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Atomic-scale investigation of interface-facilitated deformation twinning in severely deformed Ag-Cu nanolamellar composites

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We report an atomic-scale investigation of interface-facilitated deformation twinning behaviour in Ag-Cu nanolamellar composites. Profuse twinning activities in Ag supply partial dislocations to directly transmit across the Ag-Cu lamellar interface that promotes deformation twinning in the neighbouring Cu lamellae although the interface is severely deformed. The trans-interface twin bands change the local structure at the interface. Our analysis suggests that the orientation relationship and interfacial structure between neighbouring Ag-Cu lamellae play a crucial role in such special interface-facilitated twinning behaviour. © *2015 AIP Publishing LLC*.
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Interfaces have profound effects on the physical and mechanical properties of bimetallic nanolamellar composites including strength, thermal stability, and resistance to radiation damage and shock deformation.[1–4] Recent investigations revealed that interfaces also play a crucial role in the nucleation of deformation twins during plastic deformation.[5,6] It is well known that deformation twinning, which is one of the most important deformation mechanisms in face-centered cubic materials,[7–9] is facilitated significantly through the emissions of Shockley partial dislocations on successive {111} planes from grain boundaries (GBs) when the grain sizes are in the nanometer regime.[10] However, twinning activities vary widely when twins emanate from the interfaces of bimetallic nanolamellar composites.[5,6,9] Due to the different atomic structures at interfaces, deformation twinning may be completely suppressed or occur frequently in the Cu layers of Cu-Nb nanolamellar composites.[6,9] More intriguingly, interface-facilitated twinning in Cu is accomplished by allowing direct transmission of twinning partial dislocations from Ag layers to Cu layers in Ag-Cu nanolamellar composites during cold rolling and uniaxial compression.[11–14] Based on molecular dynamics (MD) simulations, two sets of twinning partial dislocations in a Ag layer can cross an "ideal" Ag-Cu interface, which is formed between defect/stress-free Ag and Cu single crystals and free of extrinsic defects, driving the deformation twinning in Cu while the twin transmission alters the local interfacial structures.[12]

Many bimetallic nanolamellar composites were prepared using severe plastic deformation techniques including cold rolling, accumulative roll-bonding, and high-pressure torsion (HPT).[5,11,12,14,15] This leads to intense shear deformation at the interfaces and in each bimetallic component during the processing operation. It is expected that the atomic structures at the interfaces will be remarkably changed because of the extensive interactions between various defects and the interfaces,[16] which may prominently affect the trans-interface twinning behavior. Therefore, exploring the atomic structures near the "real" Ag-Cu interface is essential in deciphering the fundamentals of such unique interface-facilitated twinning behavior induced by twinning partial transmission across interfaces. In the present investigation, we prepared Ag-Cu nanolamellar composites using HPT, carried out atomic-scale observations of the twinning activities in both phases, and related the interface-driven twinning in the Cu layer to the atomic structures of the Ag-Cu interfaces.

A eutectic Ag-28 wt. % Cu alloy was selected in the present study with an average thickness of Cu and Ag layers of approximately 1 μm. The cube-on-cube and hetero-twin interfaces, both of which are with {111} habit planes, coexist in the materials and this is consistent with previous reports.[13–15] Disks of the alloy with a thickness of 0.85 mm and a diameter of 10 mm were processed via quasi-constrained HPT for 2 revolutions at room temperature under an imposed pressure of 6.0 GPa and a rotational speed of 1 rpm.[17,18] After HPT,

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cross-sectional specimens for transmission electron microscopy (TEM) and high-resolution TEM (HRTEM) investigations were taken from areas with a distance of ~1–1.5 mm from the edge of the disks, where the shear strain is approximately 55–63,[17] and prepared via ion milling using a Precision Ion-Polishing System Gatan 691 at liquid nitrogen temperature. TEM and HRTEM observations were carried out on a JEOL 3000F operating at 300 kV with a field emission gun.

