

Dislocation–twin interactions in nanocrystalline fcc metals

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Abstract

Dislocation interaction with and accumulation at twin boundaries have been reported to significantly improve the strength and ductility of nanostructured face-centered cubic (fcc) metals and alloys. Here we systematically describe plausible dislocation interactions at twin boundaries. Depending on the characteristics of the dislocations and the driving stress, possible dislocation reactions at twin boundaries include cross-slip into the twinning plane to cause twin growth or de-twinning, formation of a sessile stair-rod dislocation at the twin boundary, and transmission across the twin boundary. The energy barriers for these dislocation reactions are described and compared.

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1. Introduction

Twins have been reported to significantly affect the mechanical properties of nanostructured face-centered cubic (fcc) metals and alloys [1–10]. Importantly, twins have been shown to be able to simultaneously increase the strength and ductility of nanostructured metals, which is attributed to the dislocation interaction with and accumulation at twin boundaries. Since deformation twinning usually occurs simultaneously with the slip of perfect and partial dislocations, interactions between twins and gliding dislocations inevitably occur at twin boundaries. Nanocrystalline fcc metals have been found to deform via twinning more readily than their coarse grained counterparts [11–22]. This increases the probability of interactions between dislocations and twins in nanocrystalline fcc metals. Furthermore, nanocrystalline fcc metals usually have high strength, and the resulting high flow stress may provide enough driving force to activate some energetically

unfavorable dislocation reactions at the twin boundaries. Therefore, it is of scientific interest and practical importance to understand how the dislocations react at twin boundaries.

Dislocation reactions at twin boundaries have been observed both experimentally [2,3,23–32] and by molecular dynamics (MD) simulations [33–41]. However, no systematic investigation has been reported. It is the objective of this paper to systematically describe plausible dislocation reactions at twin boundaries.

2. Possible dislocations to react with twin boundaries

There are only four types of dislocations in the fcc structure that may react at a twin boundary. They can be described with the assistance of Fig. 1, which shows a Thompson tetrahedron on the twin boundary. Note that the twin boundary is also the (1 1 1) slip plane, i.e. the ABC plane in the Thompson tetrahedron. The other three slip planes on the tetrahedron are the ACD, ABD and BCD planes. Before a dislocation reacts at a twin boundary it first needs to slip on one of these three planes. When the

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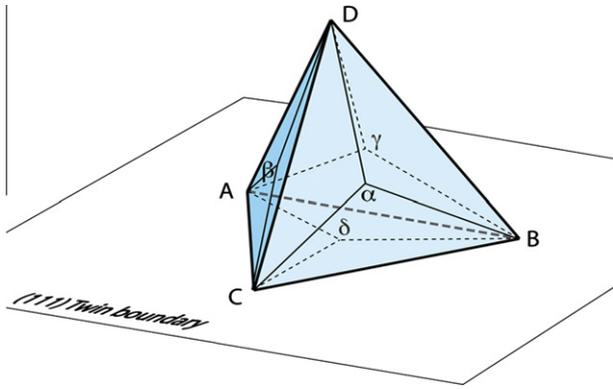


Fig. 1. Illustration of a Thompson tetrahedron on the coherent twin boundary, a (1 1 1) slip plane, which coincides with the ABC plane in the Thompson tetrahedron.

dislocation reaches the twin boundary the dislocation line should become parallel to the intersection line of the slip plane and the twin boundary, which are either AB, BC or CA. Since the three slip planes are identical close-packed planes to gliding dislocations due to the crystal symmetry for dislocation slip, we need to consider only one representative plane hereafter.

To make the discussion easier, we unfold the Thompson tetrahedron onto a two-dimensional representation, as shown in Fig. 2. Assuming that a dislocation glides on the BCD, i.e. $(\bar{1}1\bar{1})$, plane toward the twin boundary, the orientation of the dislocation line will become parallel to BC when it reaches the twin boundary. From Figs. 1 and 2 it can be deduced that this dislocation can be one of four possible types: (a) a 30° Shockley partial dislocation, i.e. the partial's Burgers vector is at a 30° angle to the dislocation line; (b) a 90° Shockley partial dislocation; (c) a screw perfect dislocation with the Burgers vector parallel to the

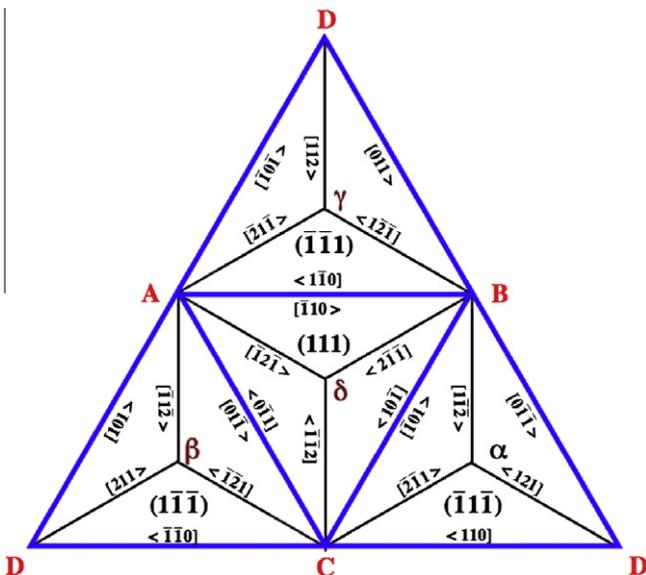


Fig. 2. Two-dimensional representation of the Thompson tetrahedron illustrating the possible slip planes and the Burgers vectors of dislocations in an fcc crystal.

dislocation line; (d) a 60° perfect dislocation. The dislocation reaction at the twin boundary is determined by both the type of dislocation and the magnitude and orientation of the applied stress. In the following sections we will describe possible reactions of each type of dislocation at the twin boundary.

3. A 30° partial at the twin boundary

Assuming that a 30° Shockley partial dislocation $B\alpha$ glides on the BCD plane towards a twin boundary, at the twin boundary it may either cross-slip into the twin boundary plane (ABC plane) or be transmitted across the twin boundary to release a dislocation on the other side of the twin boundary. Below we describe the dislocation reactions for these two scenarios.

