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Deformation Twinning Mechanisms in FCC and HCP Metals

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ABSTRACT

We report the recent work on twinning and detwinning in fcc and hcp metals based on the *in situ* and *ex situ* TEM observations and molecular dynamics simulations. Three aspects are discussed in this paper. (1) Detwinning in single-phase Cu with respect to growth twins, (2) deformation twinning in Ag-Cu composites, and (3) deformation twinning mechanisms in hcp metals. The main conclusion is that atomic structures of interfaces (twin boundaries, two-phases interface, and grain boundaries) play a crucial role in nucleating and propagating of deformation twins.

Key Words: twinning; de-twinning, interfaces; fcc; hcp

1. INTRODUCTION

Crystal twinning results in an intergrowth of two separate crystals in a variety of specific configurations (in a symmetrical manner). A twin boundary separates the two crystals. There are three modes of formation of twinned crystals, growth twins, annealing or transformation twins, and deformation or gliding twins. Growth twins are the result of an interruption or change in the lattice during formation or growth, which could be kinetically stabilized during growing for materials with even high stacking fault energy and/or energetically stabilized during growing for materials with low stacking fault energy. Deformation twinning is a typical deformation mechanism, corresponding to the glide of twinning dislocations. Deformation twinning is difficult in single-phase fcc (such as Cu) metals due to the availability of multiple slip systems that are much easier to activate, thus usually requires extreme conditions, such as shock and/or cryogenic temperatures, which generate the large stresses required to nucleate twins via pole mechanisms or dislocation dissociations. However, deformation twinning in hcp metals, i.e. twin propagation and growth are very common and important deformation mechanisms and are responsible for the hardening and texture evolution characteristic of hcp metals and alloys subjected to plastic deformation. But differing from cubic crystals, the nucleation of deformation twins in hcp metals is less of understanding.

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In this paper, we will discuss (1) de-twinning in single-phase Cu with respect to growth twins, (2) deformation twinning in Ag-Cu composites, and (3) deformation twinning in hcp metals.

2. TWINNING AND DETWINNING IN FCC METALS

The presence of twin boundaries causes the change of crystal orientations across the interface, resulting in the discontinuity of slip systems across twin boundaries, thereby strengthening materials. Recently, introducing coherent twin boundaries has attracted more attention in enhancing mechanical strength of materials. Naturally, incoherent twin boundaries will form accompanying with coherent twin boundaries. For example, $\Sigma3\{112\}$ incoherent twin boundary are often observed in nanotwinned Cu films [1].

We reported the atomistic structure of the incoherent twin boundary (ITB) in Cu by HRTEM and by molecular statics modeling [1]. The HRTEM micrograph of $\Sigma3\{112\}$ ITBs reveals that the atomic structure of $\{112\}$ ITBs has a regular repeatable pattern with a unit containing three $\{111\}$ planes. Using topological analysis and atomistic simulations, we showed that $\Sigma3\{112\}$ ITBs can be presented with a set of Shockley partial dislocations with a repeatable sequence b_2:b_1:b_3 on every (111) plane. This repeatable unit involves three adjacent $\{111\}$ planes, in good agreement with HRTEM micrograph. b_1 is equal to $\frac{1}{6}[11\bar{2}]$, a pure edge partial dislocation; b_2 and b_3 are equal to $\frac{1}{6}[\bar{2}11]$ and $\frac{1}{6}[1\bar{2}1]$, respectively, both of which are mixed partial dislocations with opposite sign of screw components. A noteworthy characteristic of the three partial dislocations is that the sum of their Burgers vectors in one unit equals to zero [2].

Using atomistic simulation, we further studied the mechanical response of ITBs. Atomistic simulations revealed that (1) ITBs can dissociated into two grain boundaries bounding with a 9R phase, which contain different arraies and numbers of Shockley partial dislocations; (2) the splitting distance is determined by stacking fault formation energy, the lower energy the wider distance; (3) for fcc metals with low stacking fault energy, the phase boundary (between 9R phase with fcc matrix phase) migrates under shear stresses parallel to ITBs, resulting in the increase in the splitting distance [3]; (4) as a consequence of the propagation of 9R phase, the both phase boundaries will migrate to reduce the system energy due to the high energy 9R phase, corresponding to migration of ITBs which is so-called detwinning [2]. (5) for fcc with high stacking energy, ITBs experience the coupled motion with sliding and migration. Correspondingly, (6) we interpolated the kinetics process in terms of the glide of grain boundary disconnection (GBD) with Burgers vector $2/3[111]\{112\}$; (7) the gliding mechanism of GBD is explored using topological model and examined with MD, showing that atoms in GB experience shuffles [3].

