

Self-thickening, cross-slip deformation twinning model

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We propose a cross-slip deformation twinning model based upon our experimental *in situ* deformation of Cu–Ge alloys using a transmission electron microscope. During the deformation, Shockley partials are emitted from the grain boundaries, which encounter an obstacle within the grain and split to nucleate deformation twins in the cross slip as well as primary planes. Upon further deformation a thickening process for twins is directly observed. The proposed model provides a dislocation mechanism for the observed simultaneous twin thickening in both the cross-slip and primary planes. The role of the proposed mechanism in the deformation of nanocrystalline materials is discussed. © 2008 American Institute of Physics.

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Twinning is an important mechanism of deformation in hexagonal-close-packed metals because of the lack of five independent slip systems. In body-centered-cubic metals, twinning is observed at lower temperatures because the yield stress rapidly increases with decreasing temperatures. In face-centered-cubic (fcc) metals, twinning is usually not observed in coarse-grained structures with medium to high stacking-fault (SF) energy at normal rates of deformation and room temperature.^{1–6} However, twinning has been observed in fcc metals under the following conditions: low-temperature deformation,⁶ high-strain rate deformation,^{6,7} severe plastic (large strain) deformation, and deformation of nanocrystalline materials.^{2,3,8–12} Contrary to coarse-grained metals, which become more difficult to deform by twinning with decreasing grain size, nanocrystalline materials may deform via partial dislocations originated from grain boundaries as elucidated by molecular dynamics simulation studies^{4,5,13,14} and experimental observations.^{1,3,8,15,16} This leads to the formation of SFs and deformation twins. It has been proposed that there is a critical size in the nanoscale regime below which dislocations cannot be created within the grain, and this limit is found to be lower for partial dislocations compared to that for perfect dislocations.¹⁷ However, *in situ* experimental observations on the formation of partial dislocations and deformation twins have been lacking.

The aim of the present work was to study the details of dislocation emission by grain boundaries and twin formation during *in situ* deformation of Cu–Ge (5 at. %) alloy. The Ge alloying reduces the SF energy so that we can study the details of dislocation emission by grain boundaries and the formation of deformation twins in large grains.

We have designed a special *in situ* deformation holder, where the specimen can be tilted along both axes during the deformation process. This feature permits us to achieve constant diffraction conditions during controlled introduction of strain into the specimen. The unique idea employed in this holder is that bending a microscope specimen prepared from a plate dimpled on one side can cause tensile deformation in the thin foil region in a controlled way. Figure 1 shows the

specimen holder in its normal position with respect to the drive mechanism, which is mounted in one of the ports of the transmission electron microscopy (TEM) specimen chamber. The drive mechanism consists of a micrometer which primarily transmits rotary motion to the screw drive on the holder and also provides readout for the estimation of specimen strain. A telescoping drive shaft is attached to the micrometer shaft with a universal joint, and the ball and pin arrangement of the screw drive couples into a slotted socket on the drive shaft to give a universal joint held in mesh by spring extension of the drive shaft. This combination of universal joints and telescoping drive shaft provides complete freedom of the stage translation and tilting motions. The micrometer can be manually operated, however, it was found preferable to employ the motor drive shown in Fig. 1, which consists of a 1 turn/min motor, gear reduced to 0.1 turn/min. From the specimen geometry and the mechanical displacement, estimates of the strain introduced can be made and reproducible increments of strain in the range of 10^{-5} s^{-1} are introduced in a controlled way.

Figures 2(a) and 2(b) show illustrative examples of bright-field electron micrographs from the same area with an incremental strain. There were no SFs or twins observed before the deformation. During the deformation, a partial dislocation was emitted from the grain boundary labeled G1 into the grain along the primary $\{111\}$ plane P1. Subse-

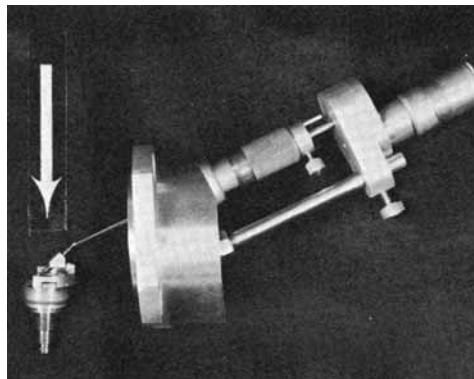


FIG. 1. *In situ* TEM deformation holder coupled with external drive mechanism.