A typical microstructure of the alloy after HPT processing exhibits Ag-Cu nanolaminates with an average layer thickness of approximately 30 nm, as revealed in Fig. 1(a), while individual layer thicknesses vary from ~5 nm to ~50 nm. Parallel with earlier investigations, the thickness of each layer was significantly reduced due to the imposition of substantial shear strain.[15] The interfaces were also severely deformed and became rugged. Deformation twins formed in some Ag and Cu nanolayers are marked by arrows in Fig. 1(b). Apparently, much higher twinning propensity was observed in the Ag layers than in the Cu layers due to the smaller stacking fault energy (SFE) in Ag (22 mJ m^{-2}) than Cu (45 mJ m^{-2}).[12–15] The lower SFE makes Ag prone to deformation twinning and various twinning activates were apparently initiated in the Ag nanolayers.

It is clearly notable that several stacking faults are embedded in twins, as indicated by arrows in Fig. 1(c), implying a heterogeneous twinning process in Ag nanolayers during HPT processing. In fact, most deformation twins formed via the emission of Shockley partial dislocations from the Ag-Cu interface and propagate across the Ag nanolayers, which is similar to those originating from the GBs in single-phase nanocrystalline (NC) materials.[19,20] Intrinsic interfacial defects including misfit dislocations and atomic steps can provide partial dislocation sources for nucleating twins,[5,6,12] while extensive interactions between defects and interfaces during HPT will leave the interface in a nonequlibrium and unstable state, thereby facilitating partial dislocation emissions to relieve local stress concentration.[21] Besides the random emissions of partial dislocations from interfaces, some deformation twins stemmed from the nucleation of the $\Sigma3\{112\}$ incoherent twin boundaries (ITBs) from the interface, as illustrated in Fig. 1(d). Although deformation-induced ITBs nucleation from GBs has been reported in coarse-grained Ag and NC Cu alloy,[22,23] they were seldom investigated in the nanolamellar structures with hetero-interfaces. As is well documented, the nucleation of $\Sigma3\{112\}$ ITBs is through the synchronized emission of a set of Shockley partial dislocations with a repeatable sequence as "zonal" twinning dislocations from a boundary.[22–24] SFE, boundary structures and the local stress state play crucial roles in their formation.[24,25] In the present investigation, the low SFE of Ag, the special interface structures, and the high resolved shear stress provided by the HPT may favor the nucleation of ITBs from interfaces and their propagation promotes deformation twinning. Moreover, unlike most nanolayered materials in which only one set of twinning systems is activated,[5,13,14] Fig. 1(e) demonstrates the formation of multifold deformation twins in some Ag nanolayers. Apparently, the interface was subjected to large shear deformation and part of the interface deviated significantly from the original interfacial plane, resulting in large stress concentrations. Emitting partial dislocations can lower the strain energy of the highly stressed/unstable interface. Furthermore, the HPT processing offers variations in the local stress orientations, providing another critical requirement for the activation of multiple twinning systems.[26,27] Overall, low SFE and severely deformed interfaces essentially boost the profuse twinning activities in the Ag nanolayers during HPT.

Although the twinning propensity significantly increases when grain size is refined to the nanometer range,[10] deformation twinning in Cu is not initiated as readily as in Ag due to its medium SFE. As exhibited in Figs. 1(b) and 2, fewer deformation twins were detected in the Cu nanolayers. This signifies that SFE is one of the most crucial factors dominating the deformation mechanisms even in the nanoscale.[10,27] Fig. 2 also reveals that there are two distinct mechanisms

