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Deformation of magnesium during c-axis compression at low temperatures

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In this study, large scale atomistically informed three-dimensional (3D) discrete dislocation dynamics (DDD) simulations were conducted to investigate the mechanical response of single crystal magnesium (Mg) during c-axis compression at low temperatures. In these simulations the plastic anisotropy of slip on pyramidal planes were accounted for to quantify the effects of misorientation, dislocation climb, and pyramidal (c + a) dislocation mobility. The simulation results show that a simple mobility rule based on the properties of edge and screw dislocations will lead to drastically different predictions of the response of Mg during c-axis compression as compared to a more rigorous dislocation orientation dependent mobility rule suggested by atomistic simulations. In addition, the current simulations suggest that plasticity is predominantly mediated by (c + a) slip on pyramidal I planes with less contribution from slip on pyramidal II planes. Furthermore, dislocation climb is observed to have an important effect even at low temperatures. A misorientation of the loading axis within a few degrees is shown to have a negligible effect on the results. The predicted dislocation microstructure are also shown to be in qualitative agreement with experimental results. Finally, the current simulations indicate that (c + a) pyramidal I slip cannot be neglected in crystal plasticity simulations.

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1. Introduction

Magnesium (Mg) and its alloys, owing to their light-weight, are prime candidates for their potential use in automotive and defense applications. Crystallographically, pure Mg has a hexagonal close-packed (hcp) structure, which exhibits lower symmetries than face-centered (fcc) and body-centered (bcc) cubic metals. Consequently, single crystal Mg exhibits a strong plastic anisotropy. Furthermore, Mg single crystals loaded parallel to the c-axis cannot fully satisfy the Taylor criterion, which requires at least five independent slip systems to accommodate homogeneous plastic deformation [1].

Early experimental studies of Mg single crystals under c-axis compression suggested that plasticity in this orientation is predominantly mediated by {10T1} and {10T2} twinning and slip deformation was not observed [2,3]. This view was subsequently challenged with several experimental studies showing unequivocally that c-axis compression of Mg is accommodated by slip on pyramidal planes along the (c + a) direction [4,5]. It is interesting to note that in those later studies twinning was not observed and slip was quantified based on slip trace analysis to be caused by (c + a) dislocation glide on second order pyramidal planes (pyramidal II). Pyramidal II slip traces were also reported during c-axis compression of bulk Mg crystals [6], although it should be noted that those analysis were performed only on samples before yield. These suggestions of the predominance of slip on pyramidal II planes was disputed more recently with further detailed reanalysis of the slip traces from the original work of Obara et al. [5] as well as by more recent experiments that showed that at room temperature (c + a) slip is in fact predominantly on first order pyramidal (pyramidal I) planes, and may be accompanied by a smaller contribution of (c + a) on pyramidal II planes [7,8].

Atomistic simulations have also been routinely employed to understand these conflicting observations. Tang and El-Awady [9,10] provided a comprehensive analysis of (c + a) dislocations on pyramidal I planes at 0 K and showed that in c-axis compression (c + a) slip occurs predominantly on pyramidal I planes, with cross-slip as a possible mechanism to promote slip on pyramidal II planes. In addition, it was shown that diffusionless climb of (c + a) dislocations is common even at low temperatures. Furthermore, Fan et al. [11] showed that with increasing temperature (c + a) slip on
pyramidal II planes increases, which could explain the high ductility observed at temperatures above 500 K [5]. On the other hand, the thermally activated dissociation of \((c + a)\) edge dislocations onto the basal plane has been suggested as a mechanism that leads to the generation of sessile \((c + a)\) edge dislocations [9,12]. It has been suggested by some studies that this dissociation is the main cause for the strong hardening and lack of ductility in c-axis compression with increasing temperature [12]. However these conclusions are inconsistent with experimental observations that show significant ductility at high temperatures [5] as well as strong hardening observed at very low temperatures [6,13].