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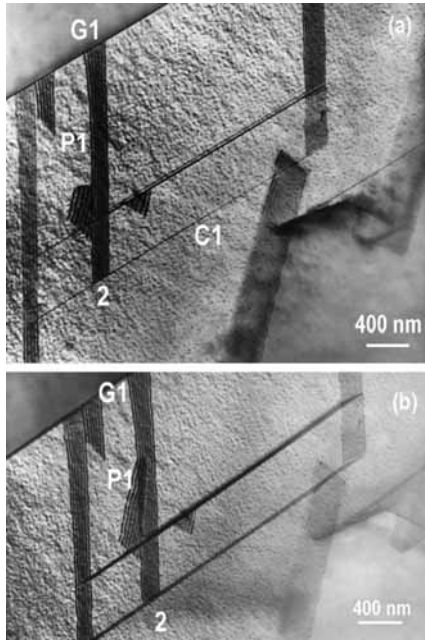


FIG. 2. Two TEM micrographs from the series of micrographs as a function of strain (with increments of about a strain of 10^{-4}) showing fringes caused by twin formation. (a) Shockley partial dislocation emission from G1 along P1 meets obstacle at 2 and cross slips along C1. (b) Thickening of twin on both planes as a function of increasing strain.

quently, the partial was observed to encounter an obstacle (at 2), where another partial was emitted and observed to slip in the cross-slip plane (C1). This process formed SFs on both the primary slip plane P1 and the cross-slip plane C1. As the deformation with an incremental strain of 10^{-5} was continued, twins were formed and grew in thickness in both C1 and P1 planes [Fig. 2(b)]. It was interesting to see that partials were generated at 2, which contributed to the thickening of the twins in both planes. The thickening of the twins in both planes can be clearly observed in Fig. 3, where the areas near G1 and 2 in Fig. 2(a) and 2 in Fig. 3(b) are shown at a higher magnification.

Based upon our experimental observations, we propose a mechanism of twin formation during *in situ* deformation. The grain boundaries provide dislocation sources where a perfect dislocation splits into a leading and a trailing Shockley partials in the primary slip plane P1, according to

$$\frac{a}{2}[1\bar{1}0](111) \rightarrow \frac{a}{6}[1\bar{2}1](111) + \frac{a}{6}[2\bar{1}\bar{1}](111). \quad (1)$$

The trailing partial stays with the boundary G1 and the leading partial encounters an obstacle within the grain at 2. Upon encountering the obstacle, the leading partial $(a/6) \times [1\bar{2}1]$ splits into a perfect dislocation (CB), and a twinning partial ($B\delta$) in the cross-slip plane C1, $(11\bar{1})$, a stair-rod dislocation ($\delta\alpha$), i.e., $C\alpha \rightarrow CB + B\delta + \delta\alpha$, according to Eq. (2) and Fig. 4. This is energetically unfavorable reaction, however, it can occur under stress concentration in the localized regions aided by *in situ* deformation,

$$\frac{a}{6}[1\bar{2}1](111) \rightarrow \frac{a}{2}[1\bar{1}0](111) + \frac{a}{6}[\bar{1}2\bar{1}](11\bar{1}) + \frac{a}{6}[\bar{1}\bar{1}0]. \quad (2)$$

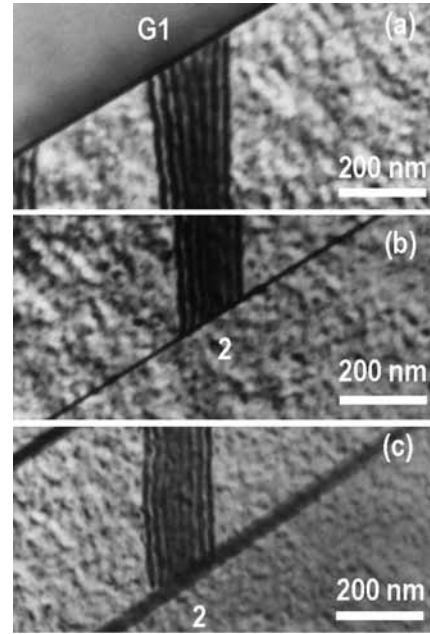


FIG. 3. Enlarged TEM images from Fig. 2. (a) and (b) are from Fig. 2(a) and (c) is from Fig. 2(b).

