Interactions between non-screw lattice dislocations and coherent twin boundaries in face-centered cubic metals

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Abstract

In a first report [Jin ZH, Gumbsch P, Ma E, Albe K, Lu K, Hahn H, et al. Scripta Mater 2006;54:1163], interactions between screw dislocation and coherent twin boundary (CTB) were studied via molecular dynamics simulations for three face-centered cubic (fcc) metals, Cu, Ni and Al. To complement those preliminary results, purely stress-driven interactions between 60° non-screw lattice dislocation and CTB are considered in this paper. Depending on the material and the applied strain, slip has been observed to interact with the boundary in different ways. If a 60° dislocation is forced by an external stress into a CTB, it dissociates into different partial dislocations gliding into the twin as well as along the twin boundary. A sessile dislocation lock may be generated at the CTB if the transited slip is incomplete. The details of the interaction are controlled by the material-dependent energy barriers for the formation of Shockley partial dislocations from the site where the lattice dislocation impinges upon the boundary.

Keywords: Dislocation; Slip; Twinning; Twin grain boundary; Molecular dynamics

1. Introduction

Strength and ductility of crystalline materials depends on slip or plastic flow mediated by the motion, interaction and multiplication of lattice dislocations. Although it is well established that slip in polycrystals is significantly affected by general grain boundaries (GBs) as well as special ones such as twin boundaries (TBs), many aspects of dislocation–GB interactions are not yet fully understood [2–9]. Recent experimental results demonstrated that in materials of low intrinsic stacking fault energies, such as Cu [10–12] and stainless steels [13], the existence of large numbers of nanoscale twins may contribute to an increase in the strength as well as to an improvement in the ductility of the material. It has been proposed that in these samples coherent twin boundaries (CTBs) provide critical energy barriers, preventing slip transits from one twin to another, therefore leading to high yield stress.

It has been evidenced that an improved understanding of dislocation–CTB interactions can be obtained by a combination of computer simulations, experiments and continuum theory in terms of slip transmission [14–17], cross-slip [18–20] and deformation twinning [7,21–23]. In particular, the interaction of screw dislocation (i.e., with Burgers vector parallel to the dislocation line) with coherent twin boundary (CTB) has been considered based on molecular dynamics (MD) simulations [1]. Two interactions were revealed at atomic levels. As a screw dislocation approaches the coherent twin boundary from one side, it may either: (1) propagate into the twin by cutting through...
the boundary; or (2) dissociate within the boundary plane into two Shockley partials propagating along the CTB into opposite directions. In contrast to Cu and Ni where both interactions may occur, only the second mechanism applies to Al. A similar conclusion has also been derived via multiscale modeling of interactions between screw dislocations and CTB as well as other types of tilt grain boundaries in Al [24].

Path techniques in combination with MD simulations have been used for Cu and Al in order to determine precisely the interaction force [25,26]. The results suggest that both the elasticity anisotropy and the response of the CTB to the dislocation fields are keys to understanding the interaction force between the dislocation and the boundary. Due to the long-range repulsion force, two dissociated partial dislocations are required to recombine into a perfect dislocation configuration when they approach to the CTB, as suggested by early simulations [27,28] and experiments [21–23,29]. However, at short distances the interaction force becomes attractive so that the slip is absorbed spontaneously by the CTB in Al, followed by cross-slip (twinning) along the boundary [1,25].

The situations will be more complicated when lattice dislocations are not pure screws. As proposed earlier, a number of possible reactions may occur at the CTB for non-screw lattice dislocations [30]. For example, a 60°/C176 perfect dislocation (i.e. with its Burgers vector inclined by 60° to the dislocation line), if not rejected back to its original grain, may be transferred directly through the boundary into the adjoining twin accompanied by emission of an additional partial dislocation along the twin boundary [7]. However, it is argued that there may be also other possibilities because those twins/TBs may act as sources of partial and perfect dislocations [31–34]. Besides, it is believed that in several nanostructured fcc metals such as Cu, Ni and Al, the dislocation slip is mediated by twin emission and/or mechanical twinning [9,35–40]. In particular, interesting questions may be raised such as: can a slip transit across the twin boundary but partly? – if yes, one still wants to know whether the remaining part of the Burgers vector can form a sessile grain boundary dislocation during the deformation and under what conditions such sessile dislocation locks may be generated and/or unlocked.