Although these MD studies as well as others [9,14,15] provided a good understanding of the characteristics of long straight individual \((c + a)\) dislocations on both pyramidal I and II planes, a large gap still exists in our understanding of how the collective motion of a large number of curved dislocations having random characters evolve and gives rise to plastic deformation in Mg. Three-dimensional (3D) discrete dislocation dynamics (DDD) simulations are well-suited to understand the collective motion of dislocations and the evolution of dislocation microstructure. Several DDD methods have already been developed to study the plastic flow in hcp metals [16–19]. Most recent DDD simulations of hcp metals like Mg have focussed on the dislocation-twin boundary interaction [20], which is more relevant for studying a-axis compression, or the reactions between various slip systems [21]. In these DDD simulations, despite the plastic anisotropy observed in MD simulations, it was assumed that \((c + a)\) dislocations do not contribute to the overall deformation. Furthermore, no distinction between the critical resolved shear stress (CRSS) of edge and screw \((c + a)\) dislocations on these planes was made in these simulations. All these assumptions are in contrast with more recent observations from MD simulations [9,22].

In addition to providing physical insights into microstructures observed in experimental studies, DDD simulations can provide the link between the atomistic and crystal plasticity (CP) simulations. In this article, we utilize 3D DDD simulations to study the plasticity of Mg under c-axis compression and specifically attempt to quantify the contribution of pyramidal I and II \((c + a)\) slip. A bottom-up approach is employed in which the CRSS of dislocations predicted from atomistic calculations are upscaled into the DDD framework. The microstructure evolution and mechanical response is then systematically investigated for bulk single crystal Mg. The effects of dislocation climb, mobility rule, and misorientation of the loading axis are then studied. Finally, the effect of switching the CRSS parameters of pyramidal I and II slip systems is discussed.

2. Methods

Simulations of the response of Mg single crystals under c-axis compression are studied here using an in-house version of the open source 3D-DDD code ParaDis [23]. The extensions of the methodology to accurately simulate dislocation mediated plasticity in hcp crystals, which are given in Ref. [19], are also included. The basic Mg properties chosen for the current simulations are: shear modulus, \(G = 17\) GPa; Poisson ratio, \(\mu = 0.29\); magnitude of the \((a)\) dislocation Burgers vector, \(b = 0.325\) nm; axial ratio, \(c/a = 1.6236\); and mass density, \(p = 1738\) kg m\(^{-3}\).

In hcp crystals dislocations can slip on one of four slip planes, namely, basal, prismatic, first-order pyramidal (pyramidal I), and second-order pyramidal (pyramidal II) planes. The basal plane has three different \((a)\) Burgers vectors. In addition, there are three prismatic planes, each has one \((a)\), one \((c)\), and two \((c + a)\) Burgers vectors. Furthermore, there are six pyramidal I planes, each has one \((a)\) and two \((c + a)\) Burgers vectors. Finally, there are six pyramidal II planes, each has one \((c + a)\) Burgers vectors. This adds up to 39 possible slip systems, which are all accounted for in the current simulations. While c-axis extension-twinning mediated plasticity and dislocation twin interaction have been incorporated in the in-house version of the ParaDis code [24,20], these were not accounted for in the current simulations since it has been shown experimentally that for c-axis compression loading plasticity is mediated by dislocation slip only [5,8].

The simulation cells are cubical with an edge length of \(l = 1.6\) \(\mu m\) or \(l = 3.0\) \(\mu m\). The z-axis of all simulation cells are aligned along the \([0001]\) c-axis direction, while the x-axis is aligned with the \([1\overline{2}10]\) direction, as shown in Fig. 1. Periodic boundary conditions (PBCs) were employed along all three directions to mimic bulk response. Initially, Frank-Read (FR) sources are randomly placed on an all slip systems in the simulation cell with a length of \(l = 800b\)

Fig. 1. Schematic of the simulation cell with Frank-Read sources randomly distributed uniformly on all slip systems. The dislocations are colored according to their Burgers vector. The crystallography of the hcp cell and the \((1\overline{1}23)\) direction, which coincides with the \((c + a)\) slip direction, are shown. The c-axis and the two offset loading directions for misorientation simulations are as indicated. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
and $\lambda = 1600b$, in the smaller and larger simulation cells, respectively. Here $b = 0.325 \text{ nm}$ is the magnitude of the (a) Burgers vector. The initial dislocation density in the smaller simulation cells were varied as $1.0 \times 10^{12} \text{ m}^{-2}$, $5.0 \times 10^{12} \text{ m}^{-2}$ and $1.0 \times 10^{13} \text{ m}^{-2}$. The simulations with an initial density of $1.0 \times 10^{12} \text{ m}^{-2}$ showed the same overall trend compared to higher dislocation densities and for the sake of brevity are not presented here. All simulations with the larger simulation cell had an initial dislocation density of $5.0 \times 10^{12} \text{ m}^{-2}$.

