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Deformation Twinning in Nanocrystalline Metals

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Deformation twins have been oberved in nanocrystalline Al processed by cryogenic ball-milling and in nanocrystalline Cu processed by high-pressure torsion at a very low strain rate. They were formed by partial dislocations emitted from grain boundaries. This paper first reviews experimental evidences and atomistic simulation results on deformation twinning and partial dislocation emissions from grain boundaries and then discusses recent analytical models on the nucleation and growth of deformation twins. These models are compared with experimental results to establish their validity and limitations.

Keywords deformation twinning, growth, models, nanomaterials, nucleation, stacking faults

1. Introduction

Nanocrystalline materials have been reported to have superior mechanical properties such as high strength, which can coexist with very good ductility (Ref 1-3). These superior mechanical properties are attributed to their unique deformation mechanisms, which are fundamentally different from those in their coarse-grained (CG) counterparts (Ref 4-8). Some deformation mechanisms, e.g., partial dislocation emission from grain boundaries, homogeneous nucleation of twins inside grain interiors, heterogeneous twin nucleation on grain boundaries, and twin lamellae formed via the splitting and migration of grain boundaries, have been predicted to operate in nanocrystalline face-centered-cubic (fcc) metals by molecular-dynamics simulations (Ref 7) and have been experimentally observed (Ref 9-13). In this paper, a review of deformation twinning and partial dislocation emissions from grain boundaries is provided. The paper concludes with a discussion of recent analytical models of the nucleation and growth of deformation twins.

2. Molecular Dynamics Simulations and Experimental Observations

Understanding of the deformation mechanisms in nanocrystalline metals was largely influenced by the results of atomistic simulations (Ref 4, 6, 7, 14-16). Such simulations predict nanocrystalline metals will deform via grain boundary sliding and rotation at very fine grain sizes (e.g., 3-10 nm) (Ref 4, 14). The grain boundary sliding and rotation were experimentally verified in nanocrystalline gold (Ref 17) and nickel (Ref 18).

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Molecular dynamics simulations also predict that partial dislocation emission from grain boundaries (Ref 7, 14) is a major deformation mechanism in grains with diameters in the range of several tens of nanometers. The activation of partial dislocations provides a critical precondition for the formation of deformation twins. Figure 1 is a high-resolution electron micrograph that shows direct evidence of partial dislocation emission from grain boundaries in nanocrystalline Cu processed by high-pressure torsion (Ref 12). As shown, there is only one twin boundary at the upper part of Fig. 1 that divides twin domains I and II. However, there are high densities of microtwins and stacking faults at the lower part of domain II. These microtwins and stacking faults do not pass across the whole grain but stop in the grain interior with Shockley partial dislocations located at the fronts of the microtwins and stacking faults. It is obvious that these twins and stacking faults were formed by partial dislocations emitted from the lower grain boundary segment. As will be discussed later, the microtwins shown in Fig. 1 were formed by heterogeneous twinning.

Deformation twins have been predicted by molecular dynamics simulations in nanocrystalline Al (Ref 7, 15), Ni (Ref 6, 14), and Cu (Ref 19). Three twinning mechanisms were predicted (Ref 7): (a) homogeneous twinning inside nanosized grains by coincidental overlapping of wide stacking fault ribbons (the stacking fault ribbons were formed by dissociated lattice dislocations, and become very wide as a result of the effect of small grain size as well as external stress (Ref 20); (b) heterogeneous twinning from the grain boundaries; and (c) twinning by grain boundary splitting and migration. The deformation twinning was recently verified in nanocrystalline Al (Ref 8-10, 20), Cu (Ref 12), and Pd (Ref 13) by high-resolution transmission electron microscopy. Al in its coarse-grained (CG) state has never been observed to deform by twinning, except at crack tips (Ref 21), due to its very high stacking fault energy. CG Cu does not deform by twinning (Ref 22, 23) except at very high strain rates (Ref 24, 25) and/or low temperatures (Ref 26). Moreover, in CG Cu, smaller grain size was found to impede deformation twinning, which is also true for many other metals (Ref 27, 28). In contrast, twinning becomes a major deformation mechanism in nanocrystalline Cu processed by high pressure torsion (HPT) at room temperature and a low strain rate (Ref 12). In addition, it was found that under the same HPT condition, twinning occurred only in crystalline domains smaller than 50 nm (Ref 29). These results indicate