To release the strain energy, it is favorable to transmit incident dislocation in one grain to the outgoing glide system in a neighboring grain. However, what actually occurs to the outgoing slip depends on a number of factors, such as the Burgers vector, the resolved shear stress, GB structure, grain size as well as presence of other dislocations. In order to understand what mechanisms actually apply, interactions between a 60° perfect lattice dislocation and a coherent twin boundary in different fcc metals are examined in this study.

2. Methods

MD simulations with simple bicrystal geometry are very useful to clarify many details of dislocation–GB interactions [27,28,41–44]. The MD geometry in our simulations (Fig. 1) is based on the matrix–twin orientation relationship for fcc lattice which is essentially identical to that used in Ref. [1]. In fcc metals, the 1/6 (110)-type perfect lattice dislocation is a combination of two 1/6 (112)-type Shockley partials. For example, the screw dislocation BA(γ) disoci-

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**Fig. 1.** Configuration of a twinned bicrystal for simulating the interactions between a perfect lattice dislocation and a coherent twin boundary in fcc metals. Two 60° dislocations DA and AD at the glide plane (K2) have been considered in this study, the Burgers vectors of which are simply reversed, each inclined by 60° to the dislocation line (ζ, parallel to the z-direction). For comparison, the screw dislocation BA or AB (see Ref. [1]) is also indicated. A homogeneous simple shear (ε_app) has been applied in the (101) shear plane which provides a constant driving force acting on the dislocation such that the motion of the dislocation is to the x-direction. Further details about the driving force, crystal orientations and dislocation reactions can be found in Appendix.
ates according to \( \mathbf{BA} = \mathbf{B} + \gamma \mathbf{A} \), where both the leading partial (\( \gamma \mathbf{A} \)) and the trailing partial (\( \mathbf{B} \)) are 30° partials of mixed character, show edge components of the same length, \( \frac{1}{2} b_s \), but in opposite directions (\( b_s = \frac{\sqrt{2}}{2} a_0 \), the Burgers vector of a Shockley partial dislocation measured in length).

In this study, we consider two non-screw dislocations, namely, \( \mathbf{DA}(\gamma) \) with \( b = \frac{1}{2}[101] \) and \( \mathbf{AD}(\gamma) \) with \( b = \frac{1}{2}[100] \). According to definition, both \( \mathbf{DA} \) and \( \mathbf{AD} \) are 60° perfect dislocations of mixed character. In MD simulations they dissociate according to \( \frac{1}{2}[101] \rightarrow \frac{1}{2}[112]+\frac{1}{2}[211] \) as an example for \( \mathbf{DA} \), or \( \mathbf{DA} = \mathbf{D} + \gamma \mathbf{A} \), where \( \gamma \mathbf{A} (\frac{1}{2}[211]) \) is the leading Shockley partial of a mixed character (30°) and \( \mathbf{D} (\frac{1}{2}[112]) \) the trailing partial of a pure edge character (90°). In general, the two Shockley partials are separated by a stacking fault ribbon and the splitting width depends on the material. The Burgers vector is merely reversed from \( \mathbf{DA} \) to \( \mathbf{AD} \), therefore, essentially they can be considered as the same lattice dislocation. But once such a dislocation moves into opposite directions, it will behave differently as the sequence of the two Shockley partials are also reversed considering their roles as leading and trailing. In particular, the leading Shockley partial is the 30° \( \gamma \mathbf{A} \) for \( \mathbf{DA} \) and it is the 90° \( \gamma \mathbf{D} \) for \( \mathbf{AD} \) (see Fig. A2 in the Appendix). Such an atomic-scale difference may lead to different dislocation reactions whence the dislocation is impinged on a CTB, which will be discussed in the next section.

All dislocations in our simulations are straight and of “infinite” length due to the periodic boundary conditions applied along the dislocation line direction. For the same reason, the twin plane is also infinite in the same direction. In general, dislocations are curved and may take any line direction. The interaction involves short segments of curved dislocations and the associated Shockley partials may show all possible characters. The curvature effects are neglected in our simulations because dislocation segments can be treated as straight according to elasticity dislocation theory [4] and the interactions dealing with other possible combinations of Shockley partials are essentially similar to what have been considered here.