Unless otherwise stated, a uniaxial compressive stress field along the c-axis direction is imposed with a strain rate of $\varepsilon = 5000 \text{ s}^{-1}$, and the initial FR sources are uniformly distributed on all possible slip systems. It should be noted that the Schmid factor during c-axis compression is non-zero only for (c+a) dislocations on pyramidal I and II planes. To quantify the effect of misorientation of the loading axis from the c-axis direction, in some simulations the loading axis was offset from the c-axis by 2, 5 and 7° for the simulation cell having edge length $l = 1.6 \mu \text{m}$. This offset is achieved by either rotating in a right hand rule about the x-axis or about the y-axis (termed hereafter “Offset I” and “Offset II”, respectively).

Atomistic simulations suggest that dislocation climb is common even at very low temperatures [9]. As such, dislocation climb is incorporated in the current simulations by using a climb drag coefficient equal to 1 Pa·s. This is four orders of magnitude higher than the drag-coefficient of gliding dislocations. The drag coefficient and the Peierls stresses for glide as predicted at 0 K for screw and edge dislocations from published MD simulations [26,27] are summarized in Table 1. No evidence of glide by (c) dislocations has been reported experimentally and thus these dislocations are assumed to be immobile. Unless otherwise stated, the parameters reported for dislocations on the basal, prismatic, and pyramidal planes, as well as (a) dislocations on pyramidal I planes are used in all current DDD simulations. The Peierls stresses for a mixed dislocation is then predicted by interpolation between the values for screw and edge dislocation by means of the following equation:

$$\tau(\theta) = \tau_{\text{screw}} \cos^2(\theta) + \tau_{\text{edge}} \sin^2(\theta)$$  (1)

where $\theta$ is the angle between the Burgers vector and the dislocation line direction. For the drag coefficient of a mixed dislocation a similar form is also used to interpolate between the edge and screw drag coefficients.

For the (c+a) dislocations on pyramidal I planes, the Peierls stress and drag coefficient was predicted from MD simulations for three different orientations, as summarized in Table 1. The Peierls stress for a mixed dislocation that is oriented about 15° in a clockwise direction from the Burgers vector direction is shown to be the lowest. This orientation has been previously termed a “near screw” orientation [9]. It should be noted that this orientation is not symmetric on the pyramidal I plane about the (c+a) Burgers vector, since the atoms on this plane in an hcp unit cell are not mirror symmetric. In view of this and given the lack of detailed MD analysis of the Peierls stress and mobility of dislocation orientations other than those reported in Table 1, in the current study for a mixed (c+a) dislocations on pyramidal I planes the Peierls stress and mobility are interpreted in a similar way to equation (1) between the screw and near-screw orientations for $0^\circ < \theta < 15^\circ$ and between the near-screw and edge orientations for $15^\circ < \theta < 90^\circ$. On the other hand, for $-90^\circ < \theta < 0^\circ$ the interpolation is performed between the screw and edge orientations. Simulations conducted with these mobilities are termed hereafter “full mobility” simulations. Another simplified rule was also utilized in some simulation. In this case only the edge and screw dislocation mobilities are input and the mobilities of all other dislocation characters are interpolated between the screw and edge orientations. This is the most common approach in DDD simulations [26–28]. Here, the parameters associated with the screw dislocations are set to equal those of the near screw dislocations. The parameters associated with any mixed dislocation would then be directly computed from a linear fit between the edge and screw orientation. Simulations conducted with these mobilities are termed hereafter “simple mobility” simulations.

A schematic description of the dislocation mobility rules on both the Pyramidal I and Pyramidal II planes is shown in Fig. 2. The corresponding underlying atomistic structure is also shown and it clearly shows that on the Pyramidal I plane there is no rotational symmetry of the near-screw direction about the (c+a) pure screw direction.

Cross-slip is another important phenomena that plays an important role in dislocation microstructure evolution and patterning [32]. Cross-slip is in principle a thermally activated process and therefore at low-temperatures dominated by the stress-contribution. In the current simulations a (c+a) screw dislocation is allowed to cross-slip between planes that share the same Burgers vector (i.e. the pyramidal I and II planes as well as the prismatic plane). Furthermore, at low-temperatures, cross-slip of screw dislocations is controlled through a purely stress-driven criteria. However, it should be noted that only allowing the dislocations to glide on the plane having the highest resolved shear stress is inaccurate because in hcp metals the intrinsic lattice resistance is highly anisotropic. Thus, a power-dissipation law is introduced according to which a screw dislocation can change its habit plane if the product of the local Peach-Koehler force and the velocity of dislocation segment plane on the cross-slip plane is higher than that on the habit plane [19]. The Peach-Koehler force contains the contributions from the applied stress as well as dislocation interaction stresses. This cross-slip model is discussed in more details elsewhere [19,20].

