Deformation Induced Microtwins and Stacking Faults in Aluminum Single Crystal

W. Z. Han, G. M. Cheng, S. X. Li, S. D. Wu,*,+ and Z. F. Zhang*,‡

Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China

(Received 4 March 2008; published 11 September 2008)

Microtwins and stacking faults in plastically deformed aluminum single crystal were successfully observed by high-resolution transmission electron microscope. The occurrence of these microtwins and stacking faults is directly related to the specially designed crystallographic orientation, because they were not observed in pure aluminum single crystal or polycrystal before. Based on the new finding above, we propose a universal dislocation-based model to judge the preference or not for the nucleation of deformation twins and stacking faults in various face-centered-cubic metals in terms of the critical stress for dislocation glide or twinning by considering the intrinsic factors, such as stacking fault energy, crystallographic orientation, and grain size. The new finding of deformation induced microtwins and stacking faults in aluminum single crystal and the proposed model should be of interest to a broad community.

DOI: 10.1103/PhysRevLett.101.115505 PACS numbers: 61.72.Nn, 61.72.Ff, 61.72.Mm, 68.37.Lp

Deformation twinning is well known from some fcc systems, such as brass, but is neither observed nor expected in aluminum single crystal and coarse-grained aluminum polycrystal, even when subjected to shock loading at low temperatures owing to the very high energy of its the planar faults [1–6]. The occurrence of deformation twinning in aluminum with a sufficiently small grain size has been suggested by recent molecular dynamics (MD) simulations [7–9]. Subsequent experiments conducted by Chen *et al.* [10], Liao *et al.* [11,12], and Wu *et al.* [13] indicate that twinning really occurred, but only in those nanocrystalline (NC) aluminum films under severe plastic deformation. In general, the reason for the nucleation of deformation twins in NC aluminum is attributed to the grain size effect [10–12]. However, whether deformation twinning can occur in pure aluminum single crystal or coarse-grained polycrystal still remains unknown.

It is well known that twinning is extremely difficult in fcc crystals because the large number (24) of slip systems makes slip a very efficient deformation mechanism. Only under very extreme conditions, such as strained at low temperature or at a high strain rate, could deformation twins nucleate in fcc metals. Numerous investigations indicate that many intrinsic and extrinsic factors have significant influence on the deformation twinning behavior of fcc metals, such as stacking fault energy (SFE), grain size, strain, strain rate, deformation temperature, deformation mode, etc. [2,3]. In addition, the effect of crystallographic orientation, one of the most important intrinsic factors in crystalline materials, has not been well understood on the deformation twinning behavior [2,3]. Recently, we have successfully acquired profuse deformation twins in a copper single crystal at room temperature and at a low strain rate through crystallographic orientation design [14]. Contrary to this result, many other researchers have processed a series of copper single crystals with random orientation by using equal-channel angular pressing (ECAP) [15,16] or other deformation methods [17–19]. Unfortunately, they detected only a few deformation twins or totally no twin in their experiments, demonstrating that crystallographic orientation does play a critical role in the nucleation of deformation twins in copper single crystals with mediate SFE. Based on the understanding of crystallographic orientation on twinning behavior in fcc crystal, it is natural to raise the interesting question of whether one can acquire deformation twins in pure aluminum single crystal deformed at room temperature and at a low strain rate through the special design of crystallographic orientation. Obviously, the corresponding experimental results will be beneficial for better understanding of the fundamental deformation mechanisms in various fcc metals.

The crystallographic orientation of the aluminum single crystal was specially designed with one of twinning systems, such as $(111)[\bar{1}\,\bar{1}\,2]$, just on the normal plane of intersection plane of ECAP die; in this case, the twinning system will acquire the maximum resolved shear stress [20], as schematically illustrated in Fig. 1(a). A sample of the aluminum single crystal with dimensions of 8 mm $\times$ 8 mm $\times$ 50 mm was prepared. Then the single crystal was extruded for only one pass by a right angle ECAP die at room temperature with extrusion rate of 5 mm/min and lubrication of MoS_2. After ECAP, the microstructures were observed by using a transmission electron microscope [(TEM), 200 kV JEM-2000FXII] and a high-resolution TEM [(HRTEM), 300 kV Tecnai G^2F30]. Thin foils for TEM were prepared by the twin-jet polishing method in a solution of 20% nitric acid and 80% carbinol in a voltage range of 8–10 V at room temperature.