The perfect $(a/2)[1\bar{1}0]$ dislocation can cross slip on the $(11\bar{1})$ C1 planes onto the adjacent (111) P1 plane (Fig. 4). After the cross slip, the perfect dislocation splits into two partials according to Eq. (3), where the leading partial $(a/6)[1\bar{2}1]$ repeats the process in Eq. (2) and the other partial $(a/6)[2\bar{1}\bar{1}]$ slips back to the grain boundary on the primary P1 plane,

$$a/2[1\bar{1}0] \rightarrow \frac{a}{6}[1\bar{2}1](111) + \frac{a}{6}[2\bar{1}\bar{1}](111). \quad (3)$$

The dislocation reactions in Eqs. (2) and (3) provide a full reaction cycle that can be repeated to simultaneously thicken the twins on the successive primary slip plane and cross-slip plane, without the need of the nucleation or emission of additional Shockley partial dislocation from the grain boundary. In other words, once a Shockley partial dislocation is emitted from a grain boundary and the partial is blocked at a barrier, this mechanism would enable the two twins to grow on a primary slip plane and a cross-slip plane by themselves. This is in contrast with a ‘‘stair-rod cross-slip’’ mechanism proposed by Fujita and Tori.¹⁸ In their model, the partial dislocation ($C\alpha$) on the primary plane P1 will form at the

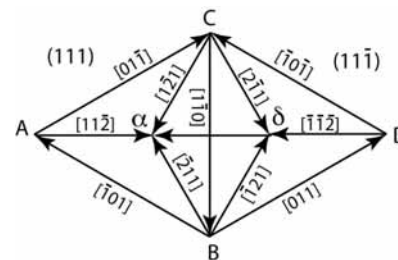


FIG. 4. Partial dislocation reactions and their reactions in the primary plane P1, (111) , and cross-slip plane C1, $(11\bar{1})$.

barrier a stair rod dislocation ($\delta\alpha$), and a partial ($C\delta$) that slips on the cross-slip plane C1, i.e., $C\alpha \rightarrow \delta\alpha + C\delta$. The model does not provide a mechanism for the twins to grow by themselves. Additional partials on successive planes need to be emitted from the grain boundary for the twins to thicken. However, this is a highly implausible, if not impossible, scenario.

The self-thickening, cross-slip twinning mechanism proposed here could play an important role in the deformation of nanocrystalline fcc materials, particularly below a critical grain size where intragrain deformation requires a very high energy (high stress). The high energy could overcome the high-stress requirement for operating the proposed mechanism. It has been reported that partial dislocation emissions and deformation twinning become significant deformation mechanisms in nanocrystalline fcc metals that have medium-to-high SF energies and usually do not deform by twinning.^{1-5,10-16} Dislocation emission from grain boundaries plays an important role in the formation of twins in nanocrystalline fcc metals,^{4,5,11} and most conventional twinning mechanisms¹⁹⁻²³ that operate in coarse-grained metals no longer operate in nanocrystalline materials. It has been a challenge to explain the sources of partials needed for twin growth since it is not plausible to nucleate partials on successive slip planes on the grain boundary. The mechanism proposed here could be one of the mechanisms for twin nucleation and growth in nanocrystalline fcc metals. Further study is under way to explore this issue.

In summary, we have proposed a self-thickening, cross-slip twinning mechanism to explain a simultaneous twinning on primary and cross-slip planes observed under *in situ* TEM experiments. The model provides a mechanism for the twins to thicken by themselves without the help of additional partials from the grain boundary. This model could play a significant role in nanocrystalline fcc metals because of the high

deformation stress and the significantly enhanced twinning activities.

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