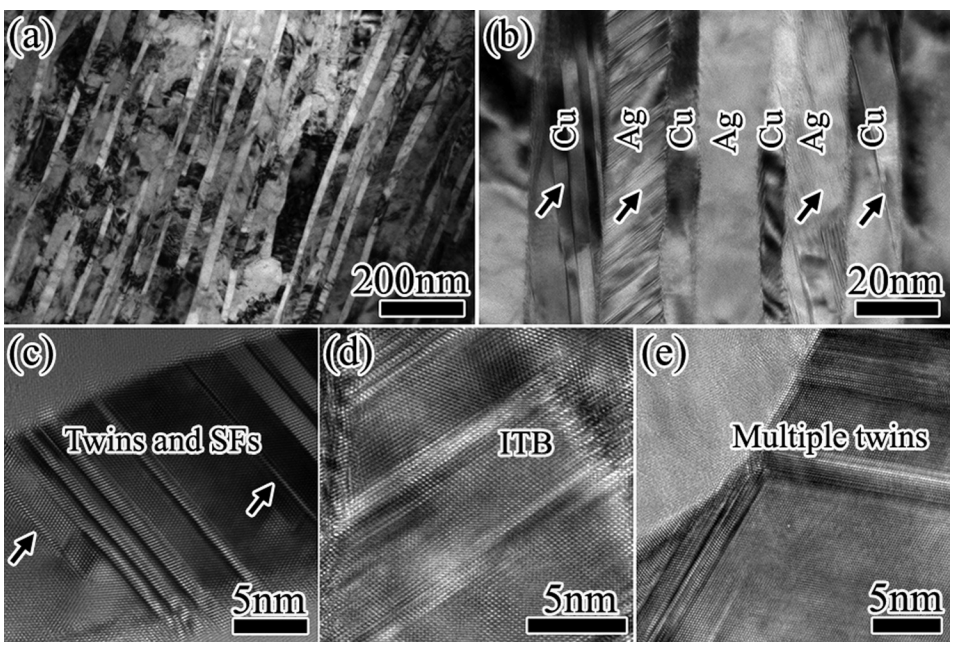

FIG. 1. (a) and (b) Typical microstructures of Ag-Cu nanolamellar composites processed by HPT. Arrows in (b) indicate twins; (c)–(e) HRTEM images showing the profuse deformation twining activates in Ag nanolayers. Arrows in (c) point to stacking faults.

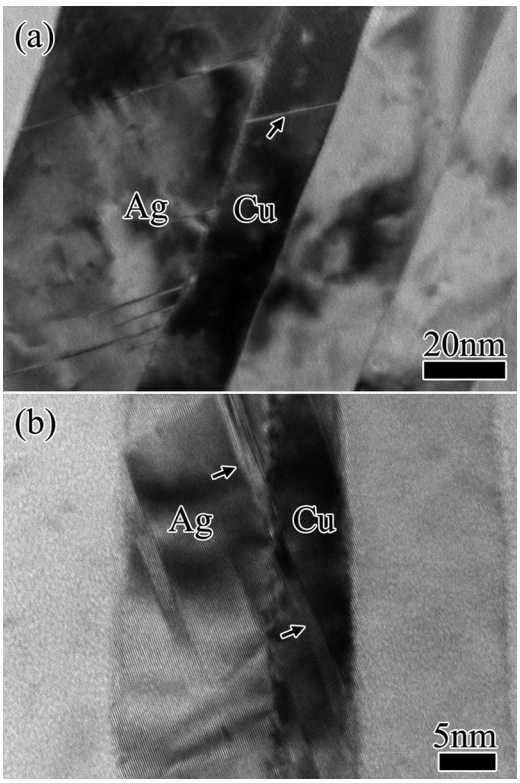

FIG. 2. (a) A deformation twin nucleated from an interface in Cu nanolayer, marked by the arrow; (b) a deformation twin in a Ag nanolayer crossed the interface and propagated in the neighboring Cu nanolayer, resulting in the formation of deformation twins in the Cu nanolayer, as marked by arrows.