After extrusion, many cell-block structures and microbands with the scale of 2 to 3 μm were developed [Fig. 1(b)]. However, in this scale, there is no any deformation twin in these microbands or cell-block substructures, which is different from the previous observations in copper single crystals [14]. The corresponding selected area dif-

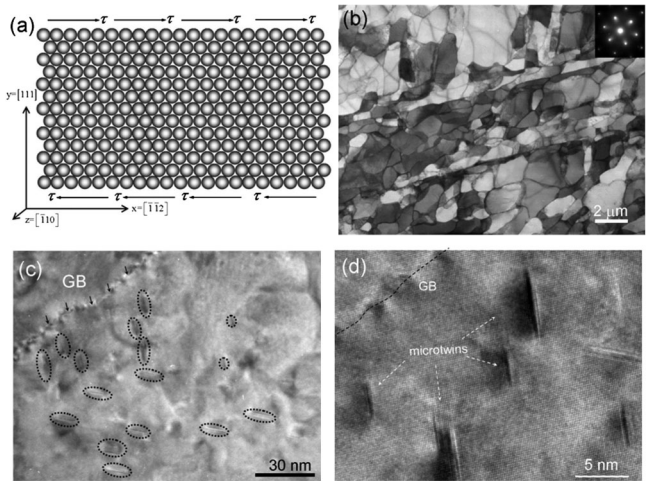

FIG. 1. Schematic illustration of the experimental design and the microstructure of as-extruded aluminum single crystal: (a) shear deformation is applied parallel to twinning plane and along twinning direction; (b) bright-field TEM micrograph showing as-extruded microstructure with subgrain size ranging from 2 to 3 μm; (c) HRTEM image of a region at the side of a subgrain boundary, two directions of strip structures can be seen, as indicated by the ellipses in the figure; (d) the magnified image of (c) at the region of subgrain boundary.

fraction pattern indicates that the misorientation among those substructures is small. HRTEM observation revealed that profuse nanoscale strips with regular shape were formed after ECAP in the interior of the subgrain, as labeled by the ellipses in Fig. 1(c). It is interesting to find that these strips mainly align along two directions with an intersecting angle of ~70°, which is very close to the dihedral angle of the two {111} planes. Figure 1(d) presents a magnified HRTEM image at the side of grain boundary (GB). It can be seen clearly that the subgrain boundary is made up of several dislocations. Further observations on the lattice image clarify that those strip structures are microtwins or stacking faults 1–2 atomic layers thick, as demonstrated in Fig. 1(d). Those with microtwins or stacking faults did not nucleate at the GB but only appeared in the interior of the subgrains.

Figure 2 shows a typical HRTEM image of the microtwins or stacking faults formed in different twinning systems, as labeled by 1 and 2 in the figure. The fast Fourier transform pattern of this region demonstrates that the stacking faults nucleate in two directions. Figures 2(b) and 2(c) are the magnified images of regions 1 and 2 in Fig. 2(a), respectively. From the atomic array pattern, it can also be confirmed that those strips are microtwins or stacking faults. Figure 3 demonstrates another HRTEM image of the microtwins or stacking faults formed in the present aluminum single crystal. Figures 3(b) and 3(d) are the magnified images of Figs. 3(a) and 3(c), respectively. Clear microtwins or stacking faults can be recognized in those figures. The current twinning mechanism in aluminum single crystal could be in accordance with the homogeneous nucleation mechanism suggested by MD simulation [7,8,21]. When the Shockley partials of two extended dislocations on the neighboring planes glide and are close to each other, the intrinsic stacking faults of the two dislocations in the overlapping region merge to form an extrinsic stacking fault [7,8,21]. This process can proceed further, for example, when the third extended dislocation joins the overlapped pair, an extrinsic stacking fault configuration transforms into a two-layer microtwin, as shown in Figs. 3(b) and 3(d).

