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Formation mechanism of wide stacking faults in nanocrystalline Al

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A full dislocation often dissociates into two partial dislocations enclosing a stacking fault (SF) ribbon. The SF width significantly affects the mechanical behavior of metals. Al has very high stacking fault energy and, consequently, very narrow SF width in its coarse-grained state. We have found that some SFs in nanocrystalline Al are surprisingly 1.4–6.8 nm wide, which is 1.5–11 times higher than the reported experimental value in single crystal Al. Our analytical model shows that such wide SFs are formed due to the small grain size and possibly also to the interaction of SF ribbons with high density of dislocations. © *2004 American Institute of Physics.*
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Nanocrystalline (nc) metals are solids with grain sizes smaller than 100 nm. They typically exhibit mechanical properties that are markedly superior to those of conventional materials, e.g., excellent superplasticity,[1] high strength,[2–6] and, in a few cases, excellent ductility.[2,5] These exceptional properties are attributed to their unique deformation mechanisms, which are derived from their unusual microstructures.[7]

Recently, there have been significant developments in understanding the deformation mechanisms of nc materials.[7–15] Atomistic simulations predict Al to deform via grain-boundary (GB) sliding at very fine grain sizes (e.g., 3–10 nm).[11,12] At several tens of nanometers, the simulations also show that partial dislocations emitted from GBs[10] dominate the deformation. Consequently, these partials form deformation twinning and partial-dislocation-enclosed stacking fault (SF) ribbons *within* grains.[10] Deformation twinning was experimentally verified in nc Al.[7,8,14] Surprisingly, SFs observed in cryogenically ball-milled nc Al (Ref. 7) were found to be much wider than both the experimental value in coarse-grained Al (Ref. 16) and the theoretical value predicted by atomistic simulations.[17] In addition, these very wide SFs also formed twins in the grain interior by coincidental overlapping.[7] Such wide SFs are unexpected because Al has very high SF energy. They will certainly affect the mechanical properties of the nc Al. The objective of this letter is to provide fundamental insight into the origin of these wide SFs.

Al powder with a purity of ~99.9 wt % was ball milled while immersed in liquid nitrogen. Readers are referred to Ref. 7 for more experimental details. The as-milled Al powder contains both elongated and equiaxed grains.[7] Figure 1 shows a SF formed from the dissociation of a screw dislocation. This type of SFs are more frequently observed than those formed from the dissociation of 60° dislocations.[7] We measured the widths of 10 SF ribbons from high-resolution transmission electron microscopy (HRTEM) images. They span a large range of 1.4–6.8 nm, with an average width of 3.5 nm. The experimental SF width from a 60° dislocation was reported to be 0.55 nm in single crystal Al (Ref. 16) and predicted to be 0.86 nm in nc Al by atomic simulation,[17] while the SF width from a screw dislocation is about one-half of the width of a 60° dislocation.[18,19] Therefore, the widths of SF ribbons observed here in nc Al are 1.5–11 times higher than the reported experimental value.[16]

Note that HRTEM can accurately reveal the width of a SF only when the two partial dislocation lines enclosing the SF are parallel to a ⟨110⟩ from which the HRTEM image was obtained. However, in a real situation, they are most likely at various angles with the ⟨110⟩ orientation, and may not even be straight, especially near the transmission electron microscopy (TEM) foil surface.[20,21] This causes two difficulties in measuring the SF width: First, it makes the SF appear wider than the real width (see line *AB* in Fig. 1), and second, it makes the lattice shift across the apparent SF line unclear. To overcome these difficulties, we only measured the widths of SFs with a clear lattice shift. In addition, we excluded the

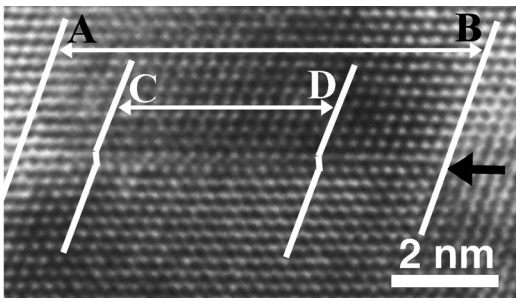

FIG. 1. An HRTEM image of a SF ribbon (as pointed out by the black arrow) viewed from a ⟨110⟩ direction. The distance *CD* was measured as the SF width.