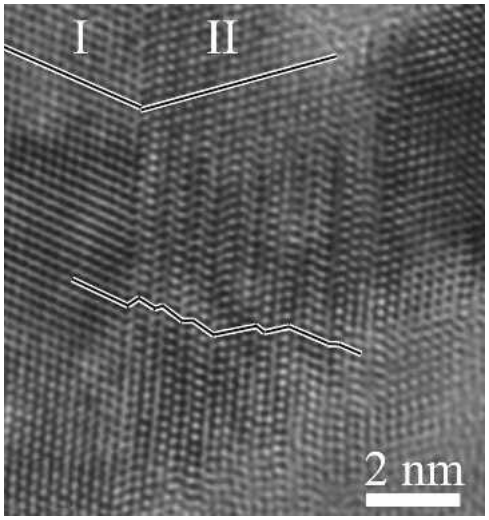

Fig. 1 [011] HRTEM image showing microtwins and stacking faults. The upper part of the image shows only two twin domains: I and II whereas the lower part of domain II has many microtwins and stacking faults with one end of the microtwin/stacking fault stops within the crystallite.

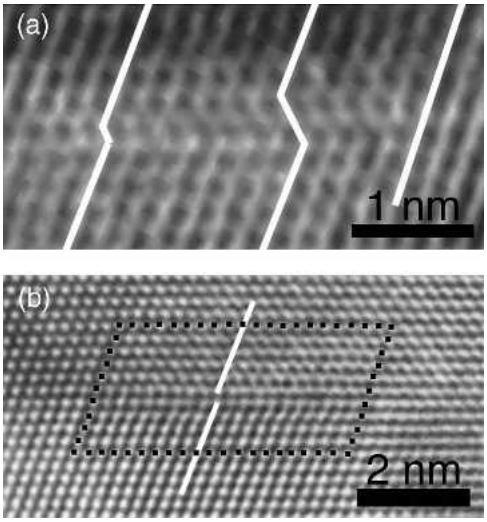

Fig. 2 (a) Deformation twin formed by the overlapping of two extended dislocations on adjacent slip planes and (b) atomic level image of a wide stacking fault

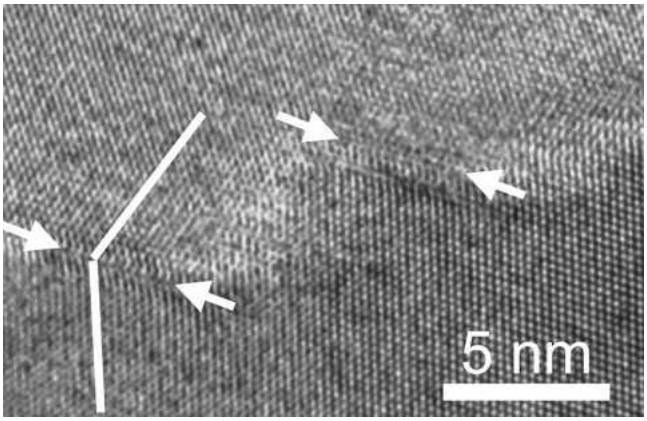

Fig. 3 HRTEM image of a twin formed by grain boundary splitting and migration. It consists of short, straight, coherent $(1\bar{1}1)$ twinning planes (marked by arrows) connected by incoherent, noncrystallographic segments

that the nanocrystalline materials indeed deform via mechanisms not accessible to their coarse-grained counterparts, and grain size plays a critical role in the formation of deformation twins.