The TEM observations above experimentally provide direct evidence confirming that microtwins or stacking faults really nucleate in aluminum single crystal deformed at room temperature and at a low strain rate, which was previously considered impossible because the SFE of aluminum is very high [1–5,7]. Regarding the twinning mechanism in fcc metals, several models have been proposed, and one of the common viewpoints is that deformation twins are created by stacking faults led by $1/6\langle 112\rangle$ Shockley partial dislocations [2,10,22–24]. Therefore, the required stress for nucleating a stacking fault or a microtwin in aluminum can be evaluated using the following

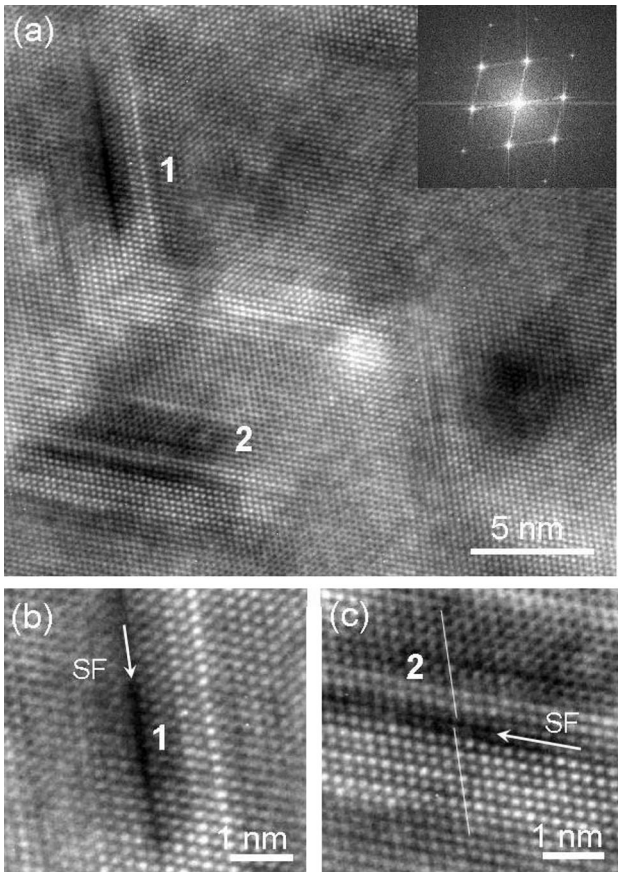

FIG. 2. (a) HRTEM micrograph showing the stacking faults formed in different twinning systems (marked by 1 and 2). (b), (c) The magnified images of regions labeled by 1 and 2 in (a), respectively. SF in (b) stands for stacking fault.

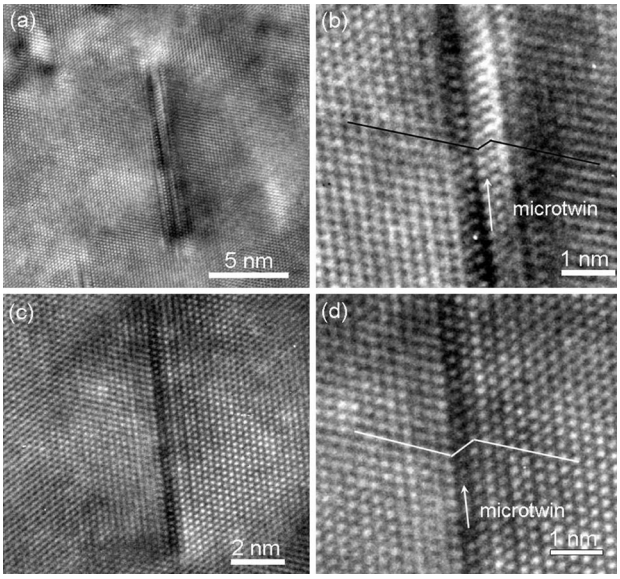

FIG. 3. HRTEM micrographs showing the formed microtwins and stacking faults in the as-extruded aluminum single crystal. (a) A microtwin or stacking fault with the length of about 10 nm formed in the interior of the subgrain. (b) The magnified image of (a). (c) Another example of a HRTEM image showing those strip structures are microtwins and stacking faults. (d) The magnified image of (c).

