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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-milling[1–3] 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) simulations[6–13] and experimental observations[4,5,14–17] 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 simulations.[6–13] 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.[4] 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.[4]

The second step starts with the emission of a 90° partial, $\mathbf{b_1}=1/6[11\bar{2}]$, from the upper GB in domain II. The partial glides on a $(11\bar{1})$ 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 $[1\bar{1}0]$ 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 defined by the twin plane K_1, shear direction η_1, undistorted plane K_2, and direction η_2. η_2 lies along the line of K_2 and the shear plane, which is normal to K_1 and contains η_1.[20] DTs in a fcc metal is of compound type, in which a twin formed by 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 Fig. 1, we can regard K_1 and K_2 as $(11\bar{1})$ and (111) slip planes, respectively. η_1 is parallel to $\mathbf{b_1}$, and η_2 is parallel to another 90° partial $\mathbf{b_2}=1/6[11\bar{2}]$. In other words, when a 90° partial $\mathbf{b_1}$ reaches the twin boundary TB1, it becomes equivalent to another 90° partial $\mathbf{b_2}$ on the (111) plane. Under an appropriate external shear stress, the $\mathbf{b_2}$ partial could glide to the left, which consequently moves the twin boundary downward by one atomic plane.
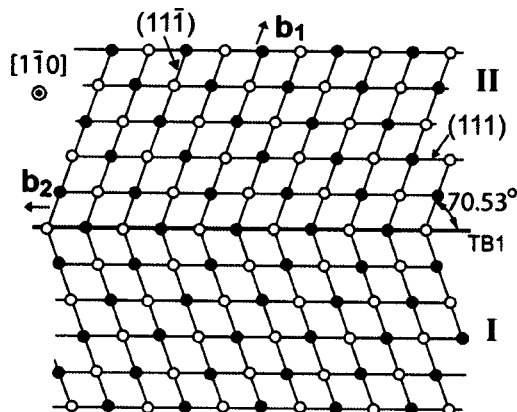

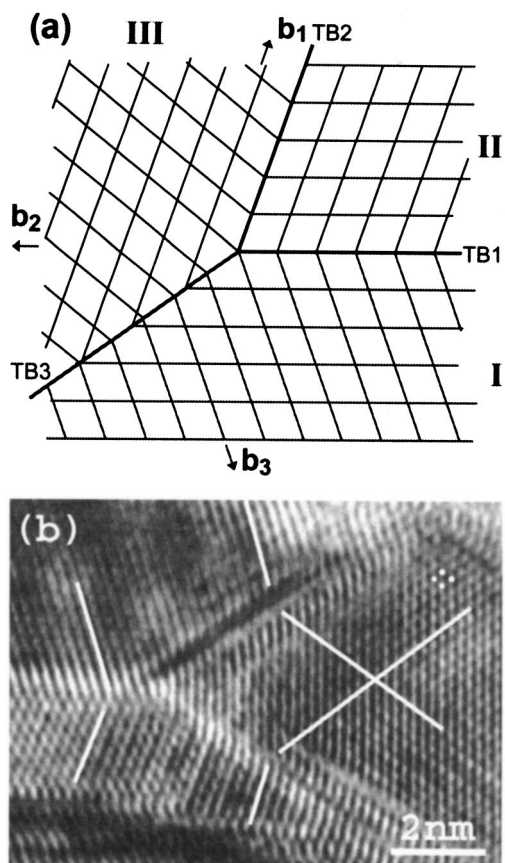FIG. 1. Illustration of a regular twin (step 1). The open and filled circles represent atoms from two adjacent $(1\bar{1}0)$ planes, respectively.

FIG. 2. (a) Illustration of a threefold deformation twin (step 2) formed by the emission of a series of 90° partials, b_1. These partials form new 90° partials with a Burgers vector b_2 on the twin boundary TB1, which glides away from TB1, forming a new twin boundary TB3; (b) HRTEM image showing a threefold twin in HPT-processed nc copper.

FIG. 3. (a) Illustration of a fourfold deformation twin (step 3) formed from a threefold deformation twin by emitting a series of 90° partials, b_3; (b) HRTEM image showing a fourfold deformation twin in HPT-processed nc copper.