### Table 1

<table>
<thead>
<tr>
<th>Slip plane</th>
<th>Dislocation character</th>
<th>CRSS (MPa)</th>
<th>Drag coefficient ($\times 10^5 \text{ Pa s}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basal</td>
<td>Edge</td>
<td>0.52 [29]</td>
<td>1.32</td>
</tr>
<tr>
<td></td>
<td>Screw</td>
<td>0.56</td>
<td>3.54</td>
</tr>
<tr>
<td>Prismatic</td>
<td>Edge</td>
<td>39.2 [30]</td>
<td>0.83</td>
</tr>
<tr>
<td></td>
<td>Screw</td>
<td>39.2 [30]</td>
<td>3.63</td>
</tr>
<tr>
<td>Pyramidal</td>
<td>Edge</td>
<td>105 [31]</td>
<td>2.08</td>
</tr>
<tr>
<td></td>
<td>Screw</td>
<td>105 [31]</td>
<td>2.08</td>
</tr>
<tr>
<td>Pyramidal</td>
<td>Edge</td>
<td>422 [20]</td>
<td>69.2</td>
</tr>
<tr>
<td></td>
<td>Near screw</td>
<td>27 [20]</td>
<td>1.48</td>
</tr>
<tr>
<td></td>
<td>Screw</td>
<td>72 [9]</td>
<td>1.48</td>
</tr>
<tr>
<td>Pyramidal</td>
<td>Edge</td>
<td>208 [20]</td>
<td>25.59</td>
</tr>
<tr>
<td></td>
<td>Screw</td>
<td>493 [20]</td>
<td>99.33</td>
</tr>
</tbody>
</table>

3. Results and discussion

The engineering stress and the dislocation density as a function of strain during c-axis compression as predicted from DDD simulations is shown in Fig. 3. All simulations were performed in a 1.6 µm simulation cell using the full mobility rule and with an initial dislocation density of $5 \times 10^{12} \text{ m}^{-2}$, which was uniformly distributed on all slip systems. For comparison the experimentally
measured engineering stress-strain curves at 77 K is also shown in Fig. 3.  

The predicted yield strength, defined here as the stress at which the stress-strain curve deviates from a linear elastic response, for the simulations with the full mobility rule is $600 \text{ MPa}$. This is 172% higher than the yield strength reported experimentally at 77 K [33]. It should be noted that the Peierls stresses of pyramidal-I and pyramidal-II dislocations as predicted from MD simulations at 0 K are about 70% higher than those predicted at 77 K [11]. Thus, the effect of temperature on the Peierls stress can not alone explain the percentage increase in yield stress as predicted in the current simulations at 0 K versus those measured experimentally at 77 K. Instead there might be other thermally activated mechanisms that would account for this softer response at 77 K.

After yield, significant parabolic-like strain-hardening is observed and the dislocation density increases by 70 times in 0.5% strain as shown in Fig. 3(b). This is qualitatively in agreement with experimental measurements, which also show parabolic-like strain-hardening that increases with increasing temperature, as shown in Fig. 3(a). Furthermore, a maximum stress is observed in the simulations at a strain level of 1.8%, after which significant softening commences. This softening is facilitated mostly by dislocation climb as will be discussed in the following subsection. It should be noted that this softening is not observed experimentally since fracture is expected to initiate before the maximum stress is reached. It has been shown experimentally that Mg single crystals during c-axis compression at 77 K show very low ductility, with fracture topically initiating at 2% strain [33]. To date, the mechanisms associated with this fracture are not fully understood, and as such fracture is not predicted by the current DDD simulations. Thus, the simulations are terminated at 2% strain or when the softening initiates, whichever is achieved first.

