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ScienceDirect
Scripta Materialia 64 (2011) 852–855
Scripta MATERIALIA
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Twinning mechanism via synchronized activation of partial dislocations in face-centered-cubic materials

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Received 25 October 2010; revised 11 January 2011; accepted 11 January 2011
Available online 14 January 2011

In situ straining in a high-resolution transmission electron microscope and molecular dynamics simulations reveal a new deformation twinning mechanism in the face-centered-cubic structure. A twin forms via the simultaneous and cooperative activation of different Shockley partial dislocations on three (1 1 1) layers. The synchronized slip produces a zero net Burgers vector; such twinning relieves local stress concentration in a shear confined to adjacent atomic layers, but induces no macroscopic shape change of the surrounding crystal.

Keywords: Twinning; Deformation structure; Partial dislocation; FCC metals

Twinning is a common and important deformation mode for the plasticity of materials [1,2]. Traditionally, twinning is believed to occur via a pole mechanism [3], where a screw dislocation pole allows layer-by-layer shearing, mediated by the successive slip of twinning dislocations (TDs) on atomically adjacent parallel planes. For face-centered-cubic (fcc) metals and alloys, the TDs are the Shockley partial dislocations on the close-packed {1 1 1} planes. For nanostructured (NS) grains, such partials can become more favorable than full dislocations, and can be emitted from grain boundaries (GBs) [4–11], instead of from poles in the interior of grains. The partials are generally described as having the same Burgers vector (BV), each gliding on a {1 1 1} plane, one at a time and one after another. This mechanism of 'monotonic activation of partials' (MAP) dictates a large twinning shear (0.707), and a 141° angle between the twinned lattice and the matrix lattice that are in mirror symmetry across the twin boundary (TB) [9,10].

However, in deformed samples such a large twinning strain is not always observed. For example, in deformed NS fcc metals only a small fraction of the grains actually show the expected shape change consistent with the crystallographic relationships above. The majority of the grains, instead, experienced much less and often no obvious global shear strain, despite the formation of many microtwins [9]. Very thin micro-twins are also observed to rapidly penetrate into the lattice but stop in the lattice interior without changing the grain shape (see below). What, then, is the mechanism at play that generates twins but produces little macroscopic strains? Must the partials move one at a time consecutively? How exactly the partials mediate twinning has broad implications for the deformation response and structural evolution in fcc materials.

A hypothesis has been put forward, invoking the random activation of partials (the RAP hypothesis [9]). When all three possible types of Shockley partial dislocations (see the three BVs, $\mathbf{b_1}$, $\mathbf{b_2}$ and $\mathbf{b_3}$, in Figure 1f) are activated separately but in equal numbers, each independently with a BV of either $\mathbf{b_1}$, $\mathbf{b_2}$ or $\mathbf{b_3}$, the net macrostrain across the entire grain becomes zero. The partials may be promoted layer-by-layer through reactions and cross-slip [10]. Also, an array of mixed Shockley partials (different BVs) can be pre-existing at the end (incoherent twin boundary, ITB) of a growth twin, or form steps or disconnections at the TB with step heights of a few (1 1 1) interplanar distances [11–15]. In

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doi:10.1016/j.scriptamat.2011.01.016

