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Nucleation and growth of deformation twins in nanocrystalline aluminum

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Deformation twins (DTs) in nanocrystalline (nc) Al were both predicted by atomic simulations, and observed experimentally. However, despite encouraging preliminary results, their formation mechanism remains poorly understood. Here we present an analytical model, based on classical dislocation theory, to explain the nucleation and growth of DTs in nc Al. A 60° dislocation system consisting of a 90° leading partial and a 30° trailing partial is found to most readily nucleate and grow a DT. The model suggests that the stress for twin growth is much smaller than that for its nucleation. It also predicts an optimal grain size for twin nucleation. The model successfully explains DTs observed experimentally in nc Al and is also applicable to other nc metals. © *2004 American Institute of Physics*. [DOI: 10.1063/1.1823042]

Recently, atomic simulations predicted partial dislocation emissions from grain boundaries (GBs) and deformation twins (DTs) in nanocrystalline (nc) Al.[1] DTs in nc Al were also observed experimentally.[2–5] However, the mechanisms that govern the nucleation and growth of DTs in nc materials are not well understood. Both atomistic simulations[1,6–8] and experiments[3,9] indicate that DTs are formed by partials emitted from GBs. However, the simulations do not reveal the critical stress or the optimal grain size needed for DT nucleation and growth. In this letter we present an analytical model based on classical dislocation theory to describe the nucleation and growth of DTs in nc Al. The model predicts critical DT nucleation stress and grain size that are consistent with experimental observations. The model can be easily applied to other face-centered-cubic metals such as Cu and Ni.

For simplicity, we consider a grain with a square (111) slip plane, as shown in Fig. 1, similar to that used in previous studies.[10,11] Under an external shear stress τ, a 90° leading Shockley partial, $\mathbf{b}_1=\mathrm{a}/6[11\bar{2}]$, is emitted from grain boundary AB, depositing two segments of partial dislocation lines (Aa and Bb) on GBs. The shear stress τ is oriented at an angle α with line ab. A trailing 30° partial, $\mathbf{b}_2=\mathrm{a}/6[\bar{2}11]$, is also emitted (line Aa′b′B). The two partials ab and a′b′ are separated by a stacking fault (SF). The two partials react to form two perfect dislocation segments, Aa′ and Bb′ at the GBs. We shall call this dislocation system a *60° I system* hereafter. *Note that* the partial segments ab and a′b′ are assumed to be straight in order to maintain mathematical considerations tractable, while avoiding an oversimplification of the associated physics.

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.[11] In the following, we shall only analyze the 60° I system in detail. The other two systems are amenable to the same procedure, and therefore we only present the final results. We ignore the Peierls stress because it is very small ($\sim 10^{-5}$ G, G is the shear modulus of Al).[12] We also ignore the differences in the core energies between partial and perfect dislocations because our calculation indicates that their effects are negligible.

To nucleate a DT we first need to create a SF that extends from a GB to the grain interior or across the whole grain. This can occur via: (1) emission of a 90° partial at a GB, (2) extending the SF ribbon across the grain. As shown later, both scenarios may occur depending on the orientation of τ. In Fig. 1, for the partial $\mathbf{b}_1$ to move, τ has to perform a work to overcome increases in both the SF energy and dislocation energy from lengthening segments Aa and Bb.[13,14] Using a procedure that is described in detail in a previous publication,[11] we can derive the critical stress for moving partial $\mathbf{b}_1$ as

$$\tau_p = \frac{1}{\sin\alpha}\left(\frac{\sqrt{6}\gamma}{a} + \frac{Ga}{2\sqrt{6}\pi d}\ln\frac{\sqrt{2}d}{a}\right), \tag{1}$$

where γ is the SF energy, a is the lattice parameter, and d is the grain size defined in Fig. 1.

The τ needed to move the SF ribbon is equivalent to τ for moving a 60° lattice dislocation, τ has to overcome the

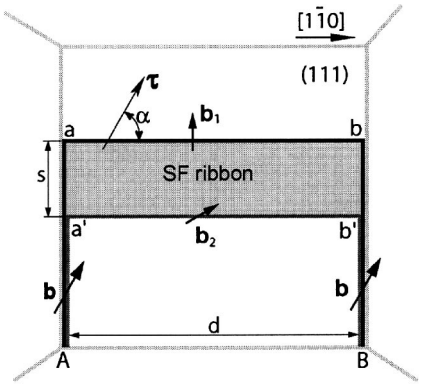

FIG. 1. A schematic illustration of the dislocation model for deformation twin nucleation.