The predicted engineering stress and the dislocation density as a function of strain for simulations using the simplified mobility rule are also shown in Fig. 3. In this case, the yield strength is on the order of 400 MPa, which is about 33% lower than that predicted from the simulations using the full mobility rule. The discrepancy in the predicted yield strength using the simplified mobility rule as compared to those predicted using the full mobility rule can be attributed to the hcp crystallography as shown in Fig. 2. In the
simplified mobility rule, it is assumed that the Peierls stress of the \( (c + a) \) dislocations on the pyramidal I plane varies uniformly with its orientation. However, in the full mobility case and based on MD simulations the Peierls stress first decreases from a higher value for the screw orientation to an absolute lower value for the near-screw and screw character, as shown schematically in Fig. 2(a). Additionally, this response is not symmetric about the screw orientation given the lack of rotational symmetry on the pyramidal I planes (see Fig. 2(b)). This leads to an anisotropic response with respect to the dislocation orientation. Thus, dislocation slip is more restricted in the full mobility case as compared to the simple mobility case, which explains the lower yield stress predicted with the simple mobility case.

It should be noted that the softer response predicted by the simplified mobility is artificial and mostly due to the crude assumption of assigning the much lower Peierls stress and mobility of the near screw dislocation to the pure screw dislocation. This is in contrast to the MD simulation predictions. As such, the results predicted from this simplified mobility should only be qualitatively compared to experiments.

The plastic strain along the c-axis direction due to \( (c + a) \) dislocation slip on pyramidal I and pyramidal II planes are shown in Fig. 4. It is observed that the contribution of slip on pyramidal I planes is at least 2 times that from slip on pyramidal II planes by the end of the simulations. This indicates that the pyramidal I slip contributes more towards plastic slip in the c-axis direction as compared to pyramidal II slip. This occurs despite the fact that the Schmid factor on the pyramidal I planes (i.e. 0.4), is lower than that on the pyramidal II planes (i.e. 0.44). The small difference in the Schmid factor of the two slip systems is countered by the difference in the CRSS of dislocations on the two slip planes. This agrees with the recent room temperature experiments of Xie et al. [8] where more slip traces are observed on pyramidal I planes as compared to pyramidal II planes.

### 3.1. The effect of simulation cell size and initial dislocation density

The effect of the simulation cell size and the initial dislocation density on the engineering stress and dislocation density versus strain are shown in Fig. 5. In the simulations, the simple mobility rule was utilized. It is observed that increasing the initial dislocation density or the simulation cell size results in a slight decrease in the strain hardening, however, the yield strength, the shape of the stress-strain curve, and the rate of increase of the total dislocation density are very similar. The decrease in the strain hardening with increasing simulation cell size or initial dislocation density can be attributed to increasing the number of available sources on both pyramidal planes, which leads to a slightly softer response.

### 3.2. The effect of dislocation climb

Recent MD simulations suggest that dislocation climb is predominant for \( (c + a) \) dislocations on pyramidal I and II planes even at very low temperatures [9]. Thus, to assess the effect of dislocation climb on the overall response of single crystal Mg during c-axis compression, a number of simulations were performed with and

![Fig. 4.](image1.png)  
**Fig. 4.** The axial plastic strain evolution along the c-axis direction, \( \varepsilon_{zz} \), due to \( (c + a) \) dislocation slip on (a) pyramidal I; and (b) pyramidal II planes, respectively. The simulations are performed in a simulation cell with edge length 1.6 \( \mu \)m and using either the full or simple mobility rules.

![Fig. 5.](image2.png)  
**Fig. 5.** The effect of the initial dislocation density and simulation cell size on (a) the engineering stress vs strain; and (b) the dislocation density versus strain. The simulations are performed using the simple mobility rules.
without climb enabled. In all cases the simulation cell edge length was 1.6 μm and the simple mobility rule was used. The engineering stress and dislocation density versus strain for the different simulated cases are shown in Fig. 6(a). It is observed that when dislocation climb is not accounted for the shape of the stress-strain curve is significantly different than the case when climb is accounted for. On one hand, the yield strength predicted for the case with no climb is on the order of 700±50 MPa, which is about 87% higher than that predicted from simulations with no climb allowed. Furthermore, after yield steady flow with no strain hardening is observed. These observations are in strong contradiction with the experimental observations at 77 K [33]. It is interesting to note that after the incipient of yield, the dislocation density in both simulations with/without climb show a significant build-up of dislocation density by over an order of magnitude within 0.5% strain, as shown in Fig. 6(b).

