Origin of deformation twinning from grain boundary in copper

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The occurrence of deformation twinning in face-centered-cubic (fcc) crystals with medium to high stacking fault energy is normally very difficult. Through specially designing the orientation of Cu single crystal, the authors do not only observe profuse nanoscale deformation twins with a tower shape originating from grain boundary but also find some of them terminated in the interior of the grain. The observations clearly prove that the deformation twinning can nucleate through successively emitting partials from grain boundaries, indicating the ubiquity of deformation twinning even in those fcc single crystals deformed at suitable conditions. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2938881]

As is well known, there are several plastic deformation modes driven by shearing, such as slipping, twinning, and kinking, in crystalline materials.[1] Twinning, one of the main plastic deformation modes, has been paid numerous attentions for more than half of century.[1–3] As far as the understanding of deformation twinning, two stages could be identified. The first stage is mainly concerned on the twinning behavior of coarse-grained (CG) materials.[2–9] Experimental studies reveal that twinning in CG face-centered-cubic (fcc) metals takes place only strained at low temperature and/or high strain rate conditions.[3–9] The main proposed twinning mechanism in this stage is the well known pole mechanism.[10,11] The second stage is the recent focus on twinning behaviors in ultrafine-grained (UFG) and nanocrystalline (nc) metals.[12–24] Molecular dynamic (MD) simulations predicted that nc metals should be more preferential for the nucleation of deformation twinning than their CG counterpart.[12–17] These predictions were, subsequently, verified in nc Al film, nc Ni, UFG Cu, and nc Ta,[18–22] indicating that grain size has an obvious influence on the twinning behaviors. The MD simulation[13,14] suggested that deformation twins in UFG and nc metals could nucleate via the dynamic overlapping of stacking fault ribbons formed by Shockley partial dislocations emitted from grain boundaries (GBs). Subsequently, several experiments[18–23] were conducted in order to clarify the deformation mechanism of UFG and nc materials. Those experimental results provide abundant evidences that the processes of twinning nucleation in UFG and nc metals have close relation with the GBs and the activity of partial dislocations, indicating that the detailed twinning mechanism is the same as the MD simulations.[18–23] From the above review, one may conclude that the twinning mechanism is the pole mechanism in CG metals and is the GB mediated mechanisms in UFG or nc metals. In the present work, the authors have made a finding of nanoscale twins with a tower shape nucleating at the GBs even in a deformed Cu single crystal subjected to equal channel angular pressing (ECAP) for only one pass. Those experimental observations may provide some convincing evidence that GB mediated twinning mechanism in UFG and nc metals may also be operational in larger grains or even in deformed single crystal.

This investigation concerns a Cu single crystal subjected to ECAP for one pass. The crystallographic orientation of the Cu single crystal was specially designed to make one of twinning systems, such as $(111)[\bar{1}\bar{1}2]$, just on the macroscopic shear deformation plane of ECAP, which has been described in more detail previously.[25,26] Such crystallographic design of the single crystal will greatly activate deformation twinning.[26] After ECAP, thin foils for transmission electron microscope (TEM) were prepared by twin-jet polishing method. High-resolution TEM (HRTEM) and TEM were performed on a 300 kV Tecnai G^2F30 and a 200 kV JEM-2000FXII, respectively. Previous investigations indicate that abundant deformation twins have nucleated in the Cu single crystal although extruded at RT and at low strain rate. Those twins can be divided into three types according to their locations and morphologies.[26] Some of deformation twins nucleated in the very fine ribbon structures in the region of shear bands, and most of them are in a scale of tens of nanometers except for few of them with a length larger than 100 nm, as reported in more detail elsewhere.[26]

Figure 1(a) is a typical bright-field TEM image showing a group of twins nucleated in a slightly larger ribbon structure in the region of shear band. Figure 1(b) is the corresponding dark-field image of Fig. 1(a). It can be found that many deformation twins nucleated at the boundaries of the wide band in the middle of Fig. 1. Some of the twins have penetrated through the whole ribbons, showing a tower shape, as marked by the large arrows in Figs. 1(a) and 1(b). While some other twins just nucleated at the GBs or already grew up, and stopped in the grain interior, as labeled by the relatively smaller arrows in Figs. 1(a) and 1(b). It is interesting to find that many deformation twins often terminated in the center of grain, rather reaching the opposite GB. Such heterogeneous nucleation of deformation twins and their morphology have been predicted in nc Al by MD simulation.[13,14] In the plot by MD simulation, twins nucleate via successively emitting Shockley partial dislocations from GBs.[13,14] At the very initial stage, those twins would grow layer by layer, forming a tower shape, so that the twin tip still stays in the interior of the grain. The present finding is well consistent with the scenario described by MD simula-