3.1. Cross-slip of the 30° partial at the twin boundary

When the 30° Shockley partial dislocation cross-slips into the ABC plane at the twin boundary, it can react at the twin boundary to grow a twin [42]. Similarly, it should also be able to cause de-twinning by moving the twin boundary towards the twin interior. The twin growth process has been described in a previous paper [42]. The de-twinning process is very similar to the twin growth process, except that the partial glides in the opposite direction after cross-slip. Here we also adopt the convention used in Fig. 2 of Zhu et al. [42], and will describe the de-twinning process only.

Fig. 3 illustrates the de-twinning process caused by the interaction of a 30° partial, $B\alpha$, with the twin boundary. Fig. 3a illustrates the partial $B\alpha$ slip on the BCD plane, leaving behind a stacking fault (SF), and stopped at the twin boundary, TB, represented by a thick black line. Under appropriate applied stress the following dislocation reaction occurs (see Figs. 1 and 2):

$$B\alpha \rightarrow B\delta + \delta\alpha \tag{1}$$

If $B\delta$ glides to the left it will move the twin boundary towards the twin interior by one atomic plane. This leaves a step and a stair-rod dislocation at the twin boundary.

The stair-rod dislocation $\delta\alpha$ could further dissociate into two partial dislocations according to the Thompson tetrahedron:

$$\delta\alpha \rightarrow \delta B + B\alpha \tag{2}$$

where the partial δB will glide on the twin boundary in the opposite direction to $B\delta$ under the same applied stress, because δB and $B\delta$ represent partials with opposite Burgers vectors.

As shown in Fig. 3c, after the δB glides to the right the twin thickness is reduced by one atomic plane, i.e. de-twinning occurred during the process. The partial $B\alpha$ advances to the new twin boundary under the original applied stress, and can repeat the above process to annihilate the whole twin.

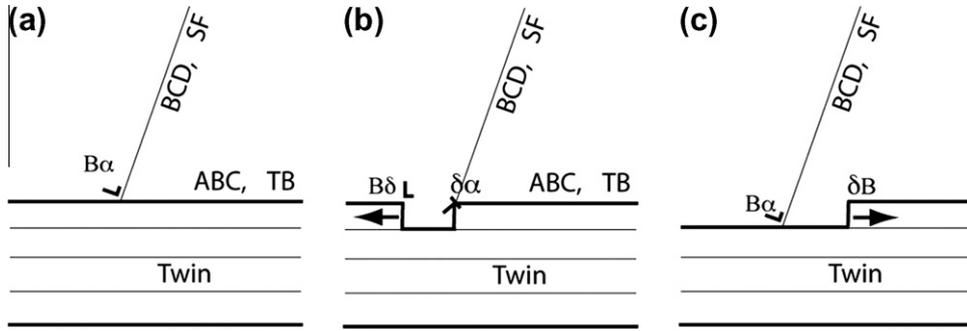


Fig. 3. De-twinning process caused by the interaction of a 30° partial, $B\alpha$, with the twin boundary. SF marks the stacking fault, TB marks the twin boundary (thick black lines). BCD and ABC represent the BCD and ABC slip planes in the Thompson tetrahedron, respectively.

There is an energy barrier to the dislocation reactions described in Eqs. (1) and (2), because the reactions increase the total energy of the dislocations. To estimate the energy barrier we invoke the isotropic elastic dislocation energy per unit dislocation line length [43]:

$$E_{\beta} = \frac{Gb^2(1 - \nu \cos^2 \beta)}{4\pi(1 - \nu)} \ln \frac{R}{r_0} \quad (3)$$

where E_{β} is the energy per unit length of a dislocation with a Burgers vector is at an angle β to the dislocation line, G is the shear modulus, ν is the Poisson's ratio, R can be estimated as the grain size d , and r_0 can be estimated as the Burgers vector b [44]. Eq. (3) can be rewritten as:

$$E_{\beta} = \frac{Gb^2(1 - \nu \cos^2 \beta)}{4\pi(1 - \nu)} \ln \frac{d}{b} \quad (4)$$

The dislocation core energy is not included in Eq. (4). For covalent and ionic crystals, the core energy is relatively high and also a strong function of orientation [45,46]. For metals with a close-packed structure, such as fcc metals, the core energy is about $0.1\text{--}0.05Gb^2$. The calculation of core energies of a dislocation is still a topic of computational and analytical study. One way to incorporate the core energy into Eq. (4) is to choose a smaller r_0 , i.e. $r_0 = b/\alpha$, where α can be calculated as [45]:

$$\alpha = \frac{\sqrt{3}e^{1+\gamma}(1 - \nu)}{\sqrt{2}[\sin^2 \beta + e^{\gamma}(1 - \nu)\cos^2 \beta]} \quad (5)$$

where $\gamma = (1 - 2\nu)/4(1 - \nu)$. Therefore, the total dislocation energy can be described as:

$$E_{\beta} = \frac{Gb^2(1 - \nu \cos^2 \beta)}{4\pi(1 - \nu)} \ln \frac{\alpha d}{b} \quad (6)$$

Note that for fcc metals the magnitudes of the Burgers vector are $a/\sqrt{2}$ for a perfect dislocation, $a/\sqrt{6}$ for a partial dislocation, and $a/3\sqrt{2}$ for the stair-rod dislocation $\delta\alpha$. These quantities will be used to estimate the dislocation energy changes for dislocation reactions.

