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The Effect of Twin Plane Spacing on the Deformation of Copper Containing a High Density of Growth Twins

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In-situ tensile straining in a transmission electron microscope was used to investigate the role of twin plane spacing on the deformation and fracture mechanism of pure copper containing a high density of nanoscale growth twins. Real-time and post-mortem observations clearly reveal that twin plane spacing plays a key role in determining the operative deformation mechanism and therefore the subsequent crack propagation path. The deformation mechanism transition, which results from changes in the twin plane spacing, has implications for interpreting the unusual mechanical behavior of the copper with a high density of nanoscale growth twins.

INTRODUCTION

It has been experimentally established that the presence of a high density of nanoscale growth twins can impart extremely high strength and hardness to a metal.¹⁻⁴ This suggests that these materials may exhibit unique plastic deformation mechanisms that are not seen in comparable, coarse-grained materials. Unlike deformation that proceeds via mechanical twinning—a topic that has been studied for many years⁵—the deformation of pre-existing twins (i.e., twin deformation) with their average twin plane spacing (TPS) at nanoscale is a relatively new area of research. Consequently, there is renewed interest in the study of twin-related deformation and fracture processes.⁶⁻¹⁵ It has been shown that TPS plays a key role in determining the final strength of these materials.¹³ There have been several studies that address the unusual mechanical behavior of

these materials by considering the interaction between dislocations and twin boundaries.^{2,11} However, direct experimental evidence on how TPS affects the deformation mechanism, especially at the nanoscale, remains elusive.

The authors investigated TPS-related

deformation and associated fracture of pulsed-electrodeposited pure copper using in-situ tensile straining in the transmission electron microscope (TEM) (for details on the experimental approach, see References 16 and 17). The high-purity copper (details of the sample preparation procedure, purity, and density can be found elsewhere²) used in the study has a high inherent density of nanoscale growth twins, which gives rise to unusual mechanical behavior—specifically high strength and ductility. Real-time and post-mortem observations clearly reveal that TPS plays a key role in determining the operative deformation mechanism and therefore the subsequent crack propagation path. For TPS larger than ~30 nm, twin boundaries (TBs) are observed to serve as both barriers to slip propagation and sources for dislocation nucleation, with a subsequent fracture pathway following clear crystallographic directions. However, when the TPS is reduced to less than ~30 nm, a transition in the mechanism of crystal plasticity occurs. Deformation is no longer dominated by the motion of full dislocation within the twins, but rather via partial dislocation motion associated with TB migration. At this point, the fracture pathway loses its strict crystallographic character.

EFFECT OF TWIN PLANE SPACING ON CRACK MORPHOLOGY

One typical example is given in Figure 1. Figure 1a is a bright-field TEM image that shows the typical path of a propagating tensile crack as it crosses twin groups with their average TPS above the critical value (i.e., ~ 30 nm).

How would you...

...describe the overall significance of this paper?

The deformation mechanism transition which results from changes in twin plane spacing has implications for interpreting the unusual mechanical behavior of copper with a high density of nanoscale growth twins.

...describe this work to a materials science and engineering professional with no experience in your technical specialty?

We report in-situ, dynamic transmission electron microscope observations of the deformation of twin copper. It was found that when the twin plane spacing is reduced to 30 nm or so, deformation is no longer dominated by the motion of full dislocation within the twins, but rather via partial dislocation motion associated with TB migration. The general application of this finding is in interpreting the extremely high strength achieved in copper with high-density nanoscale growth twins.

...describe this work to a layperson?

The tenet that "smaller is stronger" has been well known in the field of materials science. Through using in-situ tensile straining in the transmission electron microscope, we revealed that the extremely high strength of pure copper stems from the nanoscale twin plane spacing.