equation [10,22–24]:

$$\tau_{\text{required}} = \frac{1}{m}\left(\frac{Gb_P}{D} + \frac{\gamma}{b_P}\right). \quad (1)$$

Here G is the shear modulus ($\sim$35 GPa for aluminum), γ is the SFE (104–142 mJ/m^2 for aluminum [7]), b_P is the magnitude of the Burgers vector of the Shockley partial, D is the grain size, and m is the shear factor whose value varies from 0 to 1, depending on the relation between shear plane or shear direction and twinning plane or twinning direction [20]. In order to judge whether twinning can nucleate in any given fcc crystal, it is suggested that two main points should be considered. One is the required twinning stress (τ_{required}), whose value can be evaluated according to its intrinsic factors, such as SFE, crystallographic orientation, and grain size. Another one is the applied stress (τ_{applied}) by the external deformation conditions. Once the external loading mode matches the required twinning stresses ($\tau_{\text{applied}} > \tau_{\text{required}}$), deformation twins will naturally nucleate; otherwise, slipping will be the dominating deformation mechanism, as schematic illustrated in Fig. 4(a). For the present experiment, the aluminum single crystal was specially designed with a twinning system $(111)[\bar{1}\,\bar{1}\,2]$ just on one of the macroscopic shear deformation planes of ECAP [20]; hence, the present crystal acquires the most preferential orientation with the highest shear factor value ($m = 1$). After extrusion, most subgrains are refined to be approximately in the scale of $\sim$3 μm. Substituting all the parameters into Eq. (1), the required stress for nucleating a stacking fault in aluminum single crystal is evaluated to be in the range of 630 to 860 MPa. For the specially designed single crystal under severe plastic deformation, the activity of dislocation is constraint to some extent, while the resolved shear stress on the twinning system is the largest during extrusion.