The energy increase (energy barrier) for a dislocation reaction can be calculated by subtracting the total energy of the initial dislocations from that of the dislocation(s) produced by the reaction. For example, for the reaction described in Eq. (1) the energy barrier can be calculated as:

$$\Delta E_{eq,1} = E_{B\delta} + E_{\delta\alpha} - E_{B\alpha} \quad (7)$$

According to the Thompson tetrahedron both $B\alpha$ and $B\delta$ are 30° partials, i.e. $\beta = 30^\circ$, while the stair-rod dislocation $\delta\alpha$ is an edge dislocation ($\beta = 90^\circ$). Substituting Eq. (6) into Eq. (7) and using the appropriate magnitudes of Burgers vectors, the energy barrier for the dislocation reaction in Eq. (1) can be calculated as:

$$\Delta E_{Eq1}^{B\alpha \rightarrow B\delta + \delta\alpha} = \frac{Ga^2}{72\pi(1 - \nu)} \ln \frac{\sqrt{2}d}{a} + \frac{Ga^2}{72\pi(1 - \nu)} \ln 3\alpha \quad (8)$$

The first term on the right side of Eq. (8) represents the isotropic elastic energy, while the second term represents the core energy. In fact, since both $B\alpha$ and $B\delta$ are 30° partials, $E_{B\alpha} = E_{B\delta}$. This leads to $\Delta E_{Eq1}^{B\alpha \rightarrow B\delta + \delta\alpha} = E_{\delta\alpha}$. For easy comparison we will hereafter define

$$\hat{E} = \frac{Ga^2}{72\pi(1 - \nu)} \ln \frac{\sqrt{2}d}{a} = \tilde{E} \ln \frac{\sqrt{2}d}{a} \quad (9)$$

Assuming hereafter that the Poisson's ratio is approximately 1/3, which is a reasonable approximation for most fcc metals, one can easily calculate $\Delta E_{Eq1}^{B\alpha \rightarrow B\delta + \delta\alpha} = \hat{E} + 2.0\tilde{E}$. Note that \hat{E} is much larger than \tilde{E} . For example, assuming the grain size is 50 nm and a is 0.4 nm, we have $\hat{E} \approx 5\tilde{E}$.

Following a similar procedure, the energy barrier for the dislocation reaction in Eq. (2) can be calculated as:

$$\begin{aligned} \Delta E_{Eq2}^{\delta\alpha \rightarrow \delta B + B\alpha} &\approx \frac{Ga^2(10 - 9\nu)}{144\pi(1 - \nu)} \ln \frac{\sqrt{2}d}{a} + 5.5\tilde{E} \\ &\approx 3.5\hat{E} + 5.5\tilde{E} \end{aligned} \quad (10)$$

This indicates that the second reaction requires a much higher applied stress to overcome the energy barrier. If the applied stress is high enough to activate the reaction described in Eq. (1) but not the reaction in Eq. (2), then a step will be produced at the twin boundary. Twin boundaries with steps have been extensively studied experimentally and by MD simulations [33,36,37]. For example, Yamakov et al. [36] show that a partial dislocation can interact with a twin boundary, which forms a stair-rod dislocation and a step at the twin boundary and, consequently, thickens or reduces the twin by one atomic layer.

3.2. Transmission of the 30° partial across the twin boundary

To understand how the 30° partial $B\alpha$ on the BCD slip plane can be transmitted across the twin boundary we need to invoke the double Thompson tetrahedron [28], illustrated in Fig. 4. As shown, the Thompson tetrahedron above the (1 1 1) twin boundary represents matrix slip systems, while the bottom tetrahedron represents twin slip systems. The twin boundary plane is shared by the matrix above it and the twin below it. Therefore, the matrix tetrahedron and the twin tetrahedron share the same base, which is ABC. In other words, dislocations with Burgers vectors AB , BC , CA , $A\delta$, $B\delta$, and $C\delta$ can slip both in the matrix and in the twin.

From Fig. 4 the 30° partial $B\alpha$ on the BCD slip plane in the matrix, can have the following dislocation reaction to release another partial in the twin:



where $B\alpha'$ is a partial that can slip away in the twin from the twin boundary on the BCD' plane, and $\alpha'\alpha$ is a new type of stationary stair-rod dislocation across the twin boundary. Since the dislocation line is parallel to BC, it can be seen from Fig. 4 that $\alpha'\alpha$ is an edge dislocation with its Burgers vector perpendicular to both the dislocation line and the twin boundary (1 1 1). The magnitude of $\alpha'\alpha$ can be calculated from the geometry of the double tetrahedron as $2a/3\sqrt{3}$. The dislocation configuration after the reaction is illustrated in Fig. 5, which shows two stacking faults from the two sides of the twin boundary meeting at the twin boundary and connected by the stair-rod dislocation $\alpha'\alpha$.

The energy barrier of the dislocation reaction described in Eq. (11) can be calculated as:

$$\begin{aligned} \Delta E_{Eq11}^{B\alpha \rightarrow B\alpha' + \alpha'\alpha} &\approx \frac{Ga^2}{27\pi(1-\nu)} \ln \frac{\sqrt{2}d}{a} + 4.1\tilde{E} \\ &\approx 2.7\tilde{E} + 4.1\tilde{E} \end{aligned} \quad (12)$$

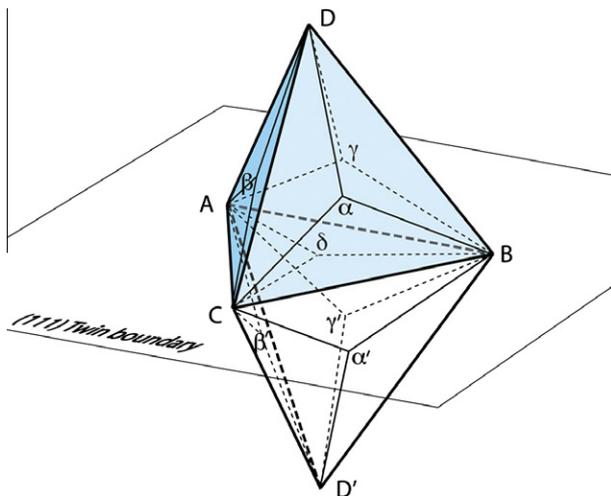


Fig. 4. Illustration of a double Thompson tetrahedron. The top tetrahedron above the (1 1 1) twin boundary represents matrix slip systems, while the bottom tetrahedron represents twin slip systems.

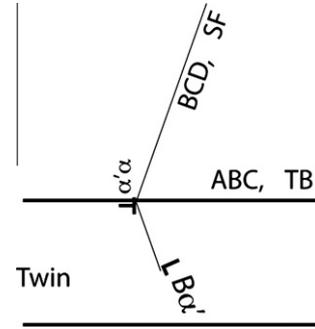


Fig. 5. The dislocation configuration after the partial $B\alpha$ penetrates the twin boundary to release another partial $B\alpha'$ on the BCD' plane inside the twin, leaving a stair-rod dislocation $\alpha'\alpha$ on the twin boundary. This configuration is viewed from the BC orientation.