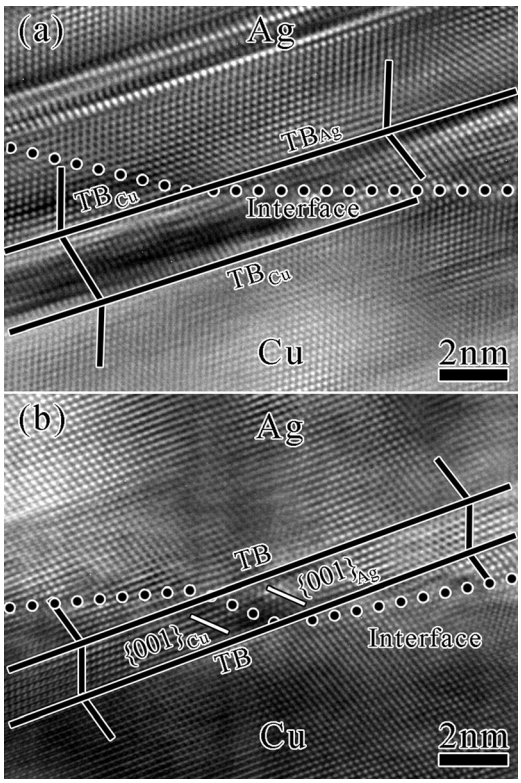

FIG. 3. HRTEM images of (a) one twin boundary and (b) a twin band with two twin boundaries transmitting across the interface from a Ag nanolayer to a Cu nanolayer. The interfaces are highlighted using dotted lines and twin boundaries are indicated using black lines.

responsible for deformation twinning in the Cu nanolayers. The first is the same as in Ag layers where the emissions of partial dislocations from interfacial defects lead to the formation of twins, as indicated by an arrow in Fig. 2(a). The other is that deformation twins in an Ag layer directly penetrate the Ag-Cu interface and propagate across the neighboring Cu nanolayer, as observed in Fig. 2(b). Considering also the earlier investigations,[11–14] it can be assumed that the Ag-Cu interface facilitated deformation twinning in Cu by allowing the transmission of twinning partials dislocations from the Ag phase to the Cu phase during deformation.

To comprehensively understand the trans-interface twinning behavior, a detailed atomic-level investigation of local structures near the interfaces was carried out. The HRTEM micrograph in Fig. 3(a) shows one twin boundary crossing an interface, which is roughly determined by the difference in the lattice parameters of Ag and Cu, while the twin thickened into a twin band with 10 atomic layers in the Cu phase. Early research suggested that twins can grow by themselves via the cross slip twinning mechanism when the twinning partial dislocations encountered an obstacle.[28] It should be noted that the cube-on-cube orientation was retained and provided perfect alignment between an active Ag twin system and a Cu twin system, although the interface was severely deformed and failed to maintain the original habit plane during HPT. Compared to one twin boundary, trans-interface twin bands with two boundaries are more easily detectable. As shown in Fig. 3(b), a twin band with 6 atomic layers transmitted across the interface from Ag to Cu although the interface was similarly subjected to extensive shear deformation, while the trans-interface twin band locally reoriented the interface plane into a {001} plane. Based on crystallographic considerations, the local structures of the interface will be changed as a result the transmission of the twin boundaries. Depending on the Burgers vector and screw/edge character of twinning partials, the Ag-Cu interface will be locally reoriented from the original (111) habit plane to either a {001} plane or another {111} plane.[12] However, concerning the defect energy of the transmitted twinning partial and residual dislocations left behind at the interface, MD simulations proposed that the reorientation into a {001} plane of the local interface plane is more energetically favorable than changing into another {111} plane.[12] Although the severely deformed interface outside of the twin band deviated from the original habit plane, the reoriented {001} plane of the interface was nearly retained since the twin boundaries across the interface can accommodate the plasticity, interact with the defects, and then protect it from severe deformation. In view of this local change of interfacial structure and crystallographic analysis,[12] it is speculated that the twin transmission occurred before the habit plane was disrupted from {111}. However, because post-deformation characterisation was carried out in the present investigation, *in-situ* investigation is necessary to unravel the puzzle.

It is apparent that providing sufficient twinning partial dislocations from one layer is a prior condition for the twin penetration into the neighboring layer.[12–14,29] Herein, profuse twinning activities in Ag due to its low SFE are the perquisite for the interface facilitated twinning process in the Cu nanolayers. Combined with earlier observations,[11–14] it can also be