Figure 2(a) shows a deformation twin formed by homogeneous twinning inside a nanocrystalline Al grain. It has a thickness of two atomic planes and is therefore a twin nucleus. It was clearly formed by dynamic overlapping of two extended partial dislocations with stacking faults on adjacent slip planes (Ref 9). As shown, the two stacking faults are only partially overlapped. This twin may grow by overlapping with more wide stacking faults. Wide stacking fault ribbons formed by dissociated lattice dislocations are a prerequisite for the formation of such twins. Such wide stacking faults are indeed found in the cryogenically ball-milled Al (Fig. 2b).

Figure 3 shows twins formed by grain boundary splitting and migration. As shown, some segments of the boundary are straight, coherent $(1\bar{1}1)$ twin boundaries as indicated by white arrows. These segments, connected by noncrystallographic segments, form a zigzag boundary between the two twinning areas. To form such twins, a grain boundary segment was dissociated into a twin boundary and a new grain boundary (Ref 16). A twin lamella was formed via the migration of the new grain boundary. The boundaries of twin lamellae formed at different time frames joined together to form the zigzag boundary. The noncrystallographic segments observed here were actually the new grain boundaries in this mechanism. Refer to the work of Yamakov et al. (Ref 16) for more detailed description on this twinning mechanism.

Deformation twins, formed by heterogeneous twinning, are shown in Fig. 1, which shows twins nucleated on the grain boundaries. Most twins observed in nanocrystalline Al and Cu are this type. The nucleation and growth of such deformation twins are not well understood. Both atomistic simulations and experimental data indicate that such deformation twins are formed by partial dislocation emissions from grain boundaries (Ref 7, 8, 10, 12, 18). However, it is not clear under what conditions the deformation twins will nucleate and grow. For example, atomistic simulations do not indicate what critical stress is needed for the deformation twin to nucleate and grow or what grain size is optimum for deformation twin nucleation. Moreover, atomistic simulations (Ref 4, 7, 14) usually use extremely high strain rates in the order of 10^6 to 10^8 s^{-1}, which correspond to explosive deformations in a real experiment. It is well known that the strain rate significantly affects the deformation mechanisms of materials (Ref 12, 19). This adds complexity to the interpretation of the atomistic simulation results. It is of interest to study the grain size effect on the deformation twinning without the complication of high strain rates. In the following section, an examination of analytical dislocations models on the formation of deformation twins will be reviewed.

3. Analytical Dislocation Models

3.1 Conventional Dislocation Models

Two similar models were proposed to explain the formation of deformation twins in nanocrystalline metals (Ref 8, 11). In

the model by Chen et al. (Ref 8), the stress needed to activate a lattice dislocation is described as:

$$\tau_L = \frac{2\eta Gb}{d} \quad \text{(Eq 1)}$$

where η is a parameter that reflects the characteristics of the dislocation ($\eta = 0.5$ for an edge dislocation and $\eta = 1.5$ for a screw dislocation), G is the shear modulus, and b is the magnitude of the Burgers vector of the lattice dislocation. The stress to activate a partial dislocation is described as:

$$\tau_P = \frac{2\eta Gb_1}{d} + \frac{\gamma}{b_1} \quad \text{(Eq 2)}$$

where b_1 is the magnitude of the Burgers vector of the partial dislocation, and γ is the stacking fault energy. When $\eta = 0.5$, these two equations become identical to those in the work by Liao et al. (Ref 11).

Because $b > b_1$, τ_P will increase at a slower rate than τ_L, which means that it will be easier to activate a partial dislocation than a lattice dislocation when the grain is below a critical size. These two models seem very straightforward in explaining the activation of partial dislocations, which is a prerequisite of deformation twinning.

Unfortunately, experimental data show that smaller grain size hinders, not promotes, deformation twinning (Ref 27, 28), which directly contradicts these two models (Ref 8, 11). It has been found that the critical stress for twinning follows a Hall-Petch relationship:

$$\sigma_T = \sigma_{To} + \kappa_T d^{1/2} \quad \text{(Eq 3)}$$

where σ_{To} is a constant and κ_T is the Hall-Petch slope for twinning. Equation 3 is similar to the well-known Hall-Petch relationship for a lattice dislocation:

$$\sigma_L = \sigma_{Lo} + \kappa_L d^{1/2} \quad \text{(Eq 4)}$$

where σ_{Lo} is a constant and κ_L is the Hall-Petch slope for the slip of a lattice dislocation.