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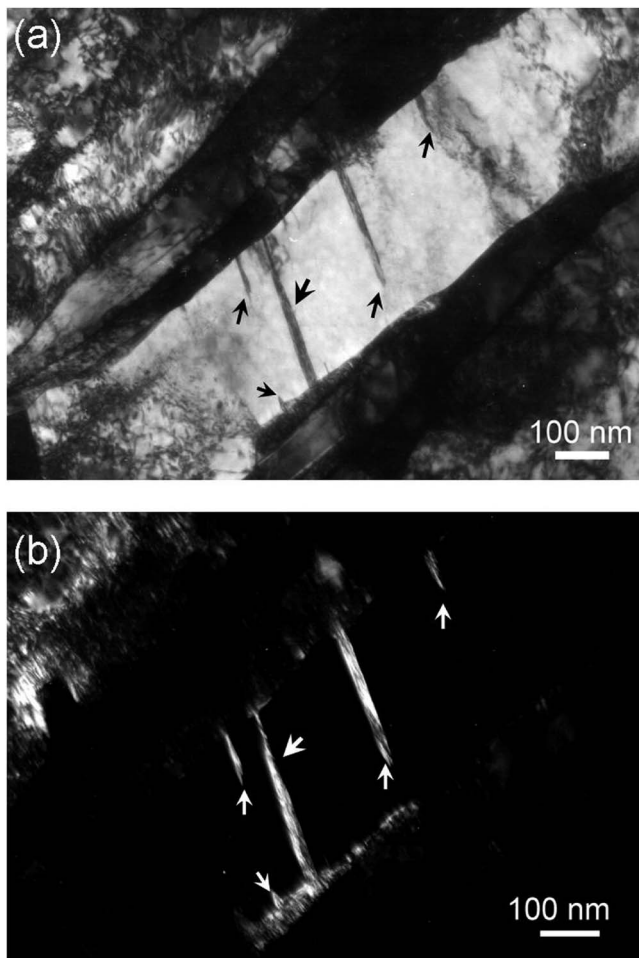
FIG. 1. (a) A typical bright-field TEM image of deformation twins nucleated at grain boundaries in a Cu single crystal after one-pass ECAP and (b) the corresponding dark-field image of (a).
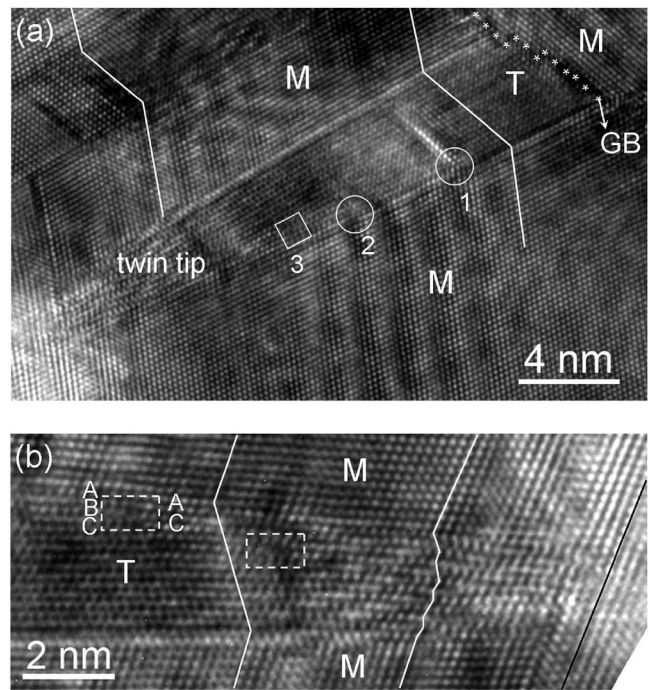

FIG. 2. (a) HRTEM [011] image of deformation twins nucleated at the grain boundary and stopped in the interior of the grain with many microtwins and stacking faults at the twin tip and (b) the magnification image of the twin tip in (a).

tion except for the difference in the length scale.[13,14] Therefore, further investigation on those twins can help us elucidate the twinning mechanism in fcc metals directly from the experimental observation.