3.3. The effect of misorientation

During c-axis loading the Schmid factors for \(\langle c+a \rangle\) dislocations on pyramidal I and pyramidal II planes are equal to 0.4 and 0.44, respectively. For all other slip systems (non-Pyramidal) the Schmid factor is equal to zero. Nevertheless, experimental results of c-axis compression always show slip traces on the basal plane [8,34]. This indicates that \(\langle a \rangle\) dislocations on the basal planes must be active during the deformation. This has been typically attributed to slight misorientation in the loading axis from the c-axis direction, in addition to the low CRSS for basal slip. To quantify these effects, in the current simulation an offset of the loading axis by 2°, 5° and 7° is introduced with respect to the c-axis. In the Offset-I case, only two of the three slip directions on the basal plane have an equal non-zero Schmid factor, while the third slip direction has a zero Schmid factor. For the Offset-II case, all three slip directions on the basal plane have an equal none zero Schmid factor. All simulations were performed for a 1.6 μm simulation cell using the simplified mobility rule and with an initial dislocation density of 5 × 10^{12} m^{-2} that was uniformly distributed on all slip systems.

The engineering stress and total dislocation density curves versus strain for the different misorientation cases are shown in Fig. 7. The reference case with no misorientation is also shown for comparison. With increasing misorientation, the external stress distribution on pyramidal I and II planes becomes more inhomogeneous and the Schmid factor on the basal slip plane increases. Furthermore, as observed in Fig. 7(a), while the overall shape of the stress-strain curve does not significantly change, the flow strength is observed to slightly decrease with increasing misorientation. However, this decrease in flow strength from the reference case is always less than 10%. In addition, there are no major differences observed between simulations with Offset-I and Offset-II. Finally, no effect of misorientation is observed on the evolution of the total dislocation density with strain.

The evolution of the cumulative dislocation density of \(\langle a \rangle\) dislocations on all basal slip systems for all Offset simulations as well as the reference case are shown in Fig. 8. It is observed that the dislocation density on the basal planes increase by two orders of magnitude in all cases. The only effect of misorientation is that the basal dislocation density starts to increase at a slightly lower strain with increasing misorientation angle. It is interesting to note that

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**Fig. 6.** The effect of climb on (a) the engineering stress-strain response; and (b) the evolution of the total dislocation density. All simulations were performed using the simplified mobility rule and the simulation cell edge length was 1.6 μm.

**Fig. 7.** The effect of offset from a perfect loading along the c-axis on: (a) the engineering stress-strain response; and (b) the evolution of the total dislocation density versus strain. All simulations were performed for a simulation cell with edge length 1.6 μm using the simplified mobility rule and an initial dislocation density of 5 × 10^{12} m^{-2} that is uniformly distributed on all slip systems.
although in the reference case the Schmid factor is zero on the basal plane, the dislocation density on the basal plane still increases significantly in a similar manner to the different offset cases. This can be attributed to dislocation reactions, as will be discussed later. In addition, since the Peierls stress for basal dislocations is very small any local stress variations due to the evolving dislocation microstructure on other slip planes can potentially lead to activation of basal slip.

It should be noted that basal slip traces observed experimentally during c-axis compression of single crystal Mg has been attributed to a misorientation within 1° from the c-axis as confirmed by Laue analysis [8]. However, the current simulations suggest that even with a misorientation up to 7° there is little effect of misorientation, and the basal slip activity can be attributed to a number of other factors including dislocation climb, dislocation reactions, low Peierls stress of basal dislocations, and the local stress variations due to the evolving dislocation microstructure.

3.4. Effect of imposing slip predominantly on pyramidal-II planes

In crystal plasticity (CP) simulations, (c + a) slip is predominately imposed on pyramidal II planes, while (c + a) slip on the pyramidal I planes is typically neglected [35–37]. This has been typically justified based on erroneous experimental interpretations of slip trace analysis after c-axis compression in Mg single crystals [5]. However, more recent experimental analysis [8] and detailed MD simulations [7,9–11] show that (c + a) slip on pyramidal I planes is more probable at and below room temperature. Hence, it is critical to address the issue of whether CP simulations imposing predominant pyramidal II slip would lead to significantly different results than those based on the more recent understanding that slip during c-axis compression is predominantly mediated by (c + a) slip on pyramidal I planes.

To address this, in the current simulations the much higher Peierls stresses and lower mobilities of (c + a) dislocations on pyramidal II planes are switched with those for (c + a) dislocations on pyramidal I planes. This will be termed hereafter the “switched case”. Simulation results with these parameters are then compared with the reference case in which the correct parameters are used. This reference case will be termed hereafter the “original case”. For these simulations two simulation cell sizes were chosen with an edge length of 1.6 μm and 3.0 μm, respectively. In both cases the simplified mobility rule was used and the initial dislocation density was $5 \times 10^{12} \text{m}^{-2}$.