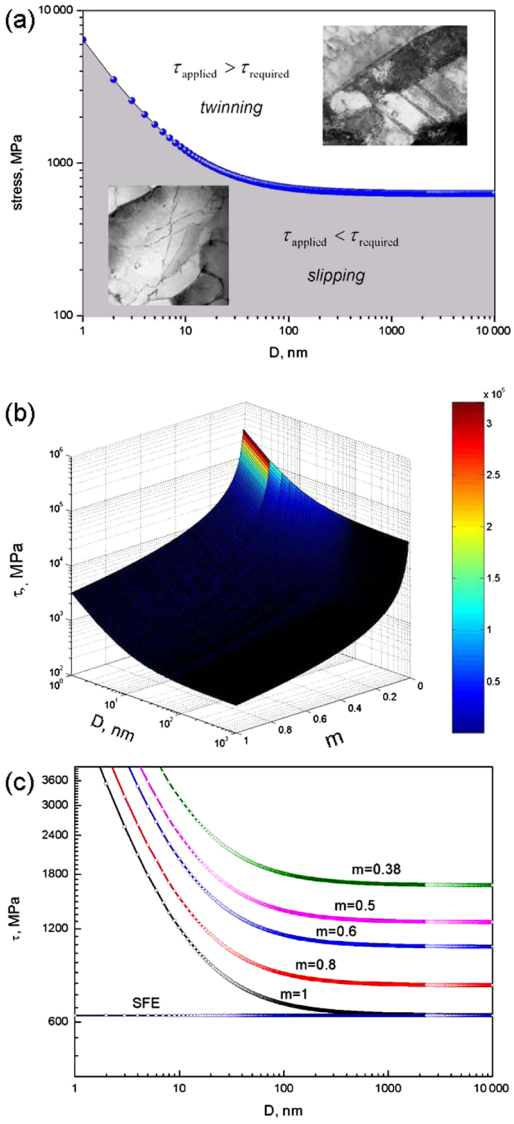

FIG. 4 (color online). (a) Schematic diagram of the correlation of slipping and twinning, in which τ_{required} is required twinning stress and τ_{applied} is the shear stress provided by the external deformation condition. The required twinning stress curve is plotted according to Eq. (1) for aluminum with $m = 1$. (b) Illustration of the required twinning stress varying with the grain size (D) and the crystallographic orientation (shear factor, m). (c) The plot for the required twinning stress of aluminum varying with the grain size for several orientations ($m = 1$, $m = 0.8$, $m = 0.6$, $m = 0.5$, $m = 0.38$), in which SFE is short for stacking fault energy. The horizontal line standing for the contribution of SFE keeps constant to twinning stress in different length scales.

Hence the local applied shear stress on a twinning system in aluminum single crystal is not difficult to accumulate to the critical value of required twinning stress, which may be the reason for the nucleation of profuse microtwins or stacking faults in the present aluminum single crystal even extruded at room temperature and at a low strain rate. In the MD simulation by Yamakov *et al.* [7,8], deformation twins nucleated at high stress level; for example, the values of applied shear stress in simulation has reached ~1 GPa in NC aluminum. Besides, the simulation conducted by Warner *et al.* [25] also demonstrates that the nucleation of deformation twins in aluminum is due to the high level of stress at the crack tip.

For simplicity, this model does not include the influence of the small Peierls-Nabarro stress and localized stress concentrations. Nevertheless, the predictions given by this model shed light on the experimentally observed trends in several ways. First, twinning stress can be evaluated according to the intrinsic factors of a certain fcc metal, such as SFE, crystallographic orientation, and grain size. Based on this, one can judge whether deformation twins can nucleate in a given fcc metal under certain deformation condition. Figure 4(b) demonstrates the required twinning stress of aluminum varying with the grain size and crystallographic orientation. If the applied shear stress is larger than the required twinning stress for certain grain size and orientation, twinning will naturally occur. Second, it can be found that, with the decrease in grain size, the twinning stress continually increases and the influence of SFE is gradually reduced, whereas the crystallographic orientation always plays an important role in deformation twinning, as schematically illustrated in Fig. 4(c). When grain size is smaller than a critical value D_C, the influence of size effect becomes larger than the contribution of SFE and will dominate the required twinning stress; hence, the difference in the SFE in various fcc metals can be neglected in this scale. Third, the present experiment indicates that crystallographic orientation has a remarkable influence on the behavior of deformation twinning in aluminum. According to Figs. 4(b) and 4(c), the twinning stress varies significantly with the crystallographic orientation; therefore, it needs more confined deformation conditions for the nucleation of deformation twins in those grains without the preferential orientations, such as in NC materials under severe plastic deformation [10–12,15]. This may be the main reason why no deformation twin was observed in aluminum by other investigators [5,6]. Finally, it is suggested that a number of deformation twins may appear in aluminum single crystal with the present preferential orientation subjected to ECAP at low temperature.

In summary, plastic deformation behaving in a twinning mode is often considered to be extremely difficult in the fcc metals with high SFE due to the prior slip deformation. The present investigation demonstrates direct evidence of twinning in aluminum single crystal and provides a new understanding on the physical nature of the fundamental plastic deformation mechanisms in various fcc metals and should be of interest to a broad community.

We are indebted to Mr. B. Wu and Ms. M. J. Zhang for their assistance in the HRTEM observations. This work was supported by the National Natural Science Foundation of China (NSFC) under Grants No. 50371090, No. 50171072, and No. 50571102. Z. F. Z. would like to acknowledge the financial support of "Hundred of Talents Project" by the Chinese Academy of Sciences and the National Outstanding Young Scientist Investigation under Grant No. 50625103.

*Corresponding author.
[+]shdwu@imr.ac.cn
[‡]zhfzhang@imr.ac.cn

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