The interaction mechanism of screw dislocations with coherent twin boundaries in different face-centred cubic metals

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Abstract

The interaction between screw dislocations and coherent twin boundaries has been studied by means of molecular dynamics simulations for Al, Cu and Ni. Depending on the material and the applied strain, a screw dislocation approaching the coherent twin boundary from one side may either propagate into the adjacent twin grain by cutting through the boundary or it may dissociate within the boundary plane. Which one of these two interaction modes applies seems to depend on the material dependent energy barrier for the nucleation of Shockley partial dislocations.

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1. Introduction

It is well established that the mechanical properties of polycrystalline metals depend on the interaction between lattice dislocations and grain boundaries [1–3], but many details of this interaction are not yet understood [4–6].

In order to study the propagation of dislocation glide across a grain boundary (GB) [7–10], we have investigated the interaction of a perfect lattice screw dislocation (Burgers vector $\mathbf{b} = \frac{a_0}{2} (110)$) with a {111} coherent twin boundary (CTB) by means of molecular dynamics (MD) simulations. The CTBs are of special interest because they control the deformation behaviour of polycrystalline metals with grown-in nano-twins [11,12] and they are closely relevant to mechanical twinning [7,13–16]. It is of fundamental interest to resolve slip transfer across GBs [17] and to be able to predict the effectiveness of these GBs in blocking and redirecting slip [18,19] in thin films, multilayers and polycrystals.

2. Methods

In the MD cell shown in Fig. 1, periodic boundary conditions (PBCs) are applied in the $z$-direction with a periodicity length, $L_z = 3\sqrt{2}a_0$, where $a_0$ is the lattice parameter. Along the other two dimensions, $L_x = 50\sqrt{6}a_0$ and $L_y = 40\sqrt{3}a_0$, respectively. Several layers of atoms at the two surfaces perpendicular to the $y$-direction are fixed. The entire MD box consists of more than 150000 atoms that are allowed to move freely. Larger MD cells do not change our observations.

About 10 outermost layers of atoms at the left side of the specimen are used to create incident dislocations. To create a screw dislocation, e.g., with $\mathbf{b} = \frac{a_0}{2} [110]$, rigid
displacements (at a speed of $\sim 50 \text{ ms}^{-1}$) are introduced above and below the central glide plane (cgp) in opposite directions. The amount of displacement at the cgp is $b_S = a_0 \sqrt{6}/6$ toward the $[211]$ direction to create the leading partial, followed by another $b_S = a_0 \sqrt{6}/6$ but shifted to a different direction, $[121]$, to create the trailing partial. The displacements are strictly confined within the $x$–$z$ planes and linearly reduced to zero at the two fixed borders in the $y$-direction. The stacking fault ribbon is automatically formed between the two straight Shockley partials with a splitting width $d$. After the dislocation has been created, positions of those rigidly displaced atoms are fixed in subsequent MD runs.

Before and after being dislocated, the system was relaxed via energy minimizations. MD-simulations have been carried out in the constant energy ensemble under a constant shear strain ($\epsilon_{\text{appl}}$) applied homogeneously to the entire MD cell at the $(111)[110]$ (or the $y$–$z$) shear plane and MD runs at any specified $\epsilon_{\text{appl}}$ are independent to each other. The motion of dislocation is always found to be subsonic. The elastic energy is released by emitting lattice waves (phonons) which lead to an increase of system kinetic energy corresponding to an effective temperature less than 10 K. The MD time step is set to be 2 fs.

Three face-centred cubic (fcc) metals (Al, Cu and Ni) and different applied stresses were used in the simulations in order to study how the dislocation/CTB interaction processes depend on the applied stress and on the chemical nature of the metal. All three metals were modelled by embedded-atom type interatomic potentials well tested [20–22]. Since temperature effects in our simulations remain insignificant, thermally activated processes (such as thermally-driven cross-slips) are suppressed. A constant shear strain $\epsilon_{\text{appl}}$, corresponding to a simple shear stress $\sigma_{\text{appl}} = \tau = \mu \epsilon_{\text{appl}}$, was applied to provide a constant driving force [23] for dislocation motion given by $f_{\text{appl}} = \tau b$, where $b = a_0 \sqrt{2}/2$ is the magnitude of the Burgers vector and $\mu \equiv \frac{1}{3} (C_{11} - C_{12} + C_{44})$, the shear modulus in the $\{111\}$ $\langle110\rangle$ shear plane.

### 3. Results

The results obtained from these simulations may be summarized as follows. When an incident screw dislocation which is composed of two Shockley partials is forced by an externally applied shear $\epsilon_{\text{appl}}$ into a CTB, it was found that two interaction modes exist:

1. Both partials are redirected into the twin boundary and split in the boundary into two Shockley partials that move along the boundary in opposite directions (Fig. 2, upper panel). In this case the screw dislocation cannot move from one grain across the CTB into the neighbouring grain (twin, Fig. 1) although the resolved driving force ($\approx 0.778 f_{\text{appl}}$) acting along such a path is more than twice as large as that along the boundary plane ($\approx 0.333 f_{\text{appl}}$). This interaction mode applies to Al.