To clarify the material dependence of the dislocation–CTB interaction we choose to consider three fcc metals, i.e. Al, Cu and Ni, which are different model materials in terms of stacking fault energies and elasticity. In our simulations the slip is always considered to be purely stress-driven. All simulations start at 0 K and thermal fluctuations remain insignificant. Strain rate effects are irrelevant. Further details concerning about the crystallography, dislocation reactions in Thompson’s notations, the driving force and MD simulations may be found in the Appendix.

3. Results

The slip remains conservative in our MD simulations of dislocation–CTB interactions. To impinge a dislocation on the CTB, the applied driving force should be high enough to overcome repulsions due to the CTB [1,25]. Therefore, the dislocation approaching to the CTB is constricted and the two separated partial dislocations are recombined into a perfect dislocation configuration at the boundary.

To predict slip transfer across the CTB, both \( K_1 \) and \( K_3 \) are involved and operate as outgoing slip planes for an incoming 60° dislocation (Fig. 1). According to twin symmetry, the corresponding dislocation reaction associated with the complete transfer of the Burgers vector \( \mathbf{DA} \) from \( K_2 \) to \( K_3 \) can be written as (see Fig. 2 and Fig. A2):

\[
\mathbf{DA} \rightarrow \mathbf{A'D'} + C\delta \quad \text{or} \quad \frac{1}{2}[101] = \frac{1}{2}[101]^t + \frac{1}{2}[112]
\]

Similarly, for \( \mathbf{AD} \) it is written as

\[
\mathbf{AD} \rightarrow \mathbf{D'A'} + \delta C \quad \text{or} \quad \frac{1}{2}[101] = \frac{1}{2}[101]^t + \frac{1}{2}[112]
\]

That is, in each case, it requires a 90° twinning partial dislocation (\( C\delta \) or \( \delta C \)) to be emitted along the twin plane (\( K_1 \)). Note again that due to the twin symmetry, the leading partial and trailing partial exchange their order after the transmission.

This indeed occurs to the dislocation \( \mathbf{DA} \) in Cu. As illustrated by MD snapshots in Fig. 3A, the observed dislocation reaction follows exactly the way shown in Fig. 2. The dissociated dislocation recombines into a perfect dislocation configuration at the CTB and then cuts through the boundary by splitting into three Shockley partials. Two of them glide in the slip plane of the twin grain (\( K_3 \)) and they

Fig. 2. The complete transfer of the Burgers vector \( \mathbf{DA} \) across the CTB. Only edge components of Burgers vectors (plotted with different colours) have been drawn because the pure screw component of the Burgers vector is invariant across the CTB. For \( \mathbf{AD} \), the vectors in this plot are simply reversed. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
belong to the same prefect dislocation (A'D'), while the third one is a twinning partial (Cδ) gliding along the twin boundary. Such observation is also well expected according to early experiments [14–17,21–23].

However, the reaction according to Eq. (1b) does not readily occur to AD. In contrast to DA, the dislocation AD in Cu penetrates the CTB but only partly (Fig. 3B). In this case, a 30° leading Shockley partial has been released from the CTB. When it proceeds, a long stacking fault ribbon is left behind. The remaining partial is pinned down and prefers to remain at the boundary, which can be identified as a sessile dislocation, a Hirth lock \( (\text{13}[\text{111}] \text{1}) \) according to the twin symmetry. This lock is featured by one row of “additional” atoms or “interstitials” and thus being called “i-type” twin lock, or an “i-lock”.

The driving force acting on the dislocation is given by Eq. (A2). To activate the observed dislocation reactions in Cu, the magnitude of the required applied shear strain is found similar for both cases, i.e. \( \varepsilon_{\text{appl}} \approx 3\% \). In terms of resolved shear stress, the corresponding values are \( \sigma_{xy} \approx 0.7 \text{ GPa} \) and \( \sigma_{xz} \approx 1.2 \text{ GPa} \).