It is worth noting that both of the twin groups indicated in Figure 1a are located in the same grain, with their boundaries parallel to each other. This ensures that the stress imposed on the two twin groups is similar and therefore validates the following comparison. Dynamic observations show that when the propagating tensile crack approaches twins with a larger TPS (typically >30 nm), it will first become blunted by the TBs. Shortly thereafter, another crack will nucleate on the other side of the TBs. Trace line analysis indicates that the matrix/twin slip system on the crack side of the TB was usually redirected onto the corresponding twin/matrix slip system on the other side. Consequently, the crack edges

usually follow specific crystallographic directions, as shown, for example, in Figure 1b and 1c, which are magnified images from the left-hand side and right-hand side areas, respectively, of the twin group indicated by arrow 1 in Figure 1a. Altogether, three twin lamellae (i, ii, and iii, as indicated in Figure 1b and 1c) were identified in this area. The thickness of twin lamellae i, ii, and iii are 56.2 nm, 26.4 nm, and 68.5 nm, respectively. The measurement errors are better than 0.2 nm based on pixel measurement. For twin lamellae i and iii, the crack edges clearly followed a specific crystallographic direction. Given that the incident beam direction was [110], the measured co-angles between the crack edges and the trace line

are roughly consistent with the theoretical values of that between $[\bar{1}10]$ and [112] directions, as indicated in Figure 1c. For lamella ii, however, although the crack path on the left-hand side (Figure 1b) followed the same crystal direction as that of lamellae i and iii, the crack edge on the right-hand side displayed some deviation by showing a curved morphology. This suggests that TPS has an important effect on the resulting crack morphology and therefore the operative deformation mechanism. The semicircular strain contrast indicated by the arrows in Figure 1b suggests sites that may serve as dislocation sources. This, plus the presence of the abundant dislocations detected post-mortem inside of the twin lamellae and at the TBs, indicates crystal plasticity is occurring mainly within the twins, consistent with the observations of plasticity via full dislocation motion for materials with larger TPS (>30 nm).

Additional observations of the effect of TPS on crack morphology are provided in Figure 1d and 1e, which are magnified images of the left-hand side and right-hand side areas of the crack indicated by arrow 2 in Figure 1a, respectively. The TPS of these four twin lamellae fell between 10 nm to 30 nm. The two protrusions, lamella III in Figure 1d and lamella I in Figure 1e, exhibited very little crystallographic character. In addition, in contrast to the frequent dislocations observed inside the twins with larger lamella thickness (Figure 1b and 1c), few dislocations can be detected inside of the smaller twin lamellae. Additionally, the TBs themselves appear to be dislocation free. This suggests that dislocation activity, such as dislocation nucleation and propagation, has been largely suppressed on the other two inclined slip planes in these narrowly spaced twin groups. However, it was at first surprising to see that the TPS on the left-hand side of the crack was much different from that of the right side. For example, the TPS of lamellae I, II, III, and IV in the left side (Figure 1d) are about 27.7 nm, 22.1 nm, 21.8 nm, and 12.6 nm, respectively. However, the corresponding values in right side (Figure 1e) are about 25.4 nm, 28.9 nm, 13.4 nm, and 22.6 nm, respectively. Measurement errors are again better than ± 0.2 nm. Be-