Table I lists the Hall-Petch slope for both twinning and for slip of lattice dislocations (Ref 27). As shown, the Hall-Petch slope for twinning is higher than that for the slip of lattice dislocation for body-centered-cubic (bcc), face-centered-cubic (fcc), and hexagonal close-packed (hcp) metals and alloys. Therefore, the models are not supported by experimental data. Moreover, these two models predict an unrealistically high critical stress for twinning (Ref 8), which reflects their problem. The models also made an inexplicit assumption that activation of partial dislocation equals formation of twinning, which, as shown later, is not correct.

3.2 Recent Model Based on the Emission of Partial Dislocation from Grain Boundaries

A recent analytical dislocation model by Asaro et al. (Ref 30) used the simulation and experimental results that partial dislocations are emitted from boundaries of nanosized grains. The critical stress needed to move a lattice dislocation is described as:

Table 1 Hall-Petch slopes for bcc, fcc, and hcp metals and alloys (Ref 27)

Material	H-P slope for slip, κ_L, MPa mm$^{1/2}$	H-P slope for twinning, κ_T, MPa mm$^{1/2}$
bcc		
Fe-3 wt.%Si	12	100
Armco Fe	20	124
Steel: 1010, 1020, 1035	20	124
Fe-25at.%Ni	33	100
Cr	10.08	67.75
Va	3.46 (20K)	22.37
fcc		
Cu	5.4 (RT)	21.66 (77K)
Cu-6wt.%Sn	7.1	11.8 (77K), 7.9 (RT)
Cu-9wt.%Sn	8.2	15.77 (77K)
Cu-10wt.%Zn	7.1	11.8 (77K)
Cu-15wt.%Zn	8.4	16.7 (295K)
hcp		
Zr	8.26	79.2
Ti	6 (78K)	18 (4K)

$$\tau_L = \frac{Gb}{d} \quad \text{(Eq 5)}$$

and the critical stress needed to move a partial dislocation is described as:

$$\tau_P \approx \frac{Gb}{3d} + (1-\delta)\frac{\gamma}{Gb} \quad \text{(Eq 6)}$$

where δ is the ratio of equilibrium stacking fault width to grain size.

This model predicts that below a certain critical grain size partial dislocations from grain boundaries need a lower stress to move than lattice dislocations in nanocrystalline metals. Most importantly, it predicts a realistic, low twinning stress obtainable under experimental conditions such as ball milling. However, the model does not address two critical issues. First, the emission of a partial dislocation does not guarantee the nucleation of a deformation twin because a trailing partial could easily follow to erase the stacking fault formed by the first partial. Second, random emissions of partial dislocations from a grain boundary would give a deformation twin equal probability to grow or to shrink, which cannot explain the deformation twin growth and the observed large deformation twins in nanocrystalline Al, Cu, and Pd (Ref 9-13).

3.3 New Model Addressing the Nucleation and Growth of Deformation Twins

To address the above two issues, an analytical model was recently developed to describe the nucleation and growth of deformation twins in nanocrystalline Al (Ref 31), and the model will be introduced in the following sections.

The model assumes a grain with a square (111) slip plane, as shown in Fig. 4, similar to that used in previous studies (Ref 20, 30). Under an external shear stress τ, a 90° leading Shockley partial, $b_1 = a/6[11\bar{2}]$, is emitted from grain boundary AB, depositing two segments of partial dislocation lines (Aa and

