shuffled cores are more favorable. However, no major differences in the Peierls stress were found between un-shuffled and shuffled cores for the near-screw and screw dislocation cores. The third conclusion is that slip of \((c+a)\) dislocations under negative shear stress requires higher stress than that under positive shear stress, exhibiting a slight shear-direction asymmetry (tension–compression asymmetry).

Considering that pyramidal II planes also have low symmetry, it is reasonable to expect the same high anisotropy for pyramidal II \((c+a)\) slip. Such a high anisotropy in pyramidal \((c+a)\) slip might be responsible for the wide range of Peierls stresses reported experimentally [3].

### 5. Conclusions

In summary, glissile core structures of pyramidal I \((c+a)\) dislocations having different characters, namely near-edge, near-screw and pure screw, were successfully reproduced/introduced based on direct MD simulations showing dislocation nucleation [18]. The Peierls stresses of these cores have also been calculated. The Peierls stresses for these glissile cores show a high anisotropy with the near-screw dislocation having the lowest Peierls stress. The shuffled near-edge dislocation core also has a significantly lower Peierls stress than the...
un-shuffled core. These findings serve as a guide for further atomistic studies in which introduction of pyramidal I \( \langle c+a \rangle \) dislocations is needed, and also provide a quantitative evaluation of pyramidal I \( \langle c+a \rangle \) slip behavior in HCP metals, which is necessary for upper length scale simulations (e.g., discrete dislocation dynamics [31], and crystal plasticity simulations [3]). In addition, the revealed high anisotropy in the Peierls stresses of pyramidal I \( \langle c+a \rangle \) dislocations, together with the transition from pyramidal I to pyramidal II slip [18] is expected to play an important role in understanding the complicated slip behavior in HCP Mg.

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