The engineering stress and the dislocation density as a function of strain for all simulated cases are shown in Fig. 9. It is observed that the yield point in both the original and switch cases are not significantly different and dislocation slip in both cases initiates almost at the same stress and strain level. However, subsequent to yielding the hardening response is significantly different. In the switched case a linear strain hardening response is observed, which is much weaker than the strain hardening observed in the original case. Furthermore, the strain hardening rate of the switch case is also lower than the strain hardening rate observed experimentally at 77 K. It should be noted that the strain hardening rate is observed experimentally to increase with decreasing temperature from 203 K to 77 K [33,38]. The switch case is thus in odds with this if the increase in strain hardening is expected to continue below 77 K. The evolution of the total dislocation density in the switched case is also shown to increase at a slower rate than that observed for the original case, as shown in Fig. 9(b). This is predominately due to that there are twice as many pyramidal I (c + a) slip systems as there are pyramidal II (c + a) slip systems.

The (c + a) dislocation microstructure after yield for the original and switched cases in a 3.0 μm simulation cell with an initial dislocation density of $5 \times 10^{12} \text{m}^{-2}$ are shown in Fig. 10(a) and (b), respectively. In the original case, screw dislocations on the
pyramidal I plane are first activated since the CRSS of edge dislocations are much higher. This leads to long-straight pyramidal I plane dislocations aligned along the intersection of the pyramidal I and basal planes. Due to cross-slip some \( (c+a) \) dislocations can be observed on the prismatic planes as well. Furthermore, due to the activity of \( (c+a) \) edge dislocations on pyramidal II planes a number of long straight \( (c+a) \) screw dislocations are observed on the intersection of the Pyramidal I and II planes but with much less frequency. On the other hand, in the switch case very few dislocations are observed on the pyramidal I plane. Instead, long straight \( (c+a) \) edge dislocations aligned at the intersection of the pyramidal II and basal planes.

The \( (c+a) \) dislocation microstructure after 0.8% plastic strain is shown in Fig. 10(c) and (d) for the original and switched cases. A 3D view of the entire dislocation microstructure after 0.8% plastic strain for the (c) original; and (d) switched cases. All simulations were conducted in a simulation cell with edge length of 3.0 \( \mu \text{m} \) using the simplified mobility rule and the initial dislocation density was \( 5 \times 10^{15} \text{ m}^{-2} \). Dislocations are colored according to their habit plane. Pyramidal I \( (c+a) \) are shown in blue, pyramidal II \( (c+a) \) are shown in red, prismatic \( (c+a) \) are shown in cyan, basal (a) in yellow, and sessile dislocations in green. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

3.5. Dislocation reactions and the formation of \( (c+a) \) loops

Recent TEM studies of c-axis compressed Mg single crystals show the formation of a large density of \( (c+a) \) dislocation loops [39]. These loops are typically bounded by a stacking fault and may also be attached to other \( (c+a) \) dislocations. Several loops having an \( (a) \) Burgers vector have also been observed [39]. Different mechanisms have been hypothesized to explain the formation of these loops. One such mechanism attributes the formation of these loops as a result of the dissociation of the \( (c+a) \) dislocations into \( (c) \) and \( (a) \) dislocations [39].

In the current DDD simulations the formation of stacking faults are not accounted for. Nevertheless, similar loops are commonly observed and their formation are attributed to an alternative mechanism involving only the interaction of \( (c+a) \) dislocations gliding on non-coplanar pyramidal planes. In Fig. 12(a), a dislocation loop having the \( (a) \) Burgers vector is shown. The loop is redrawn in bold pink color to identify it from other dislocations in the simulation cell. The ends of the loop are connected to \( (c+a) \) dislocation "arms". Other dislocation reactions marked by an "R" in the figure indicate that this reaction is commonly observed in the current simulations. These loops form after a sequence of steps involving glide and interaction of two different \( (c+a) \) dislocations on non-coplanar pyramidal slip planes in accordance to the following reaction:
Fig. 11. The axial plastic strain evolution along the c-axis direction, $\varepsilon_{zz}$, due to $(c+a)$ dislocation slip on (a) pyramidal I; and (b) pyramidal II planes, respectively. In these simulations the much higher Peierls stresses and lower mobilities of $(c+a)$ dislocations on pyramidal II planes are switched with those for $(c+a)$ dislocations on pyramidal I planes. The simulations are performed in a simulation cell with edge length 1.6 $\mu$m and 3.0 $\mu$m with an initial dislocation density of $5 \times 10^{12}$ m$^{-2}$.