As for other materials such as Al and Ni, several additional dislocation reactions have been observed in our simulations. Depending on the Burgers vector and the applied strain, the CTB may either allow complete slip transfer or act as a dislocation sink or a dislocation trap.

Fig. 4 shows our observations for Al, in which the incident dislocation DA cannot cut through the CTB entirely. Instead, a 30° twinning partial (δA) is released along the CTB at \( 1.5\% < \varepsilon_{\text{appl}} < 3.5\% \). The remaining part at the CTB can be identified as a Frank sessile dislocation \( (\text{DA}, \frac{1}{3}[\text{111}]) \). Similar reaction also occurs in other simulations [32]. In Fig. 4B, it shows that under a quite large applied strain, \( \varepsilon_{\text{appl}} \approx 4\% \), the dislocation enters the CTB and cuts through it, which is the same as observed for DA in Cu. On the other hand, in Fig. 4C the incident dislocation AD releases two twinning partials along the CTB without cutting through it. The two twinning partials (Aδ and δC) are of different characters, i.e. 30° and 90°, respectively; they repel each other and glide into opposite directions. The sessile dislocation left in the CTB is another perfect dislocation \( (\text{CD/BA, } \frac{1}{3}[\text{110}]) \).
The role of CTB as a dislocation sink or trap has also been observed in Ni (Fig. 5). At $\varepsilon_{\text{appl}} > 1.5\%$, the incoming dislocation DA releases a single twinning partial along the CTB without propagating through it, which is similar to Al (Fig. 4A). At a larger applied strain (4%), two partials will be released: one is a 30° twinning partial along the CTB and the other a 90° partial into the adjacent twin lattice. The sessile dislocation configuration left at the boundary can be identified as another kind of twin lock with Burgers vector $\frac{1}{2}[001] + \frac{1}{2}[111]$. This lock is featured by one row of “missing” atoms or “vacancies”, i.e. it may be called as a “v-lock”. For the incoming dislocation AD, the reaction...
activated at $\varepsilon_{\text{appl}} \geq 2.5\%$ appears to be the same as that for Cu shown in Fig. 3B, with an “i-lock” left at the boundary.

4. Discussions

Our MD observations suggest that besides of the complete slip-transmission, lattice dislocation forced by an external strain into the CTB can have several alternative reaction paths. As a consequence, both glissile and sessile dislocations may be created and the path actually chosen depends on the local property of the dislocation as well as the boundary. In other words, our results suggest that to carry away the elastic energy stored in lattice, the general Schmid law governing dislocation reactions [4,5] has to be applied locally.

Dislocations interacting with the CTB can not be simply treated as Volterra dislocations. No continuum elasticity theory seems presently available for predicting which path will be chosen for a given loading condition. Instead, as proposed in Ref. [1], different interaction behaviors may be understood in terms of energy barriers to nucleate partial dislocation, which are inherently material dependent.

Fig. 5. Interactions between an incoming 60° dislocation and the CTB observed in Ni. To activate these interactions requires (A) $\varepsilon_{\text{appl}} \sim 1.5\%$, or $\sigma_{xy} \sim 0.98$ GPa and $\sigma_{yz} \sim 0.57$ GPa; (B) $\varepsilon_{\text{appl}} \sim 4\%$, or $\sigma_{xy} \sim 2.62$ GPa and $\sigma_{yz} \sim 1.51$ GPa; and (C) $\varepsilon_{\text{appl}} \sim 2\%$, or $\sigma_{xy} \sim 1.63$ GPa and $\sigma_{yz} \sim 0.94$ GPa.
To understand the dislocation–CTB interaction mechanisms, displacement fields have been monitored during the interaction. Fig. 6A illustrates a fully constricted dislocation DA in Cu locating on the left hand side of the CTB. Obviously, significant atomic flow occurs at the dislocation core region. The displacement fields (or the flow fields) about the dislocation reveal that two nucleation sources for partial dislocations coexist but may cooperate differently. One source locates at the glide plane of the adjacent twin lattice at the right-hand side of CTB and the other along the common twin plane. In Cu, both sources operate effectively such that emissions of partial dislocation along both glide planes are favorable (Fig. 3A). In other metals such as Ni (Fig. 6B), only one source operates predominantly, which makes the emission of a 30°/C176 twinning partial (DA) along the CTB more favorable (cf. Figs. 4A and 5A).