Figure 2(a) presents a typical HRTEM image of a deformation twin nucleated at the GB and stopped in the interior of grain with a tower shape. It can be clearly seen that this region contains several deformation twins, the upper one has already formed, but the middle one is just in its developing stage. Figure 2(b) is the magnification image of the twin tip in Fig. 2(a). There are high densities of microtwins with the thickness of only one atomic layer, in front of the twin. These microtwins and stacking faults do not pass across the whole grain, but stop in the grain interior with Shockley partial dislocations (Burgers vectors $1/6\langle112\rangle$) located in the front boundaries of the microtwins and stacking faults, as shown in Fig. 2(b). It can be seen that there are several partial dislocations at the tilting boundary of the middle twins, as indicated by the square and circles and labeled by the number (1–3) in Fig. 2(a). The corresponding lattice image reveals that two kinds of partials might be observed, such as Shockley partials (marked by the circle) and Frank partials (marked by the square), as shown in Figs. 2(a) and 2(b). The deformation twin with a tower shape must evolve step by step through the activity of these partial dislocations. Some of them are just emitting from the boundaries, and have no sufficient energy to travel the whole grain. As a

result, they have to terminate in the interior of the grain. A series of such partials make up of the tilting boundary of the new formed twin. It is obvious that these twins should heterogeneously nucleate at a GB and grew into the grain interior via partial dislocation emission from the GB even in a plastically deformed Cu single crystal. Such heterogeneous twin nucleation and twin morphology have been predicted previously,[13,14] and were also observed in UFG or nc metals.[18–23]

Figure 3 shows another typical HRTEM image of a deformation twin nucleated at the GB and stopped in the interior of the grain. It can be seen that the twin did not grow into a tower shape. There is only one twin boundary at the upper part of Fig. 3 that divides the twin into domains I and II. Stacking faults can be discerned at the two twin boundaries. However, there are high densities of stacking faults, to some extent, which can also be regarded as microtwins with the thickness of only one atomic layer, at the lower part of domain II. These microtwins and stacking faults also stopped in the grain interior with Shockley partial dislocations located in the front boundaries of the microtwins and stacking faults. This twinning morphology is similar to the result observed by Liao *et al.*[20] in an elongated grain in nc Cu. These observations indicate that the formation of deformation twins is closely related to the activities of those stacking faults even in deformed single crystal. Our experiments suggest that the high density of GBs produced by severe plastic deformation provides numerous sources for the nucleation of twinning dislocations. In a small scale, twinning takes place by emission from the GB of successive $1/6[112]$ edge partial dislocations on adjacent (111) planes. These partial dislocations are the so-called twinning dislocations in the fcc lattice, and successively shift the (111) stacking plane, giving rise to the formation of a deformation twin. The investigations above clearly demonstrate that the twinning mechanism in
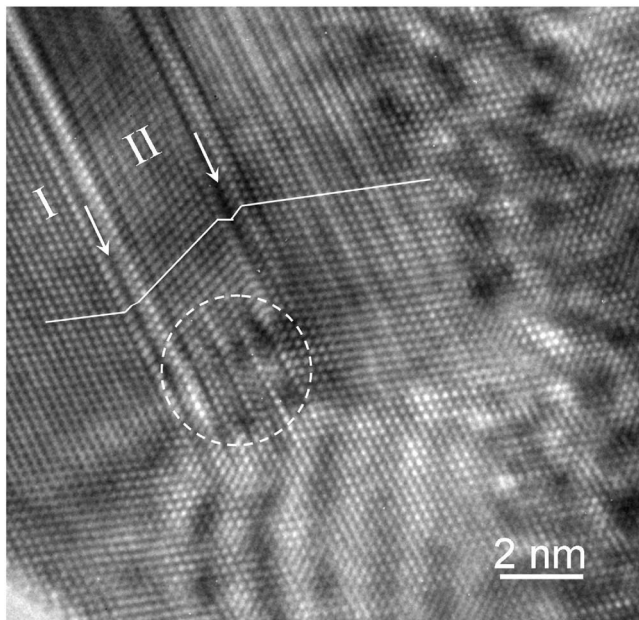
FIG. 3. A typical [011] HRTEM image of a deformation twin stopped in the interior of the grain. The upper part of the image shows only two twin domains I and II, while the lower part of II has a lot of microtwins and stacking faults ending in the interior of the grain.

deformed Cu single crystal during ECAP is identical to the prediction by MD simulations and experimental observations in UFG and nc metals.[13,14]

Finally, a remark can be made with respect to the results of previous investigation of various nc metals, where no similar twins with a tower shape were observed.[18–23] The nc metals in previous investigations have a grain size strictly under 100 nm. Simultaneously, those nc metals were, subsequently, loaded up to large strain, such as milling or rolling at cryogenic temperature.[18–23] The newly nucleated twinning partial dislocations should be driven by a high stress level to travel the relatively fine grains. While the deformation condition in the current experiment is relatively moderate. For example, the total applied equivalent strain is only $\sim$1 for one-pass ECAP.[24] The formed microstructures are slightly coarser in the ECAP experiments.[24,26] Also a special orientation was selected, which promotes deformation twinning easily. Due to the reasons above, profuse deformation twins could nucleate and some of them would just stop in the interior of grain while the loading has already completed. Therefore profuse tower-shape twins can be observed in the present specially designed experiments.