This indicates that the energy barrier for the 30° partial $B\alpha$ to be transmitted across the twin boundary is smaller than that in reaction 2, suggesting that this scenario is energetically plausible under an appropriate applied stress.

4. A 90° partial at the twin boundary

Assuming that a 90° Shockley partial dislocation $D\alpha$ glides on the BCD plane towards the coherent twin boundary, we describe plausible dislocation reactions at the twin boundary below.

4.1. Cross-slip of the 90° partial at the twin boundary

The cross-slip of 90° partials at the coherent twin boundary has been reported to be responsible for the formation of fivefold twins [47,48], which have been experimentally observed and also verified by MD simulation [49]. Since this has been reported before, we will give only a brief description here.

A deformation twin can be defined by the twin plane K_1 , shear direction η_1 , undistorted plane K_2 , and direction η_2 (see Fig. 6) [45]. Deformation twins in an fcc metal are of compound type, in which a twin formed by Shockley partials with Burgers vectors parallel to η_1 gliding on K_1 is the same as a twin formed by partials with Burgers vectors parallel to η_2 gliding on K_2 . In the current situation K_1 and K_2 correspond to the ABC and BCD planes in the Thompsons tetrahedron, respectively. η_1 is parallel to the 90° partial $A\delta$ and η_2 is parallel to another 90° partial $D\alpha$. In other words, when the 90° partial $D\alpha$ on the BCD plane reaches the twin boundary it becomes equivalent to another 90° partial $A\delta$ on the ABC plane. Under an appropriate external shear stress the $A\delta$ partial could glide to the left or right, which consequently grows or shrinks the twin by one atomic layer. Note that since both $D\alpha$ and $A\delta$ are the same type of partial, there is no energy change (barrier) in this dislocation reaction. Therefore, orientation of the applied stress becomes a critical factor influencing this cross-slip.

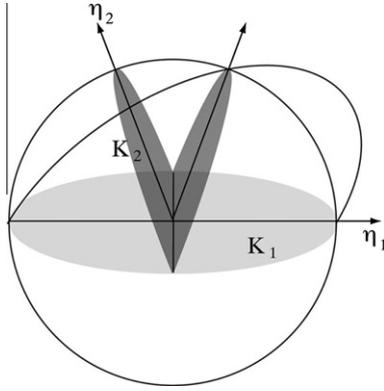


Fig. 6. Illustration of twinning elements η_1 , η_2 , K_1 and K_2 .

4.2. Transmission of the 90° partial across the twin boundary

To understand how a 90° partial $D\alpha$ can be transmitted across the twin boundary to activate a partial dislocation in the twin we need to take a careful look at the double Thompson tetrahedron to determine the dislocation reactions that can translate the Burgers vector of the 90° partial into a partial in the twin. As shown in Fig. 4, the 90° partial $D\alpha$ can dissociate as:



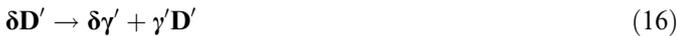
The double Thompson tetrahedron indicates that the Burgers vector $D\delta$ is identical to $\delta D'$ in the twin, i.e. $D\delta = \delta D'$, which can dissociate into a 90° partial $\alpha' D'$ and a stair-rod dislocation $\delta\alpha'$, i.e.



The 90° partial $\alpha' D'$ can glide in the twin to move away from the twin boundary. Other similar reactions that can also produce a 90° partial include:



and



The 90° partials $\beta' D'$ and $\gamma' D'$ can glide on the ACD' and ABD' slip planes, respectively, in the twin.

The magnitude of $D\delta$ and $\delta D'$ is $a/\sqrt{3}$ according to the double Thompson tetrahedron. The energy barrier of the dislocation reaction described in Eq. (13) can be calculated as:

$$\Delta E_{Eq13}^{D\alpha \rightarrow D\delta + \delta\alpha} \approx \frac{Ga^2}{18\pi(1-\nu)} \ln \frac{\sqrt{2}d}{a} + 4.4\tilde{E} = 4\hat{E} + 4.4\tilde{E} \quad (17)$$

The energy barrier of the dislocation reaction described in Eq. (14) can be calculated as:

$$\Delta E_{Eq14}^{\delta D' \rightarrow \delta\alpha' + \alpha' D'} \approx -\frac{Ga^2}{36\pi(1-\nu)} \ln \frac{\sqrt{2}d}{a} - 0.3\tilde{E} \approx -2\hat{E} - 0.3\tilde{E} \quad (18)$$

The energy barriers for the reactions in Eqs. (15) and (16) are the same as that in Eq. (14). Therefore, the dislocation reaction described in Eq. (13) has a very high energy barrier while the reactions in Eqs. (14)–(16) are energetically favorable.

The high energy barrier in Eq. (13) is caused by creation of the dislocation $D\delta$ (or $\delta D'$), which has a large Burgers vector with a magnitude of $a/\sqrt{3}$. If the dislocation reaction path changes to avoid the formation of $D\delta$ ($\delta D'$), the energy barrier will be lower. Assuming that the dislocation reactions in Eqs. (13)–(15) take place in one step without forming $D\delta$ ($\delta D'$), we can substitute Eq. (14) into Eq. (13), which yields:



Similarly, $\beta' D'$ and $\gamma' D'$ can also be formed by the following reactions:



and



The energy barrier for the reaction in Eq. (19) can be calculated as:

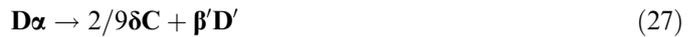
$$\Delta E_{Eq19}^{D\alpha \rightarrow \delta\alpha + \delta\alpha' + \alpha' D'} \approx \frac{Ga^2}{36\pi(1-\nu)} \ln \frac{\sqrt{2}d}{a} + 4.0\tilde{E} \approx 2.0\hat{E} + 4.0\tilde{E} \quad (22)$$

Therefore, the energy barrier for the reaction in Eq. (19) is half of the energy barrier in Eq. (13). The energy barriers for the reactions in Eqs. (20) and (21) are identical to that in Eq. (19).