The two constricted dislocation configurations shown in Fig. 6 are essentially the same. The reason that the flow fields operate in different ways with the CTB may be understood in terms of stacking fault energies. The intrinsic stacking faults (ISF) which separate the two incoming partial dislocations in Ni are at an energy level nearly five times of that for Cu. To compress a pair of partials into a perfect dislocation configuration, enhanced relaxations at the dislocation core region can be induced if the ISF energy (γS) is high. According to the assumption in Ref. [1], two dimensionless parameters may be introduced to characterize the lattice resistance for re-nucleating partial dislocations:

\[
R = \frac{\gamma_{US}}{\mu b_S} \quad \text{(at a normal glide plane)}
\]

\[
R' = \frac{\gamma_{UT}}{\mu b_S} \quad \text{(at a common twin plane)}
\]

where γUS is the unstable stacking fault energy – the energy barrier to create an intrinsic stable stacking fault on the glide plane of a perfect lattice [45]; γUT, the energy barrier to create a twin fault at a pre-existing twin plane; and μ, the shear modulus in the \{111\} \{121\} shear plane. Unstable fault energies are relevant because creating an intrinsic stable stacking fault (or a twin fault) is closely related to nucleating a Shockley partial dislocation (or a twinning dislocation), both structurally and energetically [1,45,46].

Table 1 summarizes the calculated fault energies and the resistance parameters for the three model materials. The values of R are nearly the same for Cu and Ni. Relative to R, the R' is about 89% for Cu and 74% for Ni. For Al, R ≈ 0.005 and R' is negative. To justify the reliability of interatomic potentials used for the three metals [48,49], data obtained recently via calculations based on density functional theory [50] are included. Our results suggest that, as far as these R-parameters are considered, the three model materials reproduce a trend which is in agreement with predictions based on ab initio calculations. Similar to the situation for screw dislocations [1], these parameters is applicable to explain the interactions observed for non-screw dislocations.

To cut through the CTB, a 60° perfect dislocation re-dissociates into three correlated Shockley partials (Fig. 2) if the driving force is sufficient to overcome all the three energy barriers. According to Eq. (A2) (Appendix), the resolved driving force for creating a 90° twinning partial is nearly 3.7 times of that for creating a 90° Shockley partial into the neighboring twin lattice. Therefore, a large value of R' is favorable to resist strong atomic flows along the twin path such that both partial dislocations of pure edge type may be generated. Under these conditions, our results show that the dislocation DA in Cu is indeed able to transit across the CTB entirely.

For the same dislocation (DA) in Ni, the relatively low R' may lead to enhanced relaxations along the twin path.
so a 30° twinning partial is preferentially emitted (Fig. 5A). When the driving force becomes sufficient for creating a 90° partial into the twin lattice, a “v-lock” is to be left at the boundary (Fig. 5B).

For Al, the negative $R'$ [51] suggests that relaxations along the CTB are dominant. For this reason, a CTB in Al acts as an effective trap for both non-screw dislocations (Fig. 4A and C) and screw dislocations [1,25]. On the other hand, the lattice dislocation in Al exhibits the minimum splitting width. If a dislocation is forced to impinge upon the CTB at a high velocity, the strong kinetic effects may aid it cutting through the boundary entirely, as observed for DA (Fig. 4B).

Similar arguments also apply to the dislocation AD in Cu. In this case, a 30° partial has to be first created as a leading partial, which does not rely upon significant relaxations along the boundary. When the partial slip is triggered, an “i-lock” is created at the boundary (Figs. 3B and 5C). To form an “i-lock”, the combined pressure effects due to the resolved shear strain with respect to the twin lattice are important because they may change the relevant nucleation barrier systematically.