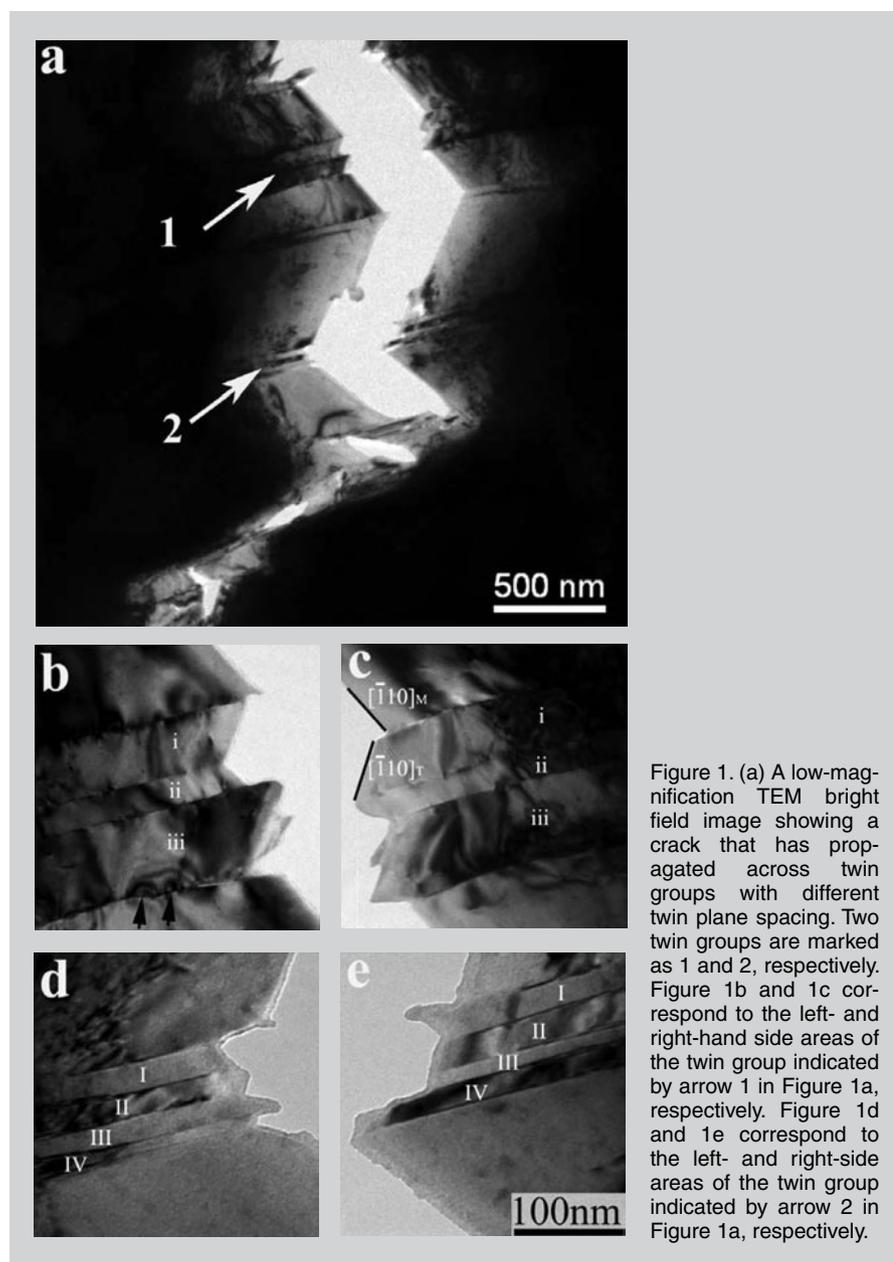
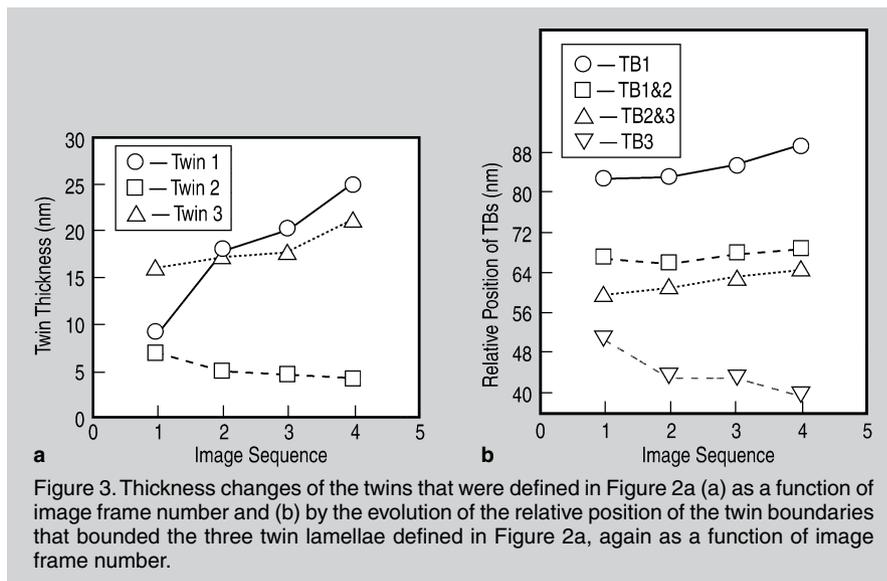


Figure 1. (a) A low-magnification TEM bright field image showing a crack that has propagated across twin groups with different twin plane spacing. Two twin groups are marked as 1 and 2, respectively. Figure 1b and 1c correspond to the left- and right-hand side areas of the twin group indicated by arrow 1 in Figure 1a, respectively. Figure 1d and 1e correspond to the left- and right-side areas of the twin group indicated by arrow 2 in Figure 1a, respectively.

cause the twin lamella of as-deposited copper always shows relatively uniform thickness,² presumably the TPS changes resulted from the migration of TBs in response to the local deformation.