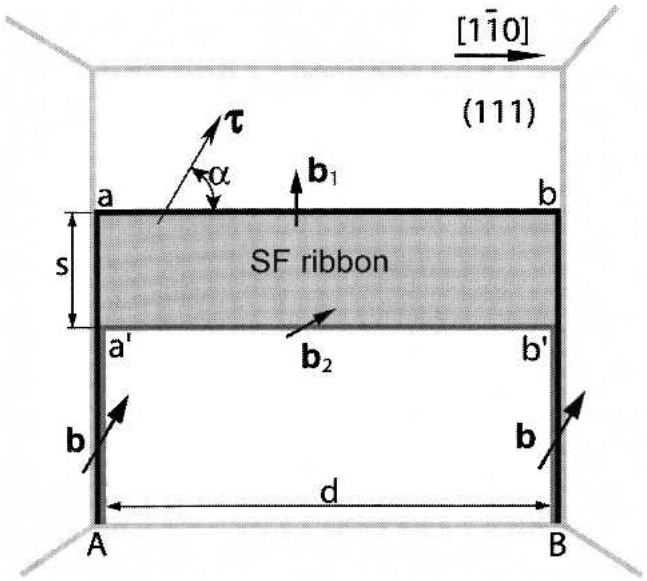

Fig. 4 Schematic illustration of the dislocation model for deformation twin nucleation

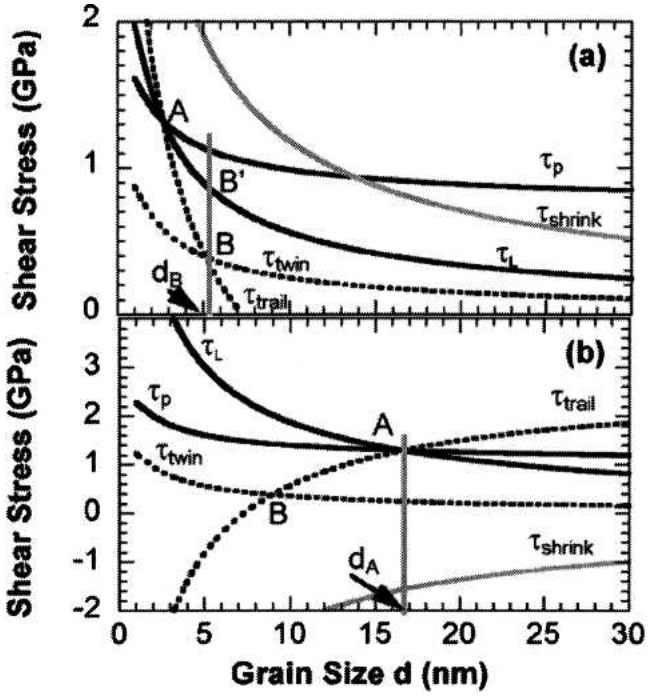

Fig. 5 Critical stresses, τ_P, τ_L, τ_{twin}, τ_{trail}, and τ_{shrink} as a function of nanocrystalline Al grain size d for a given α value of (a) 90° and (b) 135°

Bb) on grain boundaries. τ is oriented at an angle α with line ab. A trailing 30° partial, $b_2 = a/6[2\bar{1}\bar{1}]$, is also emitted (line Aa′b′B). The two partials ab and a′b′ are separated by a stacking fault. The two partials react to form two perfect dislocation segments, Aa′ and Bb′ at the grain boundaries. This dislocation system is called a 60° I system hereafter.

To nucleate a deformation twin, a stacking fault needs to be created first. This can occur via (a) emission of a 90° partial at a grain boundary or (b) extending the stacking fault ribbon in Fig. 4 across the grain. As shown later, both scenarios may occur, depending on the orientation of τ. In Fig. 4, for the partial b_1 to move, τ has to perform a work to overcome increases in both the stacking fault energy and dislocation energy from lengthening segments Aa and Bb (Ref 32, 33). The critical stress for moving partial b_1 can be derived as:

$$\tau_P = \frac{1}{\sin\alpha}\left(\frac{\sqrt{6}\gamma}{a} + \frac{Ga}{2\sqrt{6}\pi d}\ln\frac{\sqrt{2}d}{a}\right) \quad \text{(Eq 7)}$$

where γ is the stacking fault energy, a is the lattice parameter, and d is the grain size defined in Fig. 4.