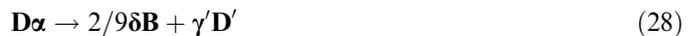
There are two stair-rod dislocations in Eqs. (19)–(21). Both stair-rod dislocations remain at the twin boundary and could react to form a dislocation structure with lower energy. With the help of the double Thompson tetrahedron the stair-rod reactions can be described by:



Substituting Eqs. (23)–(25) into Eqs. (19)–(21) yields:



and



The energy barrier for reaction in Eq. (26) is:

$$\Delta E_{Eq26}^{D\alpha \rightarrow 4/9A\delta + \alpha' D'} \approx \frac{2Ga^2}{243\pi(1-\nu)} \ln \frac{\sqrt{2}d}{a} + 1.4\tilde{E} \approx 0.6\hat{E} + 1.4\tilde{E} \quad (29)$$

The energy barriers for the reactions in Eqs. (27) and (28) are:

$$\Delta E_{Eq27,28} \approx \frac{2Ga^2(1-3\nu/4)}{486\pi(1-\nu)} \ln \frac{\sqrt{2}d}{a} + 0.2\tilde{E} \approx 0.1\hat{E} + 0.2\tilde{E} \quad (30)$$

Therefore, the energy barriers for dislocation reactions in Eqs. (26)–(28) are very low, which makes it easier for the 90° partial $\mathbf{D}\alpha$ to be transmitted across the twin boundary to emit another 90° partial in the twin. However, it is also noted that the reaction products in these equations include dislocations with Burgers vectors that are a fraction of that of a partial, which may make the energy higher than described in Eqs. (29) and (30), since they do not correspond to stable or metastable atomic positions.

5. Reaction of a perfect screw dislocation at the twin boundary

If we assume that a perfect screw dislocation \mathbf{BC} glides on the BCD plane toward the twin boundary (see Fig. 4) it could be dissociated into two 30° partials with a stacking fault in between, i.e.



when this dissociated \mathbf{BC} reaches the twin boundary it could constrict to again form a perfect dislocation. Since \mathbf{BC} is parallel to the dislocation line, it can either cross-slip into the ABC plane on the twin boundary or onto the BCD' plane in the twin, depending on the orientation of the applied stress. Therefore, a screw dislocation can easily cross-slip on the twin boundary or be transmitted across the twin boundary. The interaction of a screw dislocation with a coherent twin boundary has been observed by MD simulation [34].

6. Reaction of a perfect 60° dislocation at the twin boundary

If we assume that a perfect 60° dislocation \mathbf{BD} glides on the BCD plane towards the twin boundary (see Fig. 4) it could be dissociated into a 30° partial $\mathbf{B}\alpha$ and a 90° partial $\alpha\mathbf{D}$ with a stacking fault between them, i.e. $\mathbf{BD} \rightarrow \mathbf{B}\alpha + \alpha\mathbf{D}$. These partials ($\mathbf{B}\alpha$ and $\alpha\mathbf{D}$) with a stacking fault ribbon can glide together under an applied stress towards the twin boundary. Since the perfect 60° dislocation cannot easily cross-slip or be transmitted across the twin boundary, there are several plausible scenarios that could occur, which are described below.

6.1. Perfect dislocation \mathbf{BD} constricts before reaction

We begin by describing the scenario where the partials are constricted to form the perfect dislocation \mathbf{BD} before the dislocation reacts at the twin boundary. Such a scenario can happen more easily when the stacking fault energy is relatively high and the distance between the leading and trailing partials is small. This has been observed experimentally [32] and by MD simulations [33,35,50]. It can be seen from the double Thompson tetrahedron (Fig. 4) that \mathbf{BD} is

at a 60° angle to the dislocation line \mathbf{BC} . The dislocation reaction for \mathbf{BD} to cross-slip onto the ABC plane is:



The energy barrier for such a reaction is:

$$\Delta E_{Eq32}^{BD \rightarrow BC+CD} \approx \frac{Ga^2}{8\pi} \ln \frac{\sqrt{2}d}{a} + 7.2\tilde{E} \approx 6\hat{E} + 7.2\tilde{E} \quad (33)$$

This energy barrier is so high that such a cross-slip is almost impossible.

Another possible dislocation reaction is for \mathbf{BD} to be transmitted across the twin boundary to emit a perfect dislocation in the twin. The following analysis yields possible dislocation reactions. First, \mathbf{BD} can dissociate according to:



where $\delta\mathbf{D}$ is equivalent to $\mathbf{D}'\delta$, which can further react to emit perfect dislocations in the twin according to:



Substituting Eqs. (35)–(37) into Eq. (34), and also considering $\mathbf{B}\delta + \mathbf{A}\delta = \delta\mathbf{C}$ and $\mathbf{B}\delta + \mathbf{C}\delta = \delta\mathbf{A}$, we have:



The energy barriers for the dislocation reactions in Eqs. (38)–(40) can be described by:

$$\begin{aligned} \Delta E_{Eq38}^{BD \rightarrow 2B\delta+D'B} &\approx \frac{Ga^2(1-3\nu/4)}{12\pi(1-\nu)} \ln \frac{\sqrt{2}d}{a} + 7.5\tilde{E} \\ &\approx 4.5\hat{E} + 7.5\tilde{E} \end{aligned} \quad (41)$$

$$\begin{aligned} \Delta E_{Eq39}^{BD \rightarrow \delta C+D'A} &\approx \frac{Ga^2}{24\pi(1-\nu)} \ln \frac{\sqrt{2}d}{a} + 3.9\tilde{E} \\ &\approx 3.0\hat{E} + 3.9\tilde{E} \end{aligned} \quad (42)$$

$$\begin{aligned} \Delta E_{Eq40}^{BD \rightarrow \delta A+D'C} &\approx \frac{Ga^2}{24\pi(1-\nu)} \ln \frac{\sqrt{2}d}{a} + 3.9\tilde{E} \\ &\approx 3.9\hat{E} + 3.9\tilde{E} \end{aligned} \quad (43)$$

Therefore, the dislocation reactions in Eqs. (39) and (40) have smaller energy barriers. In these two reactions one partial will glide on the twin plane, which will grow or shrink the twin by one atomic plane and leave behind a step on the twin boundary depending on the gliding direction. At the same time a perfect 60° dislocation is emitted in the twin, which will also produce a step on the twin boundary. In comparison, the dislocation reaction in Eq. (38) will release two partials on the ABC plane, which may grow or shrink the twin by two atomic planes if they glide on two slip planes.

