Formation mechanism of fivefold deformation twins in nanocrystalline face-centered-cubic metals

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Fivefold deformation twins have been recently observed in nanocrystalline face-centered-cubic (fcc) metals and alloys synthesized by severe plastic deformation techniques. However, numerous molecular dynamics simulations in the literature have not observed fivefold deformation twins in nanocrystalline fcc metals. The discrepancy between experimental observations and molecular dynamics simulations has raised an issue on their formation mechanism and conditions. Here we propose a sequential twinning mechanism that provides a clear path for the formation of fivefold deformation twins. The mechanism requires an orientation change of applied stresses, which explains why molecular dynamics simulations under a constant load orientation do not produce fivefold deformation twins. © 2005 American Institute of Physics. [DOI: 10.1063/1.1879111]

Recently, fivefold deformation twins (DTs) have been observed in nanocrystalline (nc) face-centered-cubic (fcc) metals and alloys synthesized by severe plastic deformation techniques such as ball-milling1–3 and high pressure torsion (HPT).4,5 They are usually observed in grains with diameters of ~20 nm or smaller, indicating a grain size effect in their formation. However, their formation mechanism has been an unsolved puzzle.

Because the fivefold DTs were formed via plastic deformation, they should have been formed by a dislocation mechanism. Both molecular dynamics (MD) simulations6–13 and experimental observations14–17 indicate that partial dislocation emission from grain boundaries (GBs) becomes a major deformation mechanism in nc materials. Surprisingly, fivefold DTs have never been predicted by MD simulations6–13. This discrepancy between experiments and simulations raises two questions about the fivefold DTs: (1) What is their formation mechanism? (2) Why are they observed experimentally but not in molecular dynamics simulations? In other words, what are the conditions required for their formation?

We propose a mechanism of sequential twinning via emissions of Shockley partials from GBs and twin boundaries. The first step of this mechanism is the formation of a simple twin with twin domains I and II (Fig. 1) via partial dislocation emissions from GBs.7 As shown, the twinning plane is parallel to a (111) plane. Once a twin is nucleated, it can grow via the emission of more twinning partials.18,19 The twin described in Fig. 1 is seen ubiquitously in HPT-processed nc copper.3

The second step starts with the emission of a 90° partial, \( b_1 = 1/6[112], \) from the upper GB in domain II. The partial glides on a (111) plane toward the twin boundary TB1 (Fig. 1). For convenience, in the following discussion we assume that partial dislocation lines in all twinning steps are parallel to the [110] direction (Fig. 1). This assumption does not affect the proposed twinning process. A 90° partial has a Burgers vector perpendicular to the dislocation line.

A DT can be described by the twin plane \( K_1 \), shear direction \( \eta_1 \), undistorted plane \( K_2 \), and direction \( \eta_2 \). \( \eta_1 \) lies along the line of \( K_2 \) and the shear plane, which is normal to \( K_2 \) and contains \( \eta_1 \).6–10 DTs in a fcc metal is of compound type, in which a twin formed by partials with Burgers vectors parallel to \( \eta_1 \) gliding on \( K_1 \) is the same as a twin formed by partials with Burgers vectors parallel to \( \eta_2 \) gliding on \( K_2 \). In Fig. 1, we can regard \( K_1 \) and \( K_2 \) as (111) and (111) slip planes, respectively. \( \eta_1 \) is parallel to \( b_1 \), and \( \eta_2 \) is parallel to another 90° partial \( b_2 = 1/6[112] \). In other words, when a 90° partial \( b_1 \) reaches the twin boundary TB1, it becomes equivalent to another 90° partial \( b_2 \) on the (111) plane. Under an appropriate external shear stress, the \( b_2 \) partial could glide to the left, which consequently moves the twin boundary downward by one atomic plane.

FIG. 1. Illustration of a regular twin (step 1). The open and filled circles represent atoms from two adjacent [110] planes, respectively.

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Once the Trst partial is emitted under a high shear stress, which creates a stacking fault, it requires much less stress to activate another partial on an adjacent plane to nucleate a twin and to grow it via a stress-controlled twin growth mechanism. When a series of partials with a Burgers vector \( b_1 \) emit from the GB successively on adjacent (111) planes, with each \( b_1 \) partial converting to a \( b_2 \) partial that glides to the left, a twin domain III will form, which effectively converts the regular twin in Fig. 1 into a threefold twin as shown in Fig. 2(a). An incoherent twin boundary, TB3, is also formed. Indeed, threefold deformation twins with morphology similar to that shown in Fig. 2(a) is observed in the HPT-processed copper [Fig. 2(b)], demonstrating that the above discussed twinning process did occur.