MIGRATION OF TWIN PLANES DURING DEFORMATION

Twin boundaries, especially coherent TBs, are generally considered to be stable structures in materials due to their low energy state. However, the aforementioned analysis clearly shows that TBs experience apparent migration during deformation, especially for twins with smaller TPS (typically less than 30 nm). In order to understand the origins of this behavior, the authors focused special attention on the response of nanoscale twin groups during applied tensile deformation. One such example is shown in Figure 2. In this case, the far field external force from the tensile holder resulted in a shear stress on the twin group, with its direction approximately parallel to the TBs. At the start of the observation, more than



five twins could be identified with TPS ranging from 5 nm to 15 nm (Figure 2a). For convenience, the lower three twin lamellae are marked as 1, 2, and 3, respectively, as shown in Figure 2a. Only one load step later, twin lamella 3 was observed to double its size by “consuming” its upper neighbors (Figure 2b). Further load steps caused lamella 1 and 3 to expand and lamella 2

to shrink (Figure 2c and 2d).

To analyze the migration of the twin planes during this event quantitatively, the authors chose the corner of a large bright feature as a reference point (indicated by the white arrows in Figure 2a–d). It can be seen from Figure 2a–d that there are no obvious changes in either shape or contrast for this large bright feature during the observation period. By drawing a straight line starting from the reference point that is also perpendicular to the trace lines of the TBs (Figure 2a), both the TPS of twins and the relative position of the twin planes can be tracked. The results are plotted in Figure 3. After the first loading step, the spacing of the two planes that bounded the twin lamellae 3 increased sharply from about 9 nm to 18 nm (Figure 3a). The latter is roughly equal to the sum of lamella 3 and its two upper neighbors in Figure 2a. Other than this sharp size increase at the onset of the loading sequence, there was a steady increase of TPS of lamellae 1 and 3, and a steady decrease of TPS of lamellae 2 with increasing loading. The trend seen so far appears that larger twin lamellae grew at the expense of smaller twin lamellae. However, as shown below, this is not always the case.

Figure 3b shows the relative position of the four twin planes that bounded the three twin lamellae defined in Figure 2d. For convenience, we have defined the twin plane that connected twin lamellae *i* and *j* as TB_{*i*&*j*}, where *i*, *j* = 1, 2, and 3. It can be seen in Figure 3b that the two twin planes (TB₃