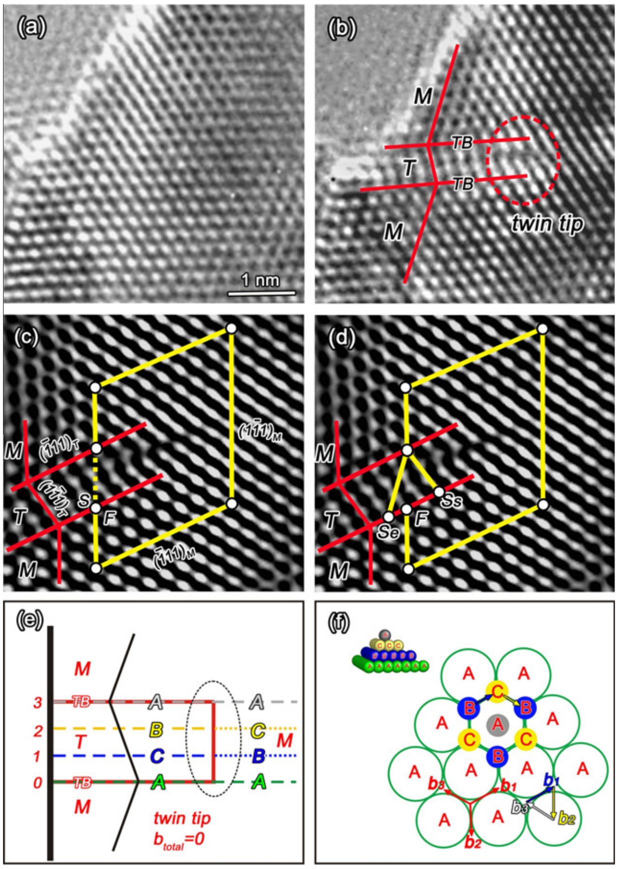

Figure 1. In situ TEM observation ([1 1 0] zone axis) of twinning in NS-Ni (grain size ~20 nm; for sample preparation, see Ref. [19]). (a) A HRTEM image of a crack tip. (b) After tensile loading, a three-layer microtwin nucleated from the crack tip, and the twin tip (enclosed by the dotted circle) stopped in the grain interior. (c) A Fourier-filtered image of the twin (T), with a Burgers circuit drawn around the twin tip along the $(1\,\bar{1}\,1)_M$ and $(\bar{1}\,1\,1)_M$ matrix (M) lattice fringes, showing circuit closure with $\boldsymbol{F}$ meeting $\boldsymbol{S}$. To avoid the influence of the crack during filtering, a rotation of ~26° angle is involved relative to the orientation in (b). In (d), two Burgers circuits are drawn following Howe et al. [16]: the magnitude of the closure failure vector $\overline{FSe}$, one lattice spacing, indicates the circuit encloses one 90° partial dislocation, whereas that (two lattice spacing) of the vector $\overline{FSs}$ indicates the circuit encloses two 30° partials [16]. (e) Schematic illustration of partials emitting from the left GB/free surface and stopped in the grain interior, converting the matrix (...ABCABC...) into a three-layer twin (...ACBABC...) with zero net BV at the tip. (f) The stacking sequence (inset), the three possible Shockley partials (summing up to zero, see the closed vector triangle), and the layer slips involved in the three-layer twinning process.

particular, using molecular dynamics (MD) simulations Wang et al. [13,14] have described a specific type of ITB composed of pre-existing Shockley partials with a particular $\mathbf{b}_2$, $\mathbf{b}_1$, $\mathbf{b}_3$ triplet unit, and a zero net BV in one unit. In this case, the motion of such steps/ends can cause detwinning, accomplished by the dissociation of the ITB via a move–drag mechanism. Specifically, under stress the middle partial moves out first in one direction whereas the other two move in the other direction. The movement stops when the stress diminishes due to the relaxation associated with the dislocation motion; the three partials are then pulled to align together due to their interactions. The repeated stop/start mechanism results in detwinning [13,14].

However, for microtwin nucleation under stress as that shown in Figure 1, there is no pre-existing growth twin, nor the particular aligned triplet partials. The formation of the three-layer twin lattice is accomplished by a single action all at once, as seen in the in situ observations in Figures 1 and 2. In these homogeneous lattices it is not understood how all the three partials, $\mathbf{b}_1$, $\mathbf{b}_2$ and $\mathbf{b}_3$, can be activated all at once in a single shear (e.g. in Figure 1, $\mathbf{b}_3$ is in the opposite direction to $\mathbf{b}_1 + \mathbf{b}_2$) [9,13,14]. For example, Figure 1 shows a three-layer twin nucleating and propagating in fcc Ni, in the region in front of a crack tip with no pre-existing growth twins. This in situ transmission electron microscopy (TEM) observation reveals the emission and rapid propagation of a bundle of partials starting from the edge of the sample. The newly formed microtwin consists of only three atomic layers. Interestingly, the twin tip exhibits a zero net BV, as revealed by the Burgers circuit with no closure failure drawn in Figure 1. This circuit is drawn in such a way that the twin is treated as if it were a single stacking fault. For the twin formation, multiple partial dislocations are expected to be involved. To identify what kind of partials are actually involved, the method developed by Howe [16] was applied, as illustrated in Figure 1 and its caption. The closure failures of the two separately drawn Burgers circuits indicate the presence of two 30° and one 90° Shockley partials. This suggests the presence of all three types of Shockley partials, summing up to a zero net BV ($\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3 = 0$).

A second example is presented for another fcc metal Cu in Figure 2 (for sample details, see Ref. [11]). In this case, the twinning process occurred inside a grain far away from the crack, and the stress was applied in-plane during straining inside the electron microscope. The in situ observation reveals that a bundle of partials was emitted from the corner of an existing twin, and the twin tip propagated over a large distance, penetrating deep into the surrounding virgin lattice. Again, Burgers circuits have been drawn in Figure 2 following Howe [16]. As explained in the figure caption, the circuits reveal the presence of two 30° and one 90° Shockley partials, and a net BV of zero. The TEM movies did not show any other dislocations leaving or interacting with the twin. In the literature, zero-BV steps that mediate twin widening have also been seen in Al [17] and in a CuTi alloy [18].

We emphasize that the zero-sum process here is confined to the scale of three atomic layers in a single bundle of partials. This is very different from the hypothesis of individual partials activated randomly in equal numbers of $\mathbf{b}_1$, $\mathbf{b}_2$ and $\mathbf{b}_3$ across the grain to produce a zero net macrostrain (the RAP hypothesis [9]). In the following we illustrate a new TB migration (for twin growth and detwinning) mechanism, based on these in situ TEM observations as well as insight from MD simulations (see below). This mechanism involves cooperatively activated partials (CAP). Specifically, this particular CAP process entails synchronized activation of partials (SAP), i.e. the simultaneous activation of three (e.g. $\mathbf{b}_1$, $\mathbf{b}_2$ and $\mathbf{b}_3$) Shockley partials with different BVs, for coordinated slip on adjacent {1 1 1} layers. The