Once the first 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.[19] When a series of partials with a Burgers vector b_1 emit from the GB successively on adjacent $(11\bar{1})$ 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 first 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.[21]
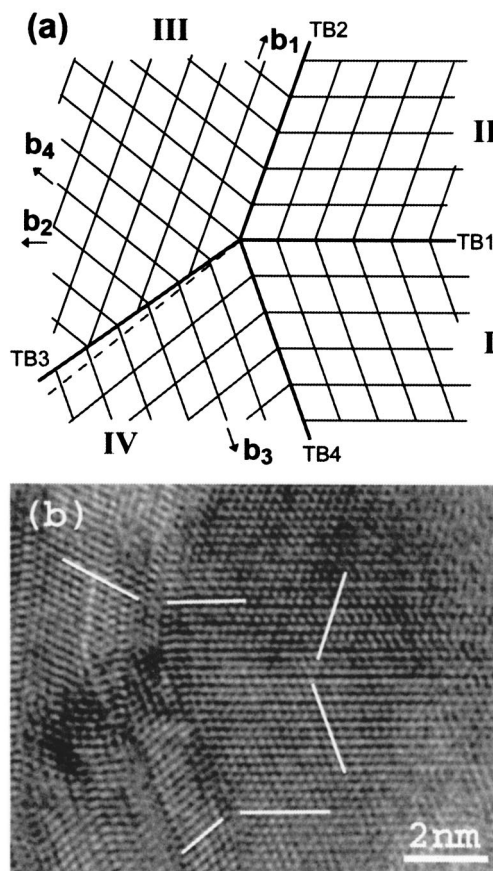
The importance of this edge dislocation in the DSC lattice will be revealed later.

The fourfold deformation twin can be transformed into a fivefold 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 fivefold twin. It is also possible that the b_3 and b_4 partials are activated simultaneously, directly transforming a threefold DT into a fivefold 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_3, 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 first 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
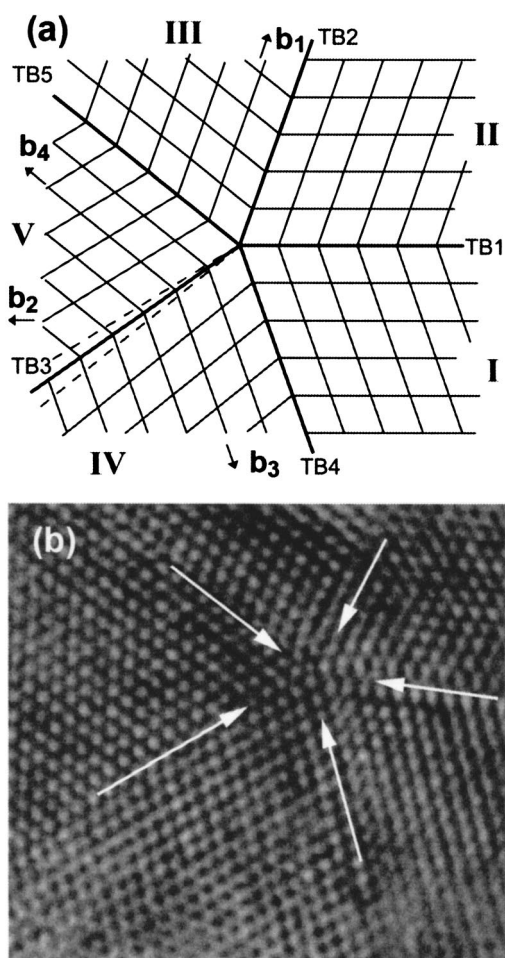
FIG. 4. (a) Image of a fivefold deformation twin (step 4) formed from a fourfold deformation twin by emitting a series of 90° partials, b_4. The dotted lines form an angle of 7.33°, which must be accommodated by elastic strain; (b) HRTEM image showing a fivefold deformation twin in HPT-processed nc-copper. The white lines mark the twin boundaries.

the emission of a b_3 partial will leave a $-b_3$ partial on the twin boundary. This $-b_3$ 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 fivefold twin 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 first partial. Therefore, the probability of transforming a threefold twin into a fourfold and fivefold twin via the partial emission from twin boundaries should be significant.

Note that the above ideal twinning process would leave a 7.33° 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°, which is 1.47° smaller than the 72° that is required to cover 360° by five twins. This angle is accommodated by elastic strain.[22,23] Figure 4(b) shows a fivefold DT 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 fivefold DT 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 fivefold DTs in nc-fcc metals.[1–5] However, MD simulations are mostly performed by assuming a uniaxial stress, which is why no fivefold DT is predicted.[6–13]

Note that fivefold DTs 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 fivefold DTs, which explains why fivefold 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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