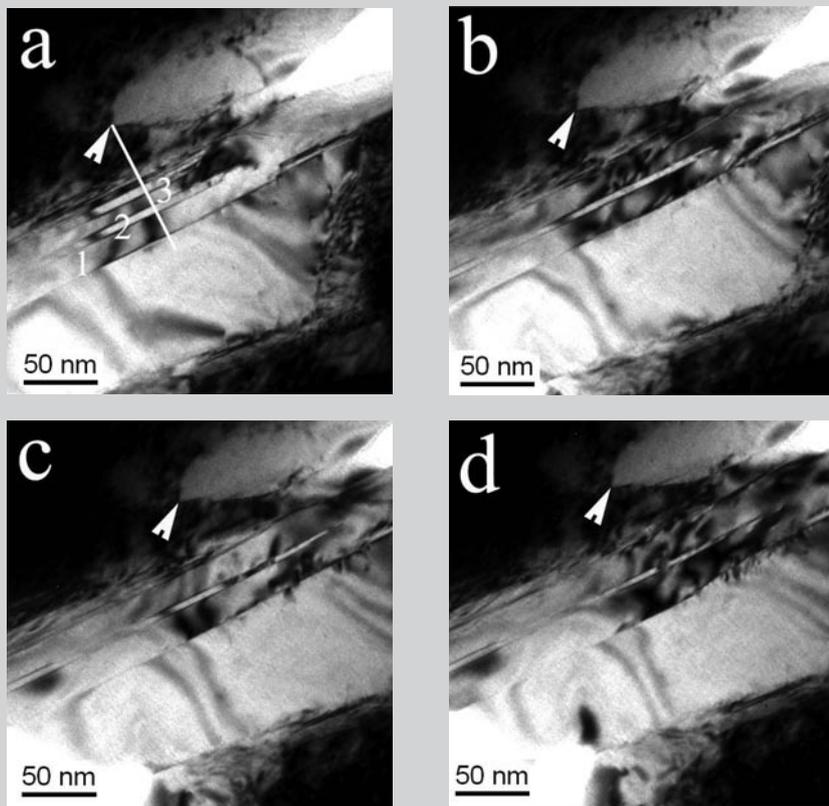


Figure 2. A sequence of still images captured during an in-situ deformation test in the TEM. Images a–d show the twin plane spacing evolution with the increasing loading steps.

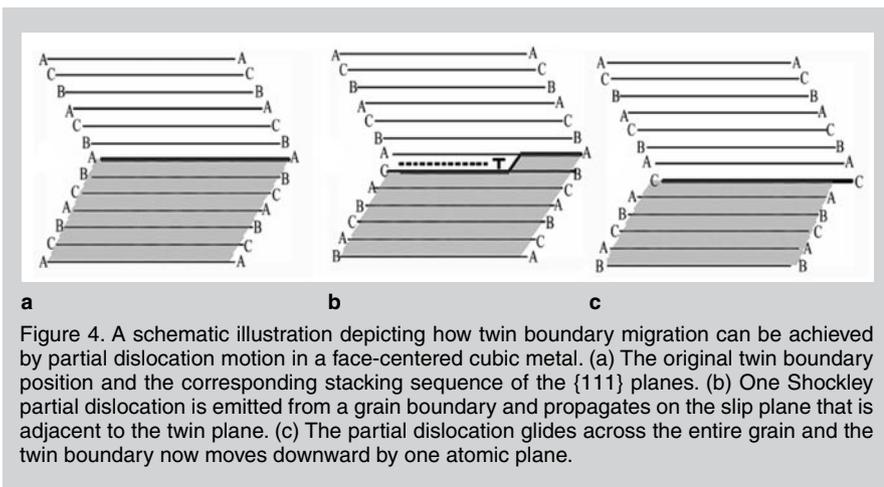


Figure 4. A schematic illustration depicting how twin boundary migration can be achieved by partial dislocation motion in a face-centered cubic metal. (a) The original twin boundary position and the corresponding stacking sequence of the {111} planes. (b) One Shockley partial dislocation is emitted from a grain boundary and propagates on the slip plane that is adjacent to the twin plane. (c) The partial dislocation glides across the entire grain and the twin boundary now moves downward by one atomic plane.

and $TB_{2\&3}$) that bounded twin lamella 3 moved outward under the influence of the external applied stress. This is consistent with the observation that larger twins grew at the expense of the smaller twins adjacent to them. However, TB_1 and $TB_{1\&2}$ do not seem to follow this rule. Both of these TBs moved toward the side with larger TPS. This simply suggests that it may not be the TPS, but the local stress condition that decides the migrating direction of the twin planes.

So far, the observations presented in this paper strongly indicate that TB migration or even annihilation will most likely occur for twin lamellae with TPS less than 30 nm or so. This is qualitatively consistent with the results of molecular dynamics simulations which have shown that the presence of grown-in twins in nanocrystalline aluminum enhance plastic deformation by means of TB migration.¹⁸ For the face-centered-cubic (fcc) copper studied here, a TB can be defined as the plane at which the normal ABCABC stacking sequence of (111) planes is reversed, creating a (111) mirror plane: ABCAB-CACBACBA (as indicated in Figure 4a). From a crystallographic viewpoint, the TB migration process can be schematically illustrated as shown in Figure 4. The solid lines represent the (111) planes and the original twin boundary plane is highlighted with a bold solid line (Figure 4a). Initially, the (111) planes have an ACBACBACBACBA sequence and the twin plane consists of atoms on A positions. Under the influence of an external applied force (presumably a shear stress on the twin plane), a Shockley partial dislocation