3. INTERFACE-FACILITATED TWINNING IN Ag-Cu COMPOSITES

Since twins are difficult in single-phase Cu, the present work alternatively considers a two-phase Ag-Cu composite and the role of the Ag-Cu interface in

facilitating extensive deformation twinning in Cu during room temperature, low strain-rate loading conditions. In this way, twins in Ag can provide an ample supply of twinning partials to Cu to support and sustain twin growth in Cu during deformation.

Ag-Cu eutectic-layered composites are synthesized via a flux-melting technique (an Ag-Cu composite of eutectic composition: 60-40 at% Ag-Cu) and then rolled. Individual Ag and Cu layer thicknesses lay within the submicron regime before and after rolling. After rolling, X-ray diffraction texture results revealed the formation of a brass-type texture for both the Ag and Cu phases, suggesting deformation twinning in both phases [4]. We hypothesize that twinning partials in Cu are either transmitted across or directly nucleated from the Ag-Cu interface. TEM-based analyses show that (1) the Ag and Cu crystals maintain a cube-on-cube orientation relationship, (2) the interface habit plane reorients from (111) to (020) and (3) fine twins are present in both Ag and Cu. The most intriguing result is the reorientation of the interface plane normal from (111) to (020) while maintaining the cube-on-cube orientation relationship. A purely crystallographic argument shows that this result can only arise when both adjoining layers twin completely. The topological analysis demonstrates that the shared (111) interface plane will reorient to (020) should the neighboring Ag and Cu crystals both twin by the same twin variant [5]. MD simulations reveal that this 'ideal' Ag-Cu interface allows transmission of twinning partials from the Ag phase into the Cu phase. In agreement with the crystallographic analyses, the transmission event is seen to reorient the interface plane from the initial {111} plane to a {100} plane. As a consequence, the proposed twin nucleation and growth processes transform the interface plane and slightly misorient the neighboring Ag and Cu crystals by creating an array of closely spaced disconnections (residual dislocations) with a relatively small Burgers vector (compared to a twinning partial). In actuality, the interface will not sustain such a finely distributed array of residual defects, as it will be driven to recover coherency over large portions of its area. Provided with thermal and/or mechanical energy, these tiny interfacial steps must eventually 'migrate' in order to rearrange and combine with the intrinsic misfit dislocations already present at the interface. These processes result in the fine twins that appeared in the Ag and Cu layers in connection with the (010) interfaces in the deformed material [5].

4. TWINNING AT GRAIN BOUNDARY IN HCP METALS

Using a topological analysis, molecular static/dynamics (MS/MD), and density functional theory (DFT), we studied twin nucleation in HCP Mg, Zr and Zn [6, 7]. The results show that a twin nucleus must consist of at least 6 atomic layers for it to be stable and that a single twinning dislocation cannot glide alone in a perfect HCP crystal, but only on a pre-existing twin boundary plane. The important conclusions from these studies are: 1) the pole mechanism for twin nucleation is not feasible for HCP metals; and 2) twin nucleation is energetically unlikely to occur inside the grain because it involves a zonal dislocation with a large Burgers vector, supported by extensive experimental Electron Back Scattering Diffraction (EBSD).

This result led us to examine the atomic structure of symmetrical tilt grain boundaries (STGBs), and study dislocation-GB interactions using MD [7]. The important finding from the MS simulation is that for tilt angles, θ, greater than 28°, STGBs of Mg can be characterized as a low energy coherent boundaries plus an array of grain boundary dislocations (GBDs). The Burgers vectors of the GBDs within STGBs are large in comparison to an <a> lattice dislocation, and can potentially dissociate into twinning partials to produce a twin nucleus. For a 17° STGB, MD simulations show that the leading dislocation in a pile up reacts with the GB and nucleates a few small $(\bar{1}012)$ twin embryos, which coalesce with time to form a sizable and stable twin nucleus [7]. These results demonstrate that: 1) twins can nucleate from grain boundaries; 2) the grain boundary misorientation, by way of its atomic structure, has a significant influence on the mechanism for twin nucleation; and 3) pile-ups constitute a plausible nucleation-triggering mechanism.

5. CONCLUSIONS

Coupling atomistic simulations with TEM observations, we discussed twinning and de-twinning mechanisms in fcc and hcp metals, as well as their composites. The main conclusion is that atomic structures of interfaces (twin boundaries, two-phases interface, and grain boundaries) play a crucial role in propagating and nucleating of deformation twins.

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