2. A second mode of interaction was noted in Cu and Ni. The incident screw dislocation cuts through the CTB without causing any slip in the boundary plane. The cutting process results in a dissociated screw dislocation in the twin crystal (Fig. 2, lower panel).

These two modes of interaction also differ as far as the applied strain, $\epsilon_{\text{appl}}$, is concerned that is required to initiate
the interaction processes between the lattice dislocation and the CTB. The first mode of interaction occurs spontaneously in Al once the dislocation arrives at the CTB. The second mode requires a material specific threshold strain. For Cu, this threshold strain is found to be about 1.0–1.1% (corresponding to a stress of about 465–510 MPa); for Ni, the corresponding values are 0.4–0.5% (or 300–380 MPa).

4. Discussion

The interaction between the screw dislocation and the CTB may be viewed as a three-step process (Fig. 2, middle panel). During the first step, an initially dissociated screw dislocation (consisting of two parallel Shockley partial dislocations, the leading and trailing partial [23,24]) approaching the {111} CTB is forced to enter the CTB. However, it cannot just pass through the CTB into the twin lattice because the mirror symmetry of the CTB [24] requires that the leading and trailing partials exchange their order. As a consequence, the leading partial is stopped at the boundary, and the trailing partial has to catch up. In the second step, a perfectly straight screw dislocation results when the two Shockley partials are fully constricted and coincide at the CTB. Only in this stage one of the two possible paths is chosen by renucleating Shockley partials either on the boundary or in the twin lattice. During the third step, the two newly formed Shockley partials redissociate.

The interaction process may be considered as a stress-driven cross-slip process in a perfect fcc lattice [25,26]. In our case the Shockley partial dislocations situated at the
CTB remain perfectly straight in the recombination and redissociation processes. This significantly simplifies the corresponding analyses which have been addressed as follows.

The incident screw dislocation is repelled by the CTB. This repulsion originates from the atomic structure of the boundary and the elastic anisotropy of the two crystals forming the CTB. The leading partial can only enter the boundary if sufficiently high shear stresses are applied. These are found to be about 100 MPa for Al and about 300 MPa for both Cu and Ni.

For Al with a high stacking fault energy $\gamma_S$ and a narrow splitting width between the partials, cross-slip occurs spontaneously when the dislocation enters the CTB (Fig. 2). For Cu and Ni, however, further increase of the applied stress is required to compress the two partials into a fully constricted configuration. The corresponding applied strain, $\varepsilon_{\text{appl}}$, is shown in Fig. 3. For Cu, the splitting distance and $\varepsilon_{\text{appl}}$ are found to be linearly related. According to linear continuum elasticity theory [23,25], the splitting distance $d$ is determined by a balance between the attraction caused by the stacking fault (independent of distance) and the repulsion caused by elastic interaction between the two partials (increasing inversely with $d$). Thus, it is energetically more difficult to recombine two partial dislocations if the equilibrium splitting distance $(d_0)$ is large [27]. As $d$ goes to zero, the theoretical prediction based on linear elastic treatment of two Volterra dislocations [23] is no longer justified because the two partial dislocation cores start to overlap into a perfect lattice screw dislocation [27]. In any case, whatever intrinsic force needs to be overcome to recombine the two partials, only the part exceeding the attractive force exerted by the stacking fault $\gamma_S$ needs to be supplied externally.

Since the twin symmetry requires that the leading and trailing partials exchange their roles, renucleation of a dislocation in the twin grain occurs as the trailing partial overlaps the leading partial at the twin boundary. Similarly, cross-slip is activated at the CTB at $d = 0$. We also consider the cross-slip process as a dislocation renucleation process.

Taking the formation of the constriction and the renucleation of the new partials together, we propose that the two distinct interaction modes between a screw dislocation and a CTB are determined by the following criteria:

(i) The critical stress to pass a screw dislocation through a CTB from the parent grain into the twin grain is determined by the fault energy difference $\gamma_{US} - \gamma_S$, so that the full screw dislocation may redissociate into two Shockley partials connected by an intrinsic stacking fault along the glide plane in the twin grain.

(ii) Alternatively, the critical stress to form a constricted screw dislocation and renucleate two Shockley partials on the twin plane is determined by the fault energy difference $\gamma_{UT} - \gamma_S$, such that the dislocation may redissociate into two Shockley partials that lie in the twin plane and are connected by a newly formed twin fault ribbon.

In these assumptions, $\gamma_{US}$ is termed as the unstable stacking fault energy [28,29], the energy barrier to create an intrinsic stable stacking fault from a prefect lattice [29,30], and $\gamma_{UT}$ is the corresponding energy barrier to create a twin fault along a pre-existing twin plane. Creating an intrinsic stable stacking fault (or a twin fault) is equivalent to nucleating a Shockley partial (or twinning) dislocation with $b_S = a_0\sqrt{6}/3$ (Fig. 4).