6.2. 30° leading partial $\mathbf{B}\alpha$ reacts first at the twin boundary

If we assume that the 60° dislocation \mathbf{BD} glides on the BCD plane toward the twin boundary it can be dissociated

as $\mathbf{BD} \rightarrow \mathbf{B}\alpha + \alpha\mathbf{D}$, with the 30° partial $\mathbf{B}\alpha$ as the leading partial. The leading partial $\mathbf{B}\alpha$ could either cross-slip onto the twin boundary plane or be transmitted across the twin boundary. We will discuss these two cases below.

6.2.1. Leading 30° partial $\mathbf{B}\alpha$ cross-slip onto the twin boundary plane

When the stacking fault energy is relatively low and under an appropriate applied stress $\mathbf{B}\alpha$ can cross-slip onto the ABC twin boundary plane to emit a partial $\mathbf{B}\delta$ following the dislocation reaction described in Eq. (1), leaving behind a stair-rod dislocation $\delta\alpha$ and the 90° partial $\alpha\mathbf{D}$, still on the BCD plane, as shown in Fig. 7a. Such a dislocation structure has been observed both experimentally [3,51] and by MD simulation [9,33,37], and it has been assumed to be very effective in blocking other dislocations and, consequently, causing strain hardening [9].

As shown in Fig. 7a, under a high applied stress the trailing partial $\alpha\mathbf{D}$ may be driven to the twin boundary to react with the stair-rod dislocation $\delta\alpha$:



The energy barrier for this reaction is:

$$\begin{aligned} \Delta E_{Eq44}^{\delta\alpha + \alpha\mathbf{D} \rightarrow \delta\mathbf{D}} &\approx -\frac{Ga^2}{36\pi(1-\nu)} \ln \frac{\sqrt{2}d}{a} + 0.3\tilde{E} \\ &\approx -2\hat{E} + 0.3\tilde{E} \end{aligned} \quad (45)$$

Therefore, the dislocation reaction in Eq. (44) is energetically favorable.

From the double Thompson tetrahedron $\delta\mathbf{D}$ is equivalent to $\mathbf{D}'\delta$. The latter can dissociate as:



where $\mathbf{D}'\alpha'$ can slip away on the BCD' plane in the twin. This scenario is schematically illustrated in Fig. 7b. The energy barrier for this reaction is:

$$\begin{aligned} \Delta E_{Eq46}^{\mathbf{D}'\delta \rightarrow \mathbf{D}'\alpha' + \alpha'\delta} &\approx \frac{Ga^2}{36\pi(1-\nu)} \ln \frac{\sqrt{2}d}{a} - 0.3\tilde{E} \\ &\approx 2\hat{E} - 0.3\tilde{E} \end{aligned} \quad (47)$$

This energy barrier is reasonably low for it to occur during real deformation.

Another scenario is for the stair-rod dislocation $\delta\alpha$ in Fig. 7a to further dissociate into two partial dislocations

according to Eq. (2), $\delta\alpha \rightarrow \delta\mathbf{B} + \mathbf{B}\alpha$, where the partial $\delta\mathbf{B}$ glides on the twin boundary in the opposite direction to $\mathbf{B}\delta$ to reduce the twin thickness by one atomic plane, as illustrated in Fig. 7c. Such a process can be repeated to reduce the twin, as described in Section 3.1. The energy barrier for such a reaction is about $3.5\hat{E} + 5.5\tilde{E}$, making it more difficult than the reaction in Eq. (46). The cutting of a stacking fault by a dislocation has been observed by MD simulation [36]. The de-twinning process is similar to cutting of the stacking fault, suggesting that such a scenario could happen under an appropriate applied stress.

6.2.2. Leading 30° partial $\mathbf{B}\alpha$ transmits across the twin boundary

As discussed in Section 3.2 (see Eq. (11) and Fig. 5), the 30° partial $\mathbf{B}\alpha$ may be transmitted across the twin boundary, leaving behind a large stair-rod dislocation $\alpha\alpha'$. If the trailing partial $\alpha\mathbf{D}$ remains on the BCD plane it will have a unique dislocation configuration where one stacking fault links $\alpha\alpha'$ with partial $\mathbf{B}\alpha'$, while another stacking fault links $\alpha\alpha'$ with trailing partial $\alpha\mathbf{D}$, as shown in Fig. 8a. The trailing partial $\alpha\mathbf{D}$ can also cross-slip onto the twin boundary plane, becoming a partial $\delta\mathbf{A}$ that slips to the left to increase the twin by one atomic plane (as described in Section 4.1), forming a dislocation configuration, as shown in Fig. 8b.

The trailing partial $\alpha\mathbf{D}$ can also react with the stair-rod $\alpha\alpha'$ and be transmitted across the twin boundary considering $\alpha\mathbf{D} \rightarrow \delta\mathbf{D} + \alpha\delta$ and $\alpha\alpha' \rightarrow \delta\alpha + \alpha'\delta$:



From the double Thompson tetrahedron (Fig. 4) it can be seen that $\delta\mathbf{D} = \mathbf{D}'\delta = \alpha'\delta + \mathbf{D}'\alpha'$. Therefore, Eq. (48) can be rewritten as:



The energy barrier for the reaction in Eq. (49) can be described by:

$$\Delta E_{Eq49}^{\mathbf{D}\alpha + \alpha\alpha' \rightarrow 2\alpha'\delta + \mathbf{D}'\alpha'} \approx \frac{Ga^2}{18\pi(1-\nu)} \ln \frac{\sqrt{2}d}{a} = 4\hat{E} \quad (50)$$

The dislocation reaction in Eq. (49) can release one partial ($\mathbf{D}'\alpha'$) in the twin, leaving behind a double stair-rod dislocation ($2\delta\alpha'$). However, this reaction apparently has a high energy barrier.