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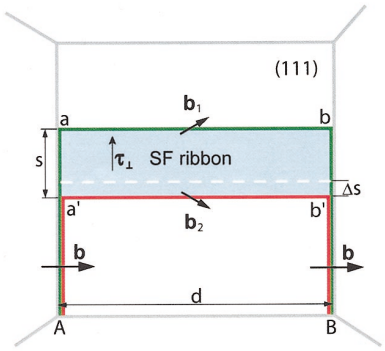

FIG. 2. (Color) A schematic illustration of the dislocation model for wide SF ribbon formation. Two Shockley partial dislocations (the green and red lines) are emitted consecutively from the GB *AB*, with their ends pinned at *A* and *B*.

segments at both ends of the SF where the lattice shift is smaller than that in the center, as demonstrated in Fig. 1. As shown in Fig. 1, we regard the length *CD* as the stacking fault width, not the longer *AB*. This procedure should give us a conservative estimate of the SF width. In other words, it is likely that our procedure gives an underestimate of the SF width. The other method to measure SF width is the weak-beam TEM technique, which is often used for coarse-grained or single-crystal materials. However, it is extremely difficult, if not impossible, to do weak-beam TEM on nc materials. Other factors that may make the SF appear wider include dislocation image force and residual stress, which are beyond the scope of this letter. The issue here is the existence of wide SFs, not their accurate measurement. The HRTEM method employed here proved the existence of these wide SFs beyond any doubt.

To understand the formation mechanisms of these unusually wide SFs, we draw on the simulation results that Shockley partial dislocations are emitted from GBs.[10,12,17] For simplicity, we consider a grain with a square (111) slip plane (see Fig. 2). Under an external stress, a leading Shockley partial dislocation, $\mathbf{b}_1 = a/6[2\bar{1}\bar{1}]$, is emitted from GB *AB* (see the green line *AabB*). The ends of the partial dislocation are pinned at the triple junctions *A* and *B* so that two segments of partial dislocation lines (*Aa* and *Bb*) are deposited on GBs. Similarly, a trailing Shockley partial dislocation, $\mathbf{b}_2 = a/6[1\bar{2}1]$, is emitted from GB *AB* and forms the red $Aa'b'B$ dislocation line. Partial dislocation lines *ab* and $a'b'$ are separated by a SF, and they would form a screw dislocation $a/2[1\bar{1}0]$ if collapsed together. The two partial dislocations react to form two full edge dislocation segments, Aa' and Bb' at the GBs. Note that the partial segments *ab* and $a'b'$ will be curved in a real situation. We assume them to be straight lines here to simplify the mathematics without sacrificing the physics.

Dislocation lines *ab* and $a'b'$ repel each other with a force f per unit length, while SF energy, γ, forces *ab* and $a'b'$ to move closer. At equilibrium, $f=\gamma$, the SF ribbon width in coarse-grained Al can be described as[17,19,22]

$$s_0 = K\mathbf{b}_1\mathbf{b}_2/\gamma, \tag{1}$$

where K is a constant.

Assuming that partial dislocation line *ab* stays stationary and line $a'b'$ moves a distance Δs to the white dotted line, the partial dislocation lines ($a'a+bb'$) will be shortened by $2\Delta s$, while the full edge dislocation lines ($Aa'+Bb'$) will be lengthened by $2\Delta s$. This will decrease the total SF energy but increase the dislocation energy because the full dislocation has higher energy than the partial dislocation. In other words, the full dislocation segments will exert a dragging force on partial dislocation $a'b'$. This has the same effect as having a lower effective SF energy, which is derived below.

The total SF energy change from the assumed motion of $a'b'$ is

$$\Delta E_{\mathrm{SF}} = -\gamma d\Delta s, \tag{2}$$

where γ is the SF energy per unit area, d is the length of $a'b'$, which is also the grain size. The total change in dislocation energy can be described as[22]

$$\Delta E_d = 2\Delta s \frac{Gb^2}{4\pi(1-\nu)}\ln\frac{R}{r_0} - 2\Delta s \frac{Gb_1^2(1-\nu\cos^2 60^\circ)}{4\pi(1-\nu)}\ln\frac{R}{r_0}, \tag{3}$$

where G is the shear modulus, b and b_1 are the length of the Burger's vector of the full dislocation and the partial dislocation 1, respectively, ν is the Poisson's ratio, R can be estimated as the grain size d, and r_0 can be estimated as b. For Al, $b=a/\sqrt{2}$, $b_1=a/\sqrt{6}$, where a is the lattice parameter. The total energy change from the SF area reduction and dislocation length change, ΔE_{te}, is the sum of ΔE_{SF} and ΔE_d:

$$\Delta E_{te} = -\left[\gamma - \frac{Ga^2(8+\nu)}{48\pi(1-\nu)d}\ln\frac{\sqrt{2}d}{a}\right]d\Delta s. \tag{4}$$

Comparing Eqs. (2) and (4), the effective stacking fault energy can be described as

$$\gamma_e = \gamma - \frac{Ga^2(8+\nu)}{48\pi(1-\nu)d}\ln\frac{\sqrt{2}d}{a}. \tag{5}$$

The width of the SF ribbon is inversely proportional to the effective SF energy,[19] i.e., the ratio of SF width in nc Al, over that in coarse-grained Al, can be described as

$$M_d = \frac{\gamma}{\gamma - \frac{Ga^2(8+\nu)}{48\pi(1-\nu)d}\ln\frac{\sqrt{2}d}{a}}. \tag{6}$$

Note that the energy difference between the partial dislocation core and the full dislocation core is ignored in the above derivation, because our calculation shows that the energy difference only has negligible effect on M_d in Eq. (6).