concluded that, irrespective of the interfacial habit plane, the trans-interface twins are crystallographically correlated with the orientation relationship across the interface, thereby implying the significance of an alignment of twinning systems in the Ag and Cu layers. As shown in Fig. 3, the cube-on-cube orientation relationship across the interface is maintained, as this is consistent with a previous study that revealed the high stability of this relationship during deformation.[13] The interfaces with such orientations, even though they were severely deformed and deviated from the original habit plane, can be consider as geometrically "transparent interface for twinning," which favors the transmission of twinning partial dislocations to form trans-interface twin bands due to the well-aligned twinning systems of the two phases across the interface.[9,13,14,29] However, another type of prevailed interfaces with the heterotwin orientation in Ag-Cu composites is not readily transmissible based on a crystallographic analysis. The HRTEM micrographs in Figs. 4(a) and 4(b) show that the heterotwin orientation of the interfaces, whose stability is lower than that of the cube-on-cube interface,[13] was roughly distinguishable. However, the twins in Ag terminated at the interfaces, while the twins in the Cu nanolayer are only those nucleated from the interfaces as revealed in Fig. 4(b). Thus, such interfaces are resistant to the penetration of twins and will readily help to initiate the nucleation of shear bands due to the defect-interface interactions with further deformation.[13,14]

The interfacial structure is another essential character critically affecting the transmissibility of interfaces.[5,9,30] As mentioned above, the interfaces suffered from severe shear deformation during HPT and many defects were substantially accumulated and stored, thereby leading to extrinsic defects at the interface. Thus, the possibility of interaction between the twinning partial dislocations and the defects at or near interfaces is significantly increased. These incoming partial dislocations are more readily trapped and absorbed via the core spreading of the dislocations, which will significantly increase the difficulty of dislocation transmission due to the interface barriers.[30] This is the reason that the trans-interface twin bands do not prevail extensively, although the cube-on-cube orientation across the interface is highly stable during deformation. Apart from these two intrinsic microstructural factors, the local stress state also largely determined whether the direct transmission of twinning boundaries was favorable or not.

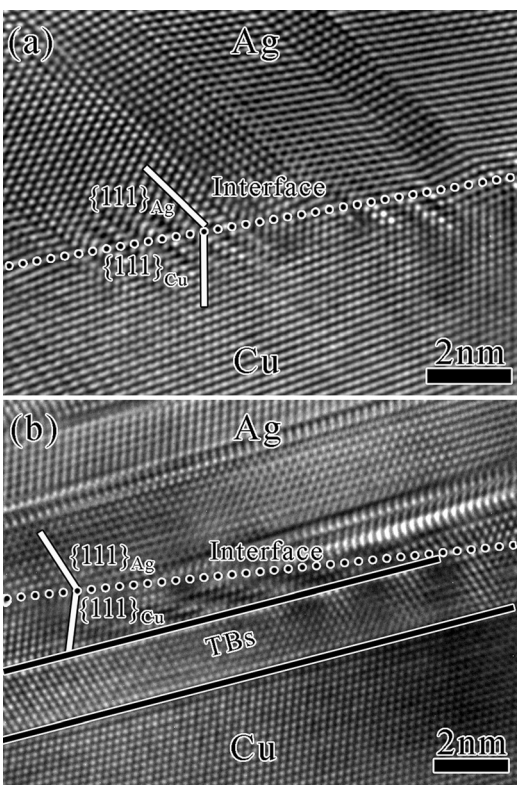

FIG. 4. (a) and (b) HRTEM images of heterotwin interfaces showing that twins in Ag layers cannot transmit across. The interfaces are highlighted using dotted lines and twin boundaries are indicated using black lines.

In summary, interface-facilitated twinning behavior in Cu-Ag nanolamellar composites processed by high-pressure torsion was investigated at the atomic scale. Due to the difference in the SFE, profuse twinning activities via partial emission from interfaces were observed in Ag nanolayers, while only a few deformation twins were found in Cu nanolayers. Some twins in Cu formed through the direct penetration of twinning partials from neighbouring Ag lamellae. Irrespective of the interface habit plane, the orientation relationship across the interface and the interface structures play a critical role in the twinning partial dislocation transmission from Ag to Cu. The trans-interface twin boundary locally changed the interface structures. Such interface-facilitated twinning behavior may open up new avenues for materials design to fine-tune the mechanical properties of the materials with heterophase interface structures through hierarchically manipulating the deformation mechanisms.

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