A threefold DT can be transformed into a fourfold DT via the emissions of a series of 90° partials from a GB in domain I or III (step 3). Assuming that a 90° partial \( b_3 \) Trst emits from a point on a GB in domain I (see Fig. 2) and moves toward the twin boundary TB3, a stacking fault will form, and a twin will nucleate and grow on both side of the stacking fault via the stress-controlled twin growth mechanism, resulting in a new twin domain IV (Fig. 3). An example of such fourfold twin in HPT-processed copper is shown in Fig. 3(b).

Note that in the above process, when a partial \( b_3 \) reaches twin boundary TB3, it becomes equivalent to an edge dislocation in the displacement shift complete (DSC) lattice with a Burgers vector parallel to the twin boundary. The importance of this edge dislocation in the DSC lattice will be revealed later.

The fourfold deformation twin can be transformed into a \( \chi \)vefold deformation twin (step 4) by emitting another series of partials \( b_4 \) from GBs in twin domain III [Fig. 3(a)], following the same process as the formation of twin domain IV. When a partial with a Burgers vector \( b_4 \) reaches the twin boundary TB3, it forms an edge dislocation in the DSC lattice, with a Burgers vector opposite to the Burgers vector of the edge dislocation previously formed by a \( b_3 \) partial in the DSC lattice. Therefore, these two types of edge dislocations will cancel each other, which converts TB3 into a coherent twin boundary. In addition, another coherent twin boundary, TB5, is also formed, which transforms the fourfold twin into a \( \chi \)vefold twin. It is also possible that the \( b_3 \) and \( b_4 \) partials are activated simultaneously, directly transforming a threefold DT into a \( \chi \)vefold DT.

In the above analysis, we have assumed that the partials, \( b_3 \) and \( b_4 \), are emitted from GBs. It is also possible for these partials to emit from the twin boundary TB3. Specifically, once a threefold twin is formed [Fig. 2(a)], the threefold node could emit a 90° partial, \( b_4 \), into domain I, under an applied external shear stress. The atoms along the threefold node should have higher energy than those on a normal twin boundary. This higher energy lowers the energy barrier for partial emission. Once a stacking fault is generated by the Trst partial from the threefold node, a twin could easily nucleate and grow via successive emission of partials from the twin boundary TB3, forming a twin domain IV. Note that...
the emission of a \( \mathbf{b}_3 \) partial will leave a \( \mathbf{b}_3 \) partial on the twin boundary. This \( \mathbf{b}_3 \) partial is also equivalent to an edge dislocation in the DSC lattice. In other words, the threefold twin can be transformed into a fourfold twin and a \( \mathbf{b}_3 \) partial by emission of partials from the twin boundary TB3, in a way similar to partial emission from GBs discussed earlier. Moreover, the higher energy and stress incompatibility at the threefold or fourfold node provide additional driving force for the emission of the \( \mathbf{b}_3 \) partial. Therefore, the probability of transforming a threefold twin into a fourfold and \( \mathbf{b}_3 \) partial via the partial emission from twin boundaries should be significant.

Note that the above ideal twinning process would leave a \( 7.33^\circ \) gap [see the angle between the two dashed lines in Fig. 4(a)]. This is because the angle between two \( <111> \) planes in a fcc metal is \( 70.53^\circ \), which is 1.47° smaller than the 72° that is required to cover 360° by \( \mathbf{b}_3 \) twins. This angle is accommodated by elastic strain.\(^{22,23}\) Figure 4(b) shows a \( \mathbf{b}_3 \) partial in HPT-processed copper. Lattice distortion from elastic strain can be clearly seen near twin boundaries.

In addition to high external shear stress discussed above, another critical requirement for forming a \( \mathbf{b}_3 \) partial in HPT-processed copper is variation in stress orientation. The mechanism discussed above requires several sets of 90° partials with various orientations and glide directions to be activated sequentially, which can only be realized under varying stress orientations. Ball-milling provides both high stress and rapid change in stress orientation. HPT applies both compressive stresses in the thickness direction and pure shear stress in the tangential direction of a sample disk. Both of these two processes can satisfy the above two requirements and have produced \( \mathbf{b}_3 \) partials in nc-fcc metals.\(^{1-3}\) However, MD simulations are mostly performed by assuming a uniaxial stress, which is why no \( \mathbf{b}_3 \) partial is predicted.\(^{6-13}\)

Note that \( \mathbf{b}_3 \) partials in electrodeposited nickel have been previously proposed to form by sequential twinning.\(^ {22}\) However, no detailed dislocation mechanism was given. In this letter, we have described a detailed mechanism that involves partial dislocation emissions from grain and twin boundaries. Such a mechanism requires both high external stress and stress orientation variation to form \( \mathbf{b}_3 \) partials, which explains why \( \mathbf{b}_3 \) partial deformation twins are observed under some experimental conditions such as ball milling and HPT, but not under uniaxial stress conditions used in most MD simulations.

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