Another factor that affects the SF width is the applied stress. The edge components of $\mathbf{b}_1$ and $\mathbf{b}_2$ in Fig. 2 are opposite to each other. Therefore, a shear stress could drive *ab* and $a'b'$ further apart,[17] increasing the SF width. Assuming the resolved shear stress on the edge component of $\mathbf{b}_1$ or $\mathbf{b}_2$ is $\tau_\perp$ (see Fig. 2), the force that drives $\mathbf{b}_1$ and $\mathbf{b}_2$ apart can be described as

$$f_\tau = 2\tau_\perp b_\perp = \frac{\tau_\perp a}{\sqrt{6}}, \tag{7}$$

where $\mathbf{b}_\perp = \mathbf{b}_1 \sin 30^\circ$ is the edge component of $\mathbf{b}_1$.

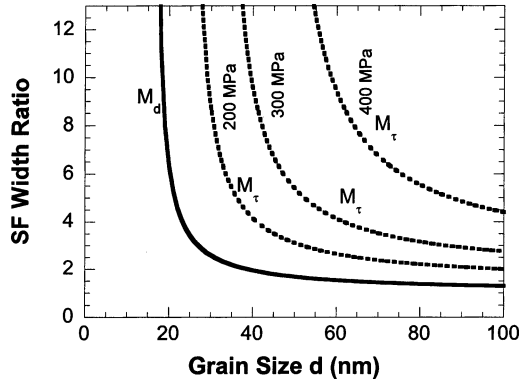

FIG. 3. The ratio of the SF width predicted by our model to that in coarse-grained Al vs grain size. The solid curve (M_d) considers only grain size effect while the dashed curves (M_τ) consider the effect of both grain size and dynamic stresses. The value of shear stress, $\tau_\perp$, is indicated near each M_τ curve. The stresses go to infinity at certain critical grain sizes, indicating that, below a certain grain size, the SF run across the whole grain and the model becomes invalid.

Taking into account this stress effect, the ratio of SF width in nc Al under stress, over that in coarse-grained Al under no stress, can be described by modifying Eq. (6) as:

$$M_\tau = \frac{\gamma}{\gamma - \dfrac{Ga^2(8+\nu)}{48\pi(1-\nu)d}\ln\dfrac{\sqrt{2}d}{a} - \dfrac{\tau_\perp a}{\sqrt{6}}}. \tag{8}$$

Using parameters appropriate for Al, G=35 GPa,[14] $\nu=0.345$, $a=0.404$ nm, $\gamma=122$ mJ/m^2,[17] we plot M_d versus d in Fig. 3 as the solid curve, which demonstrates that the SF width increases with decreasing grain size. It is also seen that with increasing stress, $\tau_\perp$, from 200 MPa to 400 MPa, the SF becomes significantly wider. Ball-milling produces random high dynamic stresses that vary in both magnitude and orientation. If allowed, after the dynamic stress vanishes, the partial dislocations would move to a SF width indicated by the solid curve in Fig. 3. However, a moving SF ribbon may frequently intersect with the high density of full dislocations[7] or other SF ribbons on three other {111} planes, creating dislocation jogs. These jogs could impede the movement of the partial dislocations after the dynamic stress vanishes. Therefore, some SFs we have observed using HRTEM may be wider than what is predicted by the solid curve in Fig. 3.

The above *semiquantitative* analysis demonstrates that the wide SFs in nc Al were formed due to small grain sizes and possibly also the interaction of SFs with a high density of dislocations inside grains.[7] Secondary factors include deformation strain rate, deformation temperature, proximity to free surfaces,[20,21] and impurities.[7] The combination of high strain rate and low temperature during cryogenic ball milling might also have promoted the SF formation in nc Al in this study.

The formation mechanisms of wide SFs presented here should also apply to other face-centered-cubic metals with high SF energy, such as Ni and Pd. However, in nc metals with low to medium SF energy, the SF ribbons may not exist inside nanograins. This is because the high SF energy is a major driving force for the emission of the trailing partial dislocations. Lower SF energy makes it easier to emit leading partials but harder to emit trailing partials. As a result, in nc metals with low to medium SF energies, SFs across the whole grain and deformation twins, instead of the SF ribbon, will be easily formed. This is exactly what happened in nc Cu (which has a medium SF energy) processed by high-pressure torsion,[9] in which no SF ribbon was observed, but deformation twins and SFs across grains were found ubiquitous.

In summary, we have investigated the formation mechanism of wide SF ribbons observed in nc Al. These SFs are surprising because their widths are 1.5–11 times higher than the experimental value in the literature.[16] These wide SFs were formed due to the grain size effect (via dislocation line tension and stress biasing effects) and possibly also due to the interactions between SFs and a high-density full dislocations. These wide SFs should also affect the mechanical behavior of nc Al, which needs further investigation.

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