Fig. 12. (a), (b) and (c) show a snapshot of reactions between the $(c+a)$ dislocations during the simulation taken from the 1.6 $\mu$m RVE sample with full mobilities. The viewing direction is parallel to the c-axis. The relevant dislocation lines are redrawn for clarity. Green corresponds to $(c+a)$ loops in all the figures. In (a), the $(c+a)$ network is shown with the end arms connected to an $(a)$ dislocation shown in magenta color. In figure (b), the $(c+a)$ dislocation loop is shown in green and red color. Two different colors for the $(c+a)$ dislocation segments are chosen to illustrate the fact that they glide on different planes. In figure (c), two separate reactions between $(c+a)$ dislocations is shown with the $(a)$ dislocation between nodes marked in circles. The black color corresponds to a $(c)$ dislocation. The reactions are marked with R. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
The loop is attached to \((c + a)\) dislocation arms in agreement with TEM observations [39].

A second reaction that is also observed in the simulations that lead to the formation of \((c + a)\) loops similar to those observed experimentally [39] is shown in Fig. 12(b). The two arms of the \((c + a)\) dislocation shown in green and red move on non-coplanar pyramidal planes and interact forming a \((a)\) dislocation that subsequently splits into two \((a)\) dislocations. These \((a)\) dislocations are shown in magenta color in Fig. 12(b). Energetically this reaction is favored and is also observed in other hcp metals, such as Be [19]. Due to dislocation climb some of these loops are non-planar, which are consistent with TEM observations [39].

A third reaction that is commonly observed in the current DDD simulations is the formation of \((c + a)\) dislocations branching into a \((c)\) and an \((a)\) dislocation, as shown in Fig. 12(c). Similar dislocation networks were also observed experimentally and were attributed to the decomposition of the \((c + a)\) dislocation following the reaction \((c + a) = (c) + (a)\) to reduce its energy [40]. However, in the current simulations this network occurs after a \((c + a)\) dislocation interactions with a pre-existing \((c)\), which leads to the following decomposition:

\[
|c_1 + a_1| + |-c_1 + a_1| = 2|a_1| \tag{2}
\]

Several such reactions are observed to form during the simulations, which lead to dislocation structures that are in qualitative agreement with experimental observations.

4. Conclusions

The current study provides a systematic investigation using three-dimensional (3D) discrete dislocation dynamics (DDD) simulations to understand the evolution of deformation during c-axis compression of single crystal Mg at low temperatures. It also provides a detailed view of our current understanding of the different deformation mechanisms on pyramidal slip systems. The Peierls stresses and dislocation drag coefficients obtained from atomistic simulations for all possible dislocations in HCP Mg have been informed into the DDD framework. A number of simulations where then performed to quantify different effect on the response of single crystal Mg during c-axis compression loading. The simulation results show that the typical approach of only providing the properties of edge and screw dislocations and utilizing a simplified fitted mobility rule for other dislocation orientations is not sufficient to accurately predict the response of Mg during c-axis compression. The simulations also show that intermediate dislocation orientations can play a very important role in the plastic slip contributions and the hardening response of Mg and must be properly accounted for. Thus, further atomistic modeling is needed to obtain the Peierls stress and drag coefficients for the entire range of \((c + a)\) dislocation orientations.

The current simulations indicate that c-axis compression is predominantly mediated by \((c + a)\) slip on pyramidal I planes. Nevertheless, even at low temperatures \((c + a)\) slip on pyramidal II planes is also expected but with much less contribution. Furthermore, dislocation climb is observed to reduce the yield strength and also leads to a parabolic stress-strain response. The effect of misorientation is shown to be negligible up to a few degrees from a perfect loading direction parallel to the c-axis. The significant basal slip activity observed experimentally is rationalized here based on the formation of \((a)\) dislocations due to \((c + a)\) dislocation reactions, as well as the high local CRSS on basal planes developing due to the evolving dislocation microstructure. All these observations seem to be qualitatively in agreement with experimental results. The current simulations also signify that in crystal plasticity simulations the pyramidal \(1\) \((c + a)\) slip cannot be neglected as has been commonly the case.

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