($\langle 112 \rangle / 6$ type) can be emitted from the intersection of a TB and a grain boundary, and can further propagate on adjacent (111) planes. If we choose the shaded area as a reference, the stacking sequence of (111) planes on the left side now becomes ACBACBACAB-CAB and the twin plane on the left side of the dislocation becomes the atomic plane with a C position (Figure 4b). Before the Shockley partial propagates throughout the entire grain, the stacking sequence on the right-hand side remains unchanged and the TB is now disconnected by a jog or step. Once the Shockley partial dislocation propagates throughout the entire grain, the step(s) on the TB will be removed and the twin plane now becomes a plane with atoms at C positions, as shown in Figure 4c. Experimentally, when viewed along the [110] direction, the TB profile is determined by the number of Shockley partials which have been emitted but have not yet propagated throughout the entire grain. The mechanistic process envisioned from the observation was confirmed recently by Y.B. Wang et al.¹⁹

CONCLUSION

It appears that at a TPS of 30 nm or so, there is a transition in plastic deformation mode. At larger sizes, dislocation nucleation and propagation within the twin lamella is dominant, while at smaller sizes, twin plane migration with the motion of Shockley partials tends to dominate. Presumably, this is due to the competition between the stress necessary to nucleate perfect dislocations and the stress necessary to activate the partial dislocation slip. Taking 30 nm

as the critical size, and letting it equal the source size, an estimate of the stress necessary to nucleate a full dislocation can be made from dislocation theory.²⁰ Using this simple criterion, we find this stress to be on the order of 700 MPa for copper. This value should correspond to the lower bound of the stress necessary to favor twin boundary migration via partial dislocation motion. Consequently, it is expected that a high density of nanoscale twins will impart extremely high strength, as seen experimentally in copper.²

References

1. Y.F. Shen et al., *Scripta Mater.*, 52 (2005), pp. 989–994.
2. L. Lu et al., *Science*, 304 (2004), pp. 422–426.
3. X. Zhang et al., *Appl. Phys. Lett.*, 84 (2004), pp. 1096–1098.
4. X. Zhang et al., *Acta Mater.*, 52 (2004), pp. 995–1002.
5. J.W. Christian and S. Mahajan, *Progress in Materials Science*, 39 (1995), pp. 1–157.
6. A.G. Froseth, P.M. Derlet, and H. Van Swygenhoven, *Adv. Eng. Mater.*, 7 (2005), pp. 16–20.
7. X.Z. Liao et al., *Appl. Phys. Lett.*, 84 (2004), pp. 592–594.
8. H. Rosner, J. Markmann, and J. Weissmüller, *Phil. Mag. Lett.*, 84 (2004), pp. 321–334.
9. Y.M. Wang et al., *Appl. Phys. Lett.*, 86 (2005), no. 101915.
10. N. Jia et al., *Scripta Mater.*, 54 (2006), pp. 1247–1252.
11. Z.H. Jin et al., *Scripta Mater.*, 54 (2006), pp. 1163–1168.
12. A.G. Froseth, P.M. Derlet, and H. Van Swygenhoven, *Scripta Mater.*, 54 (2006), pp. 477–481.
13. L. Lu et al., *Acta Mater.*, 53 (2005), pp. 2169–2179.
14. W.S. Zhao et al., *Scripta Mater.*, 53 (2005), pp. 745–749.
15. R.J. Asaro and S. Suresh, *Acta Mater.*, 53 (2005), pp. 3369–3382.
16. Z.W. Shan and S.X. Mao, *Adv. Eng. Mater.*, 7 (2005), pp. 603–606.
17. Z.W. Shan et al., *Science*, 305 (2004), pp. 654–657.
18. A. Froseth, H. Van Swygenhoven, and P.M. Derlet, *Acta Mater.*, 52 (2004), pp. 2259–2268.
19. Y.B. Wang, M.L. Sui, and E. Ma, *Phil. Mag. Lett.*, 87 (2007), pp. 935–942.
20. J. Weertman and J.R. Weertman, *Elementary Dislocation Theory* (New York: Oxford University Press, 1992).

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