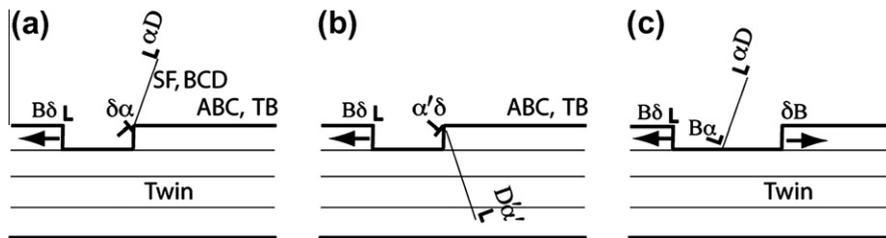


Fig. 7. Reaction of dissociated 60° dislocation \mathbf{BD} with a 30° leading partial at the twin boundary. (a) The leading partial cross-slips onto the ABC twin boundary, leaving behind a stair-rod dislocation and the 90° trailing partial still on the original BCD slip plane. (b) After the trailing partial $\alpha\mathbf{D}$ reacts with the stair-rod dislocation $\delta\alpha$ and transmits across the twin boundary (Eqs. (44) and (46)). (c) The stair-rod dislocation dissociates according to $\delta\alpha \rightarrow \delta\mathbf{B} + \mathbf{B}\alpha$ to reduce the twin by one atomic layer.

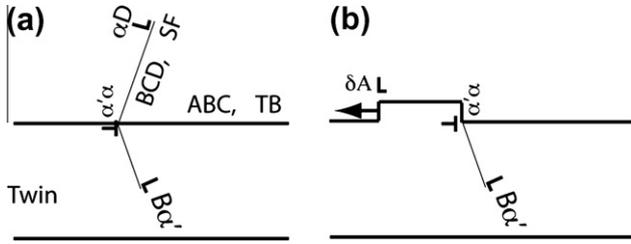


Fig. 8. (a) Dislocation configuration after the leading 30° partial $B\alpha$ transmits across the twin boundary and the trailing 90° partial αD remains on the BCD plane. (b) After the trailing partial αD cross-slips into the ABC plane to grow the twin by one atomic plane.

Similarly to Eqs. (36) and (37), δD could also dissociate according to the two equations: $\delta D = D'\delta = D'\beta' + \beta'\delta$ and $\delta D = D'\delta = D'\gamma' + \gamma'\delta$. However, the final energy barrier for such reactions will be even higher than that of the reaction in Eq. (49). Therefore, these reactions will not be described in detail here.

6.3. 90° leading partial αD reacts first at the twin boundary

If the 90° leading partial αD is the leading partial it could either cross-slip onto the twin boundary plane or transmit across the twin boundary. We will discuss these two cases below.

6.3.1. Leading 90° partial αD cross-slips onto the twin boundary plane

The leading partial αD can cross-slip to form δA , which slips on the twin boundary plane ABC as described in Section 4.1. The trailing partial $B\alpha$ can also cross-slip onto the twin boundary to form $B\delta$ on the ABC plane, following the procedure described in Section 3.1, leaving behind a stair-rod dislocation $\delta\alpha$. $B\delta$ and δA can glide together on the twin boundary with a stacking fault between them.

On the other hand, the trailing 30° partial $B\alpha$ can also be transmitted across the twin boundary to emit a partial $B\alpha'$ in the twin, as described in Section 3.2 and Fig. 5. This leaves behind a stair-rod $\alpha'\alpha$ at the twin boundary.

6.3.2. Leading 90° partial αD transmits across the twin boundary

The leading partial αD can be transmitted across the twin boundary, which is energetically not too difficult, as described in Section 4.2. With the help of Eqs. (19)–(21) in Section 4.2, which describe the dislocation reactions of $D\alpha$, the αD reactions for transmission across the twin boundary can be described by:

$$\alpha D \rightarrow \alpha\delta + \alpha'\delta + D'\alpha' \quad (51)$$

$$\alpha D \rightarrow \alpha\delta + \beta'\delta + D'\beta' \quad (52)$$

and

$$\alpha D \rightarrow \alpha\delta + \gamma'\delta + D'\gamma' \quad (53)$$

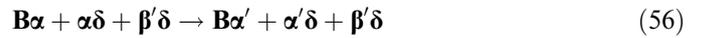
where the partial dislocations $D\alpha'$, $D'\beta'$ or $D'\gamma'$ will glide away in the twin, leaving behind two stair-rod dislocations

at the twin boundary. When the trailing partial $B\alpha$ reaches the twin boundary it can react with the stair-rod dislocation in all three cases, i.e.

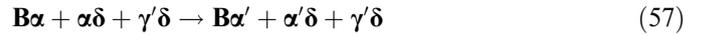


This reaction is energetically favorable with an energy reduction of $-\hat{E} - 2.0\tilde{E}$. The $B\delta$ can glide on the ABC plane, which either increases or reduces the twin thickness by one atomic plane, depending on the slip direction. The slip direction is determined by the orientation of the applied shear stress.

The trailing partial $B\alpha$ can also react with stair-rod dislocations (as shown in Eqs. (51)–(53)) at the twin boundary to release a Shockley partial dislocation in the twin:



and



At first sight the energy barrier should be 0 for the reactions in Eqs. (55)–(57) because the number of partial dislocations and stair-rod dislocations do not change. However, as described in Eqs. (23)–(25), the reacting stair-rod dislocation pairs on the left can combine to form a dislocation with lower energy, while the stair-rod dislocation pairs on the right form a dislocation with higher energy when they combine together. These energy differences can be regarded as the energy barrier, which are described by:

$$\Delta E_{Eq55} \approx \frac{23Ga^2}{486(1-\nu)} \ln \frac{\sqrt{2}d}{a} + 2.7\tilde{E} \approx 3.4\hat{E} + 2.7\tilde{E} \quad (58)$$

$$\Delta E_{Eq56,Eq57} \approx 2.8\hat{E} + 3.7\tilde{E} \quad (59)$$

Therefore, the energy barrier for the trailing 30° partial to be transmitted across the twin boundary is very high.

7. Discussion

Plausible dislocation reactions at the twin boundaries and the energy barriers associated with the reactions are listed in Table 1. It should be noted that the energy barrier is not the only factor that determines a dislocation reaction. Other factors that may play a role in the dislocation reaction include the orientation and magnitude of the applied stress, as well as the stacking fault energy of the material. If the grains are nearly randomly oriented without much texture it can be assumed that the orientation of the applied stress does not affect the global probability of which types of dislocation reaction occur.