The τ needed to move the stacking fault ribbon is equivalent to τ for moving a 60° lattice dislocation. τ has to overcome the work needed to lengthen the lattice dislocation segments Aa′ and Bb′ and can be derived as:

$$\tau_L = \frac{Ga(4-3\nu)}{8\sqrt{2}\pi(1-\nu)d\cos(\alpha-60°)}\ln\frac{\sqrt{2}d}{a} \quad \text{(Eq 8)}$$

where ν is Poisson's ratio.

After the stacking fault formation, a twin may nucleate via the emission of a second 90° partial from the grain boundary on a plane adjacent to the stacking fault. On the other hand, a trailing partial may also emit on the stacking fault plane and erase the stacking fault in its path. The critical twin nucleation stress can be derived as:

$$\tau_{twin} = \frac{Ga}{2\sqrt{6}\pi d\sin\alpha}\ln\frac{\sqrt{2}d}{a} \quad \text{(Eq 9)}$$

The trailing partial requires a stress, τ_{trail}, to move, which can be derived as:

$$\tau_{trail} = \frac{\sqrt{6}}{\cos(\alpha-30°)}\left[\frac{Ga(8-5\nu)}{48\pi(1-\nu)d}\ln\frac{\sqrt{2}d}{a} - \frac{\gamma}{a}\right] \quad \text{(Eq 10)}$$

Once a twin is nucleated, it may grow via the emission of more 90° twinning partials under stress τ_{twin}. It may also shrink via the emission of a shrinking partial b_2 on a plane adjacent to the twin boundary but on the twin side. The stress needed to move a shrinking partial can be derived as:

$$\tau_{shrink} = \frac{\sqrt{6}}{\cos(\alpha-30°)}\frac{Ga(8-5\nu)}{48\pi(1-\nu)d}\ln\frac{\sqrt{2}d}{a} \quad \text{(Eq 11)}$$

The stresses, τ_P, τ_L, τ_{twin}, τ_{trail}, and τ_{shrink}, determine the nucleation and growth of a deformation twin. For example, at $\tau_P < \tau_L$, partial dislocations will be emitted from the grain boundary, and at $\tau_{twin} < \tau_{trail}$, a twin may nucleate. In the following, Al is used as a model material to validate the model. For Al, $G = 26.5$ GPa, $\nu = 0.345$, $a = 0.404$ nm, and $\gamma = 122$ mJ/m^2 (Ref 33, 34). In Fig. 5, the stresses, τ_P, τ_L, τ_{twin}, τ_{trail}, and τ_{shrink}, are plotted as a function of grain size d for (a) $\alpha = 90°$ and (b) $\alpha = 135°$. Point B in Fig. 5(a) represents the critical grain size ($d_B = 5.16$ nm) below which a deformation twin nucleates because $\tau_{twin} < \tau_{trail}$. However, a deformation twin can nucleate only after the formation of a stacking fault. As shown, at grain size d_B, $\tau_L < \tau_P$; i.e., the lattice dislocation is operating at $\tau_L = 0.88$ GPa (point B′).

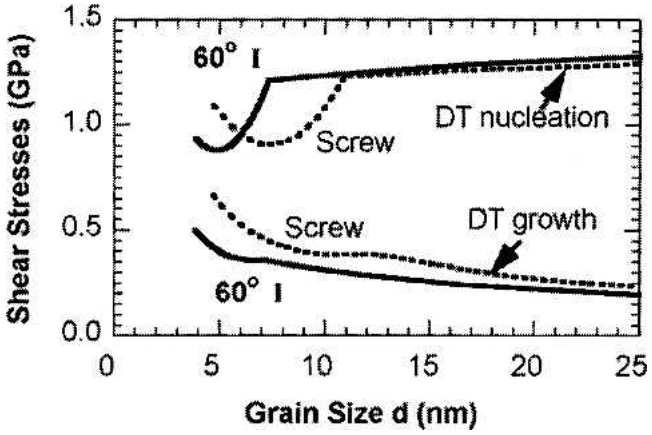

Fig. 6 Deformation map showing the critical stresses for deformation twin nucleation and growth in nanocrystalline Al as a function of grain size for the 60° I and the screw dislocation systems

The stacking fault width at τ_L is far larger than d_B (Ref 31). This means that a deformation twin nucleates after a stacking fault ribbon spreads across the grain. Interestingly, the critical grain size is larger, and the critical stress is lower for twin nucleation (point B′) than for the partial dislocation emission (point A), because the stacking fault of a dissociated lattice dislocation would spread across the grain before a partial is emitted.