According to theoretical analyses of dislocation nucleation in terms of Peierls’ model [29], the resistance encountered by a screw dislocation across the CTB may be estimated from a dimensionless parameter given by $R = (\gamma_{US} - \gamma_S)/\mu b_S$. Similarly, the resistance of a screw dislocation to cross-slip on the CTB plane corresponds to a parameter $R' = (\gamma_{UT} - \gamma_S)/\mu b_S$. We have computed the fault energies $\gamma_{US}$, $\gamma_S$, and $\gamma_{UT}$ (Fig. 4) via standard procedures [20,21,31]. Table 1 summarizes the results obtained.

If one compares the computed fault energies, one notices a difference between Al on one hand and Cu and Ni on the other hand. According to Table 1, $\gamma_S$ is higher than $\gamma_{UT}$ for Al. The negative $R$ implies that the lattice screw dislocation impinging at the CTB tends to dissociate spontaneously at the twin plane (Fig. 2), i.e., there is no barrier to redirect lattice screw dislocations into the CTB. One way to test the stability of a screw dislocation at a CTB is to introduce a perfect screw dislocation into the boundary.
at zero stress: in Al, such a dislocation is always found to dissociate along the twin boundary; in contrast, this does not occur in Cu or Ni. Another way is to apply an additional shear strain orthogonal to \( \varepsilon_{\text{appl}} \) by which the resolved shear stress acting on the CTB plane can be forced to vanish while the resolved shear strain acting on the glide plane in the twin grain is still 0.5%; we found that the screw dislocation in Al still cross-slips to the CTB plane, even though there is essentially no applied driving force acting along this path.

On the other hand, for both Cu and Ni, \( \gamma_{\text{US}} \) and \( \gamma_{\text{UT}} \) is larger than \( \gamma_8 \). This suggests that an external threshold strain is required for slip transmission, which is \( \sim 1.1\% \) for Cu and \( \sim 0.5\% \) for Ni (corresponding to an applied threshold stress of about 510 MPa and 380 MPa, respectively). The cross-slip path cutting through the CTB is preferentially chosen because the applied stress supplies a significantly larger driving force (\( \sim 0.778 f_{\text{appl}} \)) along the glide plane in the twin lattice than along the twin plane (\( \sim 0.333 f_{\text{appl}} \)), though \( R' \) is 10% lower than in Cu and nearly 30% lower in Ni (Table 1).

### 5. Summary

In general, the interaction between the screw dislocation and the CTB depends on both the externally applied strain/stress to recombine the two Shockley partial dislocations into a constricted full dislocation at the boundary and the resistance to renucleate partial dislocations along different paths from the site the dislocation enters the boundary—both depend on the chemical nature of the metals. Quantitatively, MD results presented here depend on the accuracy of those EAM potentials [20–22].

The scenario discussed above was restricted to pure screw dislocations with dislocation line directions lying parallel to the twin plane, a very special and also the easiest case. Our results suggest that slip across CTB chooses only one of the two competitive glide planes. If one considers the more general case of non-screw dislocations, partial dislocations can be emitted along both paths. Even in this case, all scenarios found in MD-simulations can be explained by the idea of dislocation renucleation as proposed in this study. Segments of curved dislocations

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Table 1

<table>
<thead>
<tr>
<th></th>
<th>( b_S (\text{Å}) )</th>
<th>( \mu (\text{GPa}) )</th>
<th>( \gamma_8 (\text{mJ m}^{-2}) )</th>
<th>( \gamma_{\text{US}} (\text{mJ m}^{-2}) )</th>
<th>( \gamma_{\text{UT}} (\text{mJ m}^{-2}) )</th>
<th>( R )</th>
<th>( R' )</th>
<th>( R'/R )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>1.651</td>
<td>27.911</td>
<td>146.149</td>
<td>168.414</td>
<td>69.533</td>
<td>0.0048</td>
<td>-0.0166</td>
<td>-3.441</td>
</tr>
<tr>
<td>Cu</td>
<td>1.471</td>
<td>46.554</td>
<td>29.498</td>
<td>185.178</td>
<td>168.677</td>
<td>0.0227</td>
<td>0.0203</td>
<td>0.894</td>
</tr>
<tr>
<td>Ni</td>
<td>1.437</td>
<td>75.630</td>
<td>125.673</td>
<td>367.878</td>
<td>303.706</td>
<td>0.0223</td>
<td>0.0164</td>
<td>0.735</td>
</tr>
</tbody>
</table>

The \( R \)-parameters (see text) may be used to explain our MD observed pathways for redirecting screw dislocations by the CTB.

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Fig. 4. Fault energy curves as a function of rigid displacement either along a normal glide plane in a perfect lattice or along a twin plane of a twinned bicrystal. They are calculated via standard procedures described in the literature (see Refs. [18] and [26]). Atoms are allowed to relax but not in the direction of rigid displacement. To map out the barriers for redirecting screw dislocations at the CTB, the compressibility dependence of fault energies is not included because such effect is insignificant.
can be considered as straight as they are deposited at a CTB and the deformation is still limited by several characteristic processes associated with perfect straight dislocations such as has been shown in this paper.

A detailed report on results for non-screw dislocations is beyond the framework of this paper and will be published separately.

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