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work needed to lengthen the lattice dislocation segments Aa′ and Bb′, and can be derived as

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

where ν is Poisson's ratio.

The partial and perfect dislocations compete with each other, and the one requiring lower stress prevails. The stacking fault width, s, under external driving force τ, can be derived following a procedure described in our previous work[11]

$$s_\tau = \frac{\gamma s_0}{\gamma - \dfrac{Ga^2(8-5\nu)}{48\pi(1-\nu)d}\ln\dfrac{\sqrt{2}d}{a} - \dfrac{\tau a}{2}\left(\dfrac{\sin\alpha}{\sqrt{6}} - \dfrac{\cos\alpha}{\sqrt{2}}\right)}, \tag{3}$$

where $s_0 = Gb^2/4\pi\gamma(1-\nu)$ is the intrinsic SF width of a 60° dislocation.[13,14]

After the SF formation, a twin may nucleate via the emission of a second 90° partial from the GB on a plane adjacent to the SF. We define this partial as a twinning partial. It generates a two-layer twin nucleus, and replaces the SF with two twin boundaries. Since the twin boundary energy is about half of the SF energy,[13] τ only needs to overcome the lengthening of partial dislocation segments. The critical twin nucleation stress can be derived as

$$\tau_{\text{twin}} = \frac{Ga}{2\sqrt{6}\pi d\,\sin\alpha}\ln\frac{\sqrt{2}d}{a}. \tag{4}$$

On the other hand, a trailing partial may also emit on the SF plane and erase the SF in its path. The trailing partial requires a stress, τ_{trail}, to move, which can be derived as

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

To nucleate a twin, the twinning partial must prevail over the trailing partial.

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, $\mathbf{b}_2$, 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

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

For Al, $G=26.5$ GPa, $\nu=0.345$, $a=0.404$ nm, and $\gamma=122$ mJ/m$_2$.[14,15] In Fig. 2, 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) $\alpha=135°$. The point B in Fig. 2(a) represents the critical grain size ($d_B=5.16$ nm) below which a DT nucleates because $\tau_{\text{twin}}<\tau_{\text{trail}}$. However, a DT can nucleate only after the formation of a SF. 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′). The SF width at τ_L calculated from Eq. (3) is far larger than d_B. This means that a DT nucleates after a SF ribbon spreads across the grain. Figure 2(b) shows the stresses versus d at $\alpha=135°$. In Fig. 2(b), 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 $\tau>\tau_p$, DT will nucleate.

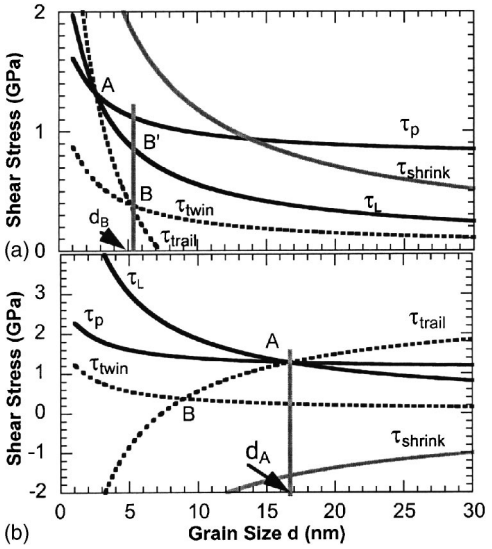

FIG. 2. The critical stresses, τ_p, τ_L, τ_{twin}, τ_{trail}, and τ_{shrink} as a function of nc Al grain size d for a given α value of (a) 90° and (b) 135°.

Following the same procedure, we can analyze the 60° II and the Screw systems. We found that the 60° II system does not operate because it requires much higher stress to nucleate a DT. Therefore we shall drop the 60° II system in the following analysis. In a polycrystalline nc sample, grains are likely to orient in all orientations. Therefore, a deformation map linking stresses of DT 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 (see Fig. 3).