Figure 5(b) shows the stresses versus d at $\alpha = 135°$. As shown, τ_{trail} or τ_{shrink} is actually the critical stress curve above which the trail or shrink partial is prohibited. At $d < d_A$ (16.66 nm) and $\tau > \tau_P$, deformation twins will nucleate.

The above equations and analysis are for the 60° I system only. There are two other possible dislocation systems: a 60° II system with a leading 30° partial and a trailing 90° partial, and a screw system with a leading 30° partial and a trailing 30° partial (Ref 20). These two systems are amenable to the same procedure, and therefore, only the final results are presented. It is found that the 60° II system does not operate because it requires much higher stress to nucleate a deformation twin. Therefore, the 60° II system was eliminated in the following analysis. In a polycrystalline nanocrystalline sample, grains are likely to orient in all orientations. Therefore, a deformation map linking stresses of deformation twin nucleation and growth with grain size is very useful and desirable. Such a map can be constructed by plotting the critical stresses against the critical grain sizes (Fig. 6).

The deformation map in Fig. 6 reveals the following four interesting points: (a) The deformation twin nucleation curves have a cup and handle geometry. The cup section is from τ orientations at which all stresses behave like those in Fig. 5(a), whereas the handle section is from τ orientations at which all stresses behave like those in Fig. 5(b). (b) The optimum grain sizes for deformation twin nucleation (the lowest stress point at cup bottom) are 4.85 nm and 7.25 nm, respectively, for the 60° I and screw systems. (c) The 60° I system has a slightly lower critical stress (0.88 GPa) than the screw system (0.91 GPa) for deformation twin nucleation. (d) The stress for deformation twin growth is much lower than that for its nucleation.

Clearly, the critical stress for deformation twin nucleation is very high (>0.88 GPa). Such a high stress can be obtained only under high strain rates and/or low temperatures, which is consistent with experimental conditions for cryogenically ball-milled nanocrystalline Al (Ref 9-11). In addition, the high nucleation stress also explains the low deformation twin density in the nanocrystalline Al.

On the other hand, the stress for deformation twin growth is low enough to be easily attained during a normal static deformation. This is consistent with a recent molecular dynamics simulation (Ref 35), which shows that deformation twins are difficult to nucleate but easy to grow. This explains why a twin would grow without the traditional pole mechanism. This new twin growth mechanism is defined as the "stress-controlled-growth" mechanism.

4. Summary

When the grain sizes of nanocrystalline materials are in the range of 10-50 nm, deformation twins will form in medium to high stacking-fault-energy fcc metals such as Al and Cu. Several types of deformation twins are predicted by molecular dynamics simulations and observed experimentally. The most common twins observed experimentally are those nucleated heterogeneously on grain boundaries via the emission of partial dislocations on the grain boundaries.

Two analytical models based on conventional dislocation theories (Ref 8, 11) are not supported by experimental data and cannot give a reasonable critical twining stress. Another model (Ref 30), based on the partial dislocation emission from grain boundaries, gives a reasonable critical stress for partial dislocation activation but does not address the nucleation and growth of deformation twins. A new model (Ref 31), which is also based on the partial dislocation emission from grain boundaries, addresses both the nucleation and growth of deformation twins in nanocrystalline fcc metals and alloys. It describes a stress-controlled mechanism for the growth of deformation twins, which explains why and how a twin grows without the conventional pole mechanism. The model can successfully explain the experimental observation of twins in nanocrystalline Al processed by cryogenic ball milling.

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