Stacking fault energy should play a significant role in determining which types of dislocation reaction predominantly occur. Specifically, if the stacking fault energy is relatively high it will be difficult for partial dislocations to nucleate and slip, which leads to fewer interactions

Table 1

Summary of dislocation reactions at twin boundaries and their isotropic energy barriers. TB = twin boundary, which is the ABC plane.

| Reaction description | Equation | Eq.# | Isotropic energy barrier |
|----------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------|------|-------------------------------------|
| 30° Partial, Bα | | | |
| Cross-slip onto the TB | Bα → Bδ + $\delta\alpha$ | 1 | $\widehat{E} + 2.0\widetilde{E}$ |
| Stair-rod dislocation dissociation | $\delta\alpha$ → $\delta B + B\alpha$ | 2 | $3.5\widehat{E} + 5.5\widetilde{E}$ |
| Transmit across the TB | Bα → Bα' + $\alpha'\alpha$ | 11 | $2.7\widehat{E} + 4.1\widetilde{E}$ |
| 90° Partial, Dα | | | |
| Cross-slip onto the TB | Dα → Aδ | | 0 |
| Transmit across the TB | Dα → $\delta\alpha + \delta\alpha' + \alpha'D'$ | 19 | $2.0\widehat{E} + 4.0\widetilde{E}$ |
| | Dα → $\delta\alpha + \delta\beta' + \beta'D'$ | 20 | $2.0\widehat{E} + 4.0\widetilde{E}$ |
| | Dα → $\delta\alpha + \delta\gamma' + \gamma'D'$ | 21 | $2.0\widehat{E} + 4.0\widetilde{E}$ |
| | Dα → $4/9A\delta + \alpha'D'$ | 26 | $0.6\widehat{E} + 1.4\widetilde{E}$ |
| | Dα → $2/9\delta BC + \beta'D'$ | 27 | $0.1\widehat{E} + 0.2\widetilde{E}$ |
| | Dα → $2/9\delta + \gamma'D'$ | 28 | $0.1\widehat{E} + 0.2\widetilde{E}$ |
| Cross-slip of perfect screw dislocation, BC | | | |
| No dislocation reaction needed | | | 0 |
| Perfect 60° dislocation | | | |
| Cross-slip onto TB | BD → BC + CD | 32 | $6.0\widehat{E} + 7.2\widetilde{E}$ |
| Transmit across the TB | BD → 2Bδ + D'B | 38 | $4.5\widehat{E} + 7.5\widetilde{E}$ |
| | BD → $\delta C + D'A$ | 39 | $3.0\widehat{E} + 3.9\widetilde{E}$ |
| | BD → $\delta A + D'C$ | 40 | $3.0\widehat{E} + 3.9\widetilde{E}$ |
| | D'δ → D'α' + $\alpha'\delta$ | 46 | $2.0\widehat{E} - 0.3\widetilde{E}$ |
| 30° Leading partial cross-slip onto TB and trailing 90° partial transmit across TB | | | |
| 30° Leading partial transmit across TB first and the 90° trailing partial transmit cross TB second | Dα + $\alpha\alpha'$ → 2$\alpha'\delta$ + D'α', | 49 | $4.0\widehat{E}$ |
| 90° Leading partial and 30° trailing partial transmit across TB sequentially | Bα + $\alpha\delta + \alpha'\delta$ → Bα' + 2$\alpha'\delta$ | 55 | $3.4\widehat{E} + 2.7\widetilde{E}$ |
| | Bα + $\alpha\delta + \beta'\delta$ → Bα, + $\alpha'\delta + \beta'\delta$ | 56 | $2.8\widehat{E} + 3.7\widetilde{E}$ |
| | Bα + $\alpha\delta + \gamma'\delta$ → Bα' + $\alpha'\delta + \gamma'\delta$ | 57 | $2.8\widehat{E} + 3.7\widetilde{E}$ |

$$*\widehat{E} = \frac{Ga^2}{72\pi(1-\nu)} \ln \frac{\sqrt{2}d}{a}, \widetilde{E} = \frac{Ga^2}{72\pi(1-\nu)}$$

between individual partials and twin boundaries. In addition, a higher stacking fault energy makes it easier for a dissociated perfect dislocation to constrict at the twin boundary before the leading partial reacts at the twin boundary. This is especially significant for perfect screw dislocations, which, once constricted, can cross-slip into the twin boundary plane or be transmitted across the twin boundary to glide on a slip plane in the twin, without any dislocation reaction.

If the stacking fault energy is very low partial dislocations can be emitted in large numbers from grain boundaries and other sources [52,53]. These partials can cross-slip into the twin boundaries with small energy barriers (see Table 1), which generate steps on the twin boundaries. It can also be seen from Table 1 that the energy barriers for 90° partials to be transmitted across twin boundaries are much lower than the energy barrier for 30° partials to be transmitted across a twin boundary. In addition, a low stacking fault energy makes it difficult for a dissociated perfect dislocation to constrict. This could produce a scenario in which the leading partial cross-slipped into the twin boundary plane or was transmitted across the twin boundary, while the trailing partial remains on the original slip plane in the matrix. Such a dislocation structure is believed to be effective in improving the work hardening rate [9].

8. Summary

In this paper we have systematically described the plausible dislocation reactions at twin boundaries. Such reactions and subsequent dislocation slips determine how the twins affect the deformation behavior of nanocrystalline fcc metals. Plausible dislocation reactions and the energy barriers associated with the reactions are listed in Table 1. It should be noted that the equations used to calculate the dislocation elastic energies are based on isotropic elasticity. Therefore, the energy barriers listed in Table 1 are isotropic energy barriers. The energy barrier determines the feasibility of a dislocation reaction. A lower energy barrier indicates that the reaction is statistically more likely to occur. However, other factors, including the orientation and magnitude of the applied stress and the stacking fault energy also play important roles. It should be noted that most of the dislocation–twin reactions described in this paper may not occur in coarse grained fcc metals and alloys because of their requirement of high applied stresses to overcome the energy barriers.

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