The deformation map in Fig. 3 reveals the following four interesting points: (i) The DT *nucleation* curves have a cup and handle geometry. The cup section is from τ orientations at which all stresses behave like those in Fig. 2(a), while the handle section is from τ orientations at which all stresses behave like those in Fig. 2(b); (ii) The optimum grain sizes for DT nucleation (the lowest stress point at cup bottom) are 4.85 and 7.25 nm, respectively, for the 60° I and Screw systems; (iii) The 60° I system has a slightly lower critical stress (0.88 GPa) than the Screw system (0.91 GPa) for DT nucleation; (iv) The stress for DT growth is much lower than that for its nucleation.

Clearly, the critical stress for DT nucleation is very high (>0.88 GPa). Such a high stress can only be obtained under high strain rates and/or low temperatures, which is consistent with experimental conditions for cryogenically ball-milled

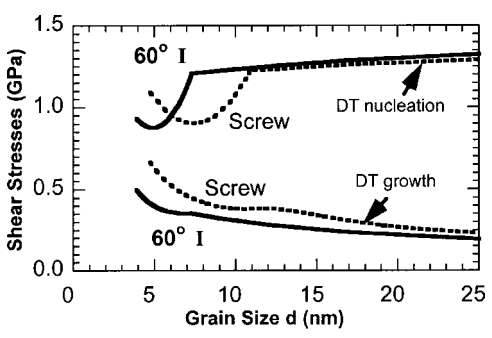

FIG. 3. A deformation map showing the critical stresses for DT nucleation and growth in nc Al as a function of grain size for the 60° I and the Screw dislocation systems.

nc Al.[2,3,5] In addition, the high nucleation stress also explains the low DT density in the nc Al.

Our model shows that the stress for DT growth is low enough to be easily attained during a normal static deformation. This is consistent with a recent MD simulation,[16] which shows that DTs are difficult to nucleate but easy to grow. However, the MD simulation attributed the difficult twin nucleation to high unstable twin fault energy.[16,17] Our analytical model can be further refined by considering the unstable SF energy and unstable twin fault energy, when their values can be more reliably obtained from the literature.[16]

In this model, we have made several assumptions to render the mathematics tractable, including a square grain geometry and straight dislocation lines. Moreover, we have also ignored any possible interactions between the twinning dislocations with grain boundaries and interactions between dislocations. These assumption and simplifications render the present model semiquantitative. Moreover, it is worth noting that the dislocation line energy, as derived from classic dislocation theory, is itself semiquantitative. One critical issue is whether the equation used to describe dislocation line energy, which is based on long-range dislocation stress field, is still valid for the nano-sized grains relevant in this model. A recent atomic simulation shows that it remains valid at grain sizes down to 2 nm,[18] which validates our use of the equation. In this model we also bypassed the dislocation nucleation from GBs. This can be best studied by atomic simulations.[7,13] We have used these simulation results to formulate our assumptions such as partial dislocation emission from GBs.[1,5–7]

The final criterion for judging the validity of a model is how well it explains experimental observations. Our current model does very well in this aspect: (1) It predicted a realistc DT nucleation stress (>0.88 GPa), which is obtainable under experimental conditions (cryogenic ball milling).[2,3] (2) The DT is not a major deformation mechanism in nano Al because of the required high stress for twin nucleation. (3) The model predicted that once a twin is nucleated, it requires relatively low stress to grow, which explains how a twin can be formed without the traditional pole mechanism. In other words, this explains why a partial would emit from a plane adjacent to the twin plane, making the twin grow, instead of emitting from any plane to generate random SFs. We name this DT growth mechanism the *stress-controlled twin growth mechanism*. Note that a recently proposed "double-cross-slip" twinning mechanism cannot operate in nc Al because when the grain size is very small, say, <50 nm, the grain interior is usually dislocation free.[19] If such a source is formed by dislocations on the GBs, the twinning partial will not be able to form the necessary faulted loop. To summarize, the current model provides a rational explanation for the formation of DTs that have been observed in nc Al.

In summary, we have developed an analytical model based on classical dislocation theory to describe DT nucleation and growth in nc Al. Our model indicates that the optimum grain size for DT nucleation in nc Al is around 4.85 or 7.25 nm. The nucleation of a DT requires very high shear stress (>0.88 GPa). Once a DT is nucleated, it is not likely to shrink because a shrinking partial requires higher stress to operate than a twinning partial. The DT grows at much lower stresses via the emission of twinning partials from GBs on slip planes adjacent to the twin boundary via the stress-controlled twin growth mechanism.

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