In summary, we report an experimental observation on deformation twins nucleated at GB in deformed Cu single crystal via the mechanism of successive emitting of Shockley partials. The present study provides some evidences that the GB mediated twinning mechanism may also be operational in larger grains, even in deformed single crystal. Besides, profuse deformation twins can be produced in the specially designed Cu single crystal subjected to ECAP for only one pass at RT and at low strain rate, demonstrating that the crystallographic orientation plays a critical role in the process of nucleating deformation twins.

[1]R. W. K. Honeycombe, *Plastic Deformation of Metals* (Cambridge University Press, Cambridge, 1969).
[2]J. W. Christian and S. Mahajan, Prog. Mater. Sci. **39**, 1 (1995).
[3]R. E. Reed-Hill, J. P. Hirth, and H. C. Rogers, *Deformation Twinning* (Gordon and Breach, New York, 1964).
[4]T. H. Blewitt, R. R. Coltman, and J. K. Redman, J. Appl. Phys. **28**, 651 (1957).
[5]G. T. Gray III, P. S. Follansbee, and C. E. Frantz, Mater. Sci. Eng., A **111**, 9 (1989).
[6]G. T. Gray III and J. C. Huang, Mater. Sci. Eng., A **145**, 21 (1991).
[7]M. A. Meyers, R. U. Andrade, and H. A. Chokshi, Metall. Mater. Trans. A **26**, 2881 (1995).
[8]M. A. Meyers, O. Vohringer, and V. A. Lubarda, Acta Mater. **49**, 4025 (2001).
[9]Y. S. Li, N. R. Tao, and K. Lu, Acta Mater. **56**, 230 (2008).
[10]A. H. Cottrell and B. A. Bilby, Philos. Mag. **7**, 573 (1951).
[11]J. A. Venables, Philos. Mag. **6**, 379 (1961).
[12]J. Schiøtz and K. W. Jacobsen, Science **301**, 1357 (2003).
[13]V. Yamakov, D. Wolf, S. R. Phillpot, A. K. Mukherjee, and H. Gleiter, Nat. Mater. **1**, 1 (2002).
[14]V. Yamakov, D. Wolf, S. R. Phillpot, and H. Gleiter, Acta Mater. **50**, 5005 (2002).
[15]K. Jacobsen and J. Schiøtz, Nat. Mater. **1**, 15 (2002).
[16]A. G. Froseth, P. M. Derlet, and H. Van Swygenhoven, Adv. Eng. Mater. **7**, 16 (2005).
[17]J. Wang and H. C. Huang, Appl. Phys. Lett. **85**, 5983 (2004).
[18]M. W. Chen, E. Ma, K. J. Hemker, H. W. Sheng, Y. M. Wang, and X. M. Cheng, Science **300**, 1275 (2003).
[19]X. Z. Liao, F. Zhou, E. J. Lavernia, S. G. Srinivasan, M. I. Baskes, D. W. He, and Y. T. Zhu, Appl. Phys. Lett. **83**, 632 (2003).
[20]X. Z. Liao, Y. H. Zhao, S. G. Srinivasan, Y. T. Zhu, R. Z. Valiev, and D. V. Gunderov, Appl. Phys. Lett. **84**, 592 (2004).
[21]X. Z. Liao, F. Zhou, E. J. Lavernia, S. G. Srinivasan, M. I. Baskes, D. W. He, and Y. T. Zhu, Appl. Phys. Lett. **83**, 5062 (2003).
[22]X. L. Wu and E. Ma, Appl. Phys. Lett. **88**, 061905 (2006).
[23]Y. M. Wang, A. M. Hodge, J. Biener, A. V. Hamza, D. E. Barnes, K. Liu, and T. G. Nieh, Appl. Phys. Lett. **86**, 101915 (2005).
[24]C. X. Huang, K. Wang, S. D. Wu, Z. F. Zhang, G. Y. Li, and S. X. Li, Acta Mater. **54**, 655 (2006).
[25]W. Z. Han, Z. F. Zhang, S. D. Wu, and S. X. Li, Acta Mater. **55**, 5889 (2007).
[26]W. Z. Han, Z. F. Zhang, S. D. Wu, C. X. Huang, and S. X. Li, "Orientation design for enhancing deformation twinning in Cu single crystal subjected to equal channel angular pressing," Adv. Eng. Mater. (unpublished).