Our separate calculations suggest that compressions (or dilations) along the glide plane normal tend to increase (or decrease) the energy barrier in both Ni and Cu. According to Eq. (A2), with an $\varepsilon_{\text{appl}}$ of about 3%, the resolved strain ($\varepsilon_{\text{appl}}$) on the glide plane $K_1$ is about 1%, which is compressive; that ($\varepsilon_{\text{appl}}$) on the glide plane $K_3$ is about 1.5%, which is tensile. For dislocation DA, the energy barrier is reduced by 10–20% for creating a leading Shockley partial into the adjacent twin lattice and the energy barrier is increased by nearly the same amount for creating a twinning partial at the twin plane, aiding either the transmission of the entire slip (Fig. 3A) or a 90° partial dislocation (Fig. 5B) into the twin grain.

In contrast, the opposite trend is expected for the dislocation AD because in this case the driving force is in an opposite direction to that for DA. With increasing the $\varepsilon_{\text{appl}}$, the barrier in the twin lattice tends to increase but that along the CTB tends to decrease, suggest that whence an “i-lock” is formed it remains to be sessile at the CTB. To release the “i-lock”, a uniform tensile strain ($\varepsilon_{\text{y}}$, cf. Fig. A1) may help, which is found to be about 2% according to our MD simulations. Alternatively, a second AD forced gliding in the same slip plane may also remove the lock by emitting a 90° partial into the twin lattice and pushing away a twinning partial along the CTB; however, it generates a new lock at the CTB by releasing another 30° partial into the twin lattice.

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Appendix

A.1. Twin crystallography

Perfectly twinned lattices with invariant (111) planes are separated by the coherent twin boundary ($K_1$ or CTB). The (111)$^T$ plane ($K_3$) in the twin lattice is the reflected mirror image of the (111) plane ($K_2$) in the matrix lattice (Fig. A1). The two glide planes are conjugate to each other and coincide by a rotation of 180° about z. The transformation of lattice orientations from the matrix $(hkl)$ to twin $(h'k'l')$ is uniquely defined [47] as

\[
\begin{pmatrix}
  h' \\
  k' \\
  l'
\end{pmatrix}
= T
\begin{pmatrix}
  h \\
  k \\
  l
\end{pmatrix},
\text{with } T = \frac{1}{2}
\begin{pmatrix}
  -1 & 1 & 2 \\
  1 & -1 & 2 \\
  2 & 2 & 0
\end{pmatrix}
\]  

(A1)

A.2. Dislocation reactions in Thompson’s notation

The Burgers vector of the perfect dislocation will change from the matrix lattice to the twin lattice (see Fig. 2). We illustrate the dislocation reaction paths by referring Thompson’s triangles (Fig. A2) for those glide planes ($K_1$, $K_2$, and $K_3$). The two triangles ($K_2$ and $K_3$) are conjugates to each other about the common twin plane ($K_1$). Due to the twin symmetry, Burgers vectors of both Shockley partials and perfect dislocations have to be converted 180° across the CTB. As a consequence, the two Shockley partials exchange their roles as leading partial and trailing partial when they cutting through the CTB.

Table 1

<table>
<thead>
<tr>
<th>$a_0$ (Å)</th>
<th>$\mu$ (GPa)</th>
<th>$\gamma_s$ (mJ m$^{-2}$)</th>
<th>$\gamma_{US}$ (mJ m$^{-2}$)</th>
<th>$\gamma_{UT}$ (mJ m$^{-2}$)</th>
<th>$R$</th>
<th>$R'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>EAM$^a$</td>
<td>4.05</td>
<td>27.9</td>
<td>146</td>
<td>168</td>
<td>70</td>
</tr>
<tr>
<td></td>
<td>DFT</td>
<td>4.05</td>
<td>25.1$^b$</td>
<td>112</td>
<td>140</td>
<td>85</td>
</tr>
<tr>
<td>Cu</td>
<td>EAM$^b$</td>
<td>3.60</td>
<td>46.6</td>
<td>29.5</td>
<td>185</td>
<td>167</td>
</tr>
<tr>
<td></td>
<td>DFT</td>
<td>3.635</td>
<td>40.8$^b$</td>
<td>36</td>
<td>138</td>
<td>143</td>
</tr>
<tr>
<td>Ni</td>
<td>EAM$^c$</td>
<td>3.52</td>
<td>75.6</td>
<td>126</td>
<td>368</td>
<td>304</td>
</tr>
<tr>
<td></td>
<td>DFT</td>
<td>3.52</td>
<td>74.6$^c$</td>
<td>133</td>
<td>258</td>
<td>186</td>
</tr>
</tbody>
</table>

The $R$ parameters are calculated according to Eq. (2). The shear modulus is given by $\mu = \frac{1}{2}(c_{11} - c_{12} + c_{44})$, where $c_{11}$, $c_{12}$ and $c_{44}$ are elastic constants.  

$^a$ Interatomic potentials with embedded-atom methods (EAM) [48].  
$^b$ Interatomic potentials with embedded-atom methods (refitted) [1,49].  
$^c$ Literature data taken from Ref. [3].
A.3. Applied shear strains and the driving force

The driving force on the dislocation is determined by a constant simple shear \( \varepsilon_{\text{appl}} \) applied homogeneously to the entire MD cell along the Burgers vector direction of the incident dislocation (Fig. 1). In terms of the engineering strain \( \varepsilon, i = 1, 6 \), the resolved strains on glide planes \( K_i \) and \( K_3 \) (Fig. A1) are given by

\[
\begin{pmatrix}
0 \\
0 \\
0 \\
\varepsilon_{xz}
\end{pmatrix} \rightarrow \begin{pmatrix}
\frac{2\sqrt{2}}{3} \varepsilon_{xy} \\
\frac{2\sqrt{2}}{3} \varepsilon_{xy} \\
0 \\
\frac{1}{\sqrt{3}} \varepsilon_{yz}
\end{pmatrix} \rightarrow \begin{pmatrix}
\frac{2\sqrt{2}}{3} \varepsilon_{xy} \\
\frac{2\sqrt{2}}{3} \varepsilon_{xy} \\
0 \\
\frac{1}{\sqrt{3}} \varepsilon_{yz}
\end{pmatrix}
\]

(A2)

For screw dislocations, \( \varepsilon_{yz} = \varepsilon_{\text{appl}} \) and \( \varepsilon_{xy} = 0 \). For 60° dislocations, \( \varepsilon_y = \frac{\sqrt{3}}{3} \varepsilon_{\text{appl}}, \varepsilon_z = \frac{3}{4} \varepsilon_{\text{appl}} \). The magnitude of the applied engineering shear stresses can be given in two terms, \( \sigma_{yz} = \mu \varepsilon_{xy} \) and \( \sigma_{xz} = \mu \varepsilon_{xy} \), respectively, where \( \mu \) is the shear modulus for both the \( \{111\}\{110\} \) and \( \{111\}\{112\} \) shear plane (Table 1). Non-linear effects, i.e., the \( \varepsilon_{\text{appl}} \)-dependence of \( \mu \), and the combined anisotropy effects, which tend to be more significant with increasing \( \varepsilon_{\text{appl}} \), are neglected in our calculations.

The driving force acting on the incident unit dislocation is determined as [4]:

\[
f = \mu \varepsilon_{\text{appl}} b
\]

equivalent to the Peach–Koehler driving force, \( f = \sigma_{\text{appl}} b \). For partial dislocations, the resolved driving forces with respect to the screw component and the edge component take similar forms according to Eq. (A2).

A.4. MD simulation

To simulate dislocation–CTB interactions, the periodic boundary condition is applied to the z-direction of the MD cell (Fig. A1), with the length of the edge given by \( l_z = 3\sqrt{2}a_0 \), where \( a_0 \) is the lattice parameter. Along the other two dimensions, \( l_x = 50\sqrt{6}a_0 \) and \( l_y = 40\sqrt{3}a_0 \). The MD box contains about 150,000 “free” atoms. The “dislocator” is allowed to move but only for nucleating incident dislocations [1]. The dislocation–CTB interactions within a pre-sheared bicrystal lattice are monitored in independent simulations specified only by \( \varepsilon_{\text{appl}} \). Most of the strain energy released by the motion of dislocation ends up as heat, raising the system kinetic temperature by several kelvin. The MD time step is set to be 2 fs. EAM-type interatomic potentials given by Refs [48,49] have been used in our simulations.

References


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[51] Stacking fault energy calculations suggest that the parameter $R'$ for Al tends to be always negative, regardless homogeneous compression or dilation along the fault plane normal.