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Stability of nanoscale twins in copper under electric current stressing

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Migration of {112} incoherent twin boundary (ITB) in nanotwinned Cu under electric current stressing has been observed using *in situ* high-resolution transmission electron microscopy. The current-driven ITB migration is found to be four orders of magnitude faster than that driven thermally. We propose that electric current plays a role of shuffling Cu atoms at ITB/coherent twin boundary junctions, which enhances nucleation of {112} steps and facilitates twin boundary migration in Cu. By understanding how twin boundaries respond to electric current force we shall be able to trace the property change in nanotwinned Cu under electric current stressing, which would be an essential assessment of interconnect reliability. © *2010 American Institute of Physics*. [doi:10.1063/1.3483949]

Twin boundary (TB) is a common planar defect in face-centered cubic structured metals with low stacking fault energies, such as gold, copper, and silver. The formation of twins, in general, is associated with mechanical deformation or thermal annealing processes.[1,2] Cu foils with dense nanoscale twins have demonstrated a ten-fold increase in mechanical strength while maintaining a low electrical resistivity.[3] Twins, instead of dislocations, have been recognized to be the dominant defects which affect the mechanical properties of nanoscale materials. Moreover, the presence of triple junctions of coherent TBs (CTBs) and grain boundaries (GBs) is shown to impede current-driven atomic transport at twin-modified GBs,[4] which may suppress electromigration-induced failure of Cu lines in integrated circuits. Such excellent mechanical and electrical properties make nanotwinned Cu a perfect candidate material for compact three-dimensional integration of microelectronic devices. However, the stability of nanotwins in Cu under thermal, mechanical and electrical stressing has to be assessed because of extreme processing and operation conditions for ultralarge-scale integrated circuits. Unlike unstable GBs in nanocrystalline Cu, nanoscale twins in sputtered Cu films have shown good thermal stability as evidenced by a high hardness of 2.2 GPa after annealing at 800 °C for 1 h.[5] Nevertheless, how twinning structures evolve in response to mechanical and electrical stressing affects material mechanical properties and deserves a detailed investigation. A previous report has demonstrated stress-driven CTB migration in Cu observed using *in situ* transmission electron microscopy (TEM).[6] It suggests that the stress-driven CTB migration is associated with emission of Shockley partial dislocations from CTB/GB junctions. A molecular dynamics (MD) simulations has also been performed to predict migration dynamics of CTBs in Cu under shear stress.[7] However, the predicted CTB moving velocity seems to be impractically high (0.2–10.7 m/s), which is possibly due to the unrealistic mechanical loading conditions. In this study we investigate the stability of nanoscale twins in Cu under electric current stressing. The migration kinetics and mechanism of {112} incoherent TB (ITB) in Cu under electric current stressing are reported.

Thin Cu line specimens for *in situ* TEM observations were prepared through conventional thin film deposition, photolithography and etching processes.[4] The specimen was mounted on a specially designed TEM holder that allows for introducing an electric current through the Cu line. The sample was loaded into the TEM system (Model: JEOL 2000V UHV-TEM) and inspected at an ultrahigh vacuum environment of 3×10^{-10} torr to prevent Cu oxide formation. *In situ* TEM observations were performed when applying an electric current with an averaged density of 2×10^{10} A/m^2 through a 15-μm-wide Cu line specimen. We inspected several $(01\bar{1})$-oriented Cu grains with $\{111\}/\langle112\rangle$ type twins. The current-driven ITB behavior was video-recorded and analyzed.

Figure 1 shows snapshots from an *in situ* TEM movie of a $\{111\}/\langle112\rangle$ type twin in a $(01\bar{1})$-oriented Cu grain at different current stressing time. The incident electron beam was parallel to the $[01\bar{1}]$ direction, as indicated in Fig. 1(a). The (211) ITB moved in the direction of electron flow as an electric current was directed from right to left and approximately normal to the ITB. Figure 2 shows the change in twin length as a function of current stressing time. It is noted that the ITB moving velocity increased suddenly when the current density was raised from 2×10^{10} to 3×10^{10} A/m^2 in the final stage, as shown in Fig. 2. It indicates that the ITB migration indeed is manipulated by the electric current applied. A previous report suggests that thermally activated ITB migration involves formation of {112} steps with $3d_{(111)}$ lattice spacings in height at ITB/CTB junctions.[8] The {112}

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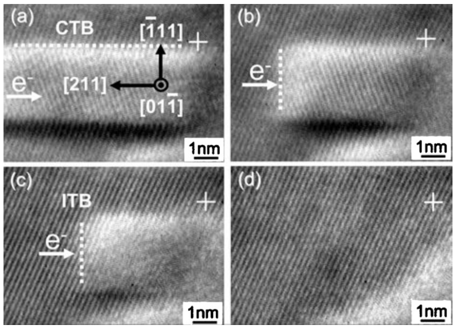

FIG. 1. High-resolution TEM images captured from an *in situ* movie of a $\{111\}/\langle 112\rangle$ type twin in a $(01\bar{1})$-oriented Cu grain at different current stressing times (a) 10 s, (b) 41 s, (c) 45 s, and (d) 48.5 s. The cross refers to a fixed point for ease of inspection.

steps result from a set of partial dislocations gliding on the $\{111\}$ planes perpendicular to the $\{112\}$ ITB.[9] As a $\{112\}$ step moves along the ITB and reaches the other ITB/CTB junction via successive dislocation gliding on the $\{111\}$ planes next to the $\{112\}$ step, the ITB eventually advances a distance of $3d_{(112)}$ and the system free energy is reduced by eliminating a portion of CTB area at both sides of the ITB. In fact, the step-motion behavior has also been predicted by MD simulations for stress-driven ITB migration.[10] The step motion is suggested to be related to the exchange of type-I and type-II kite structures at the ITB, which have similar formation energies of 547 $\mathrm{mJ/m^2}$ and 564 $\mathrm{mJ/m^2}$ for type-I and type-II kites, respectively.[8] Because the step motion does not involve marked change in the system free energy, we believe that the step nucleation rather than the step motion is the rate-limiting process of ITB migration. The measured ITB moving velocity at a current density of 2×10^{10} $\mathrm{A/m^2}$ is 0.062 nm/s that is comparable to the velocity of thermally activated ITBs at 300 °C ($\sim$0.056 nm/s).[8] Because the temperature increase due to self-heating in our electrically stressed Cu sample is below 100 °C, we extrapolate the thermally activated ITB migration data using an activation energy of 0.9 eV/atom (Ref. 8) and estimate the ITB moving velocity at 100 °C to be 3.2×10^{-6} nm/s, four orders of magnitude slower than the current-driven ITB migration. The results suggest that electric current must have strong effect on nucleation of $\{112\}$ steps at ITB/CTB junctions.

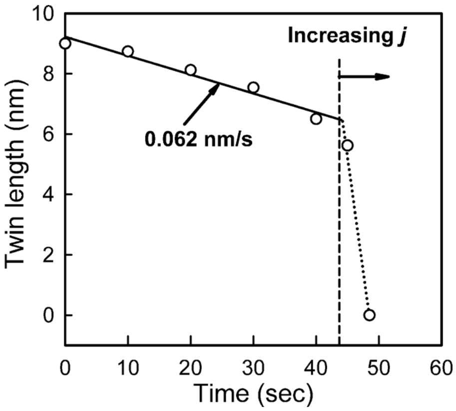

FIG. 2. The change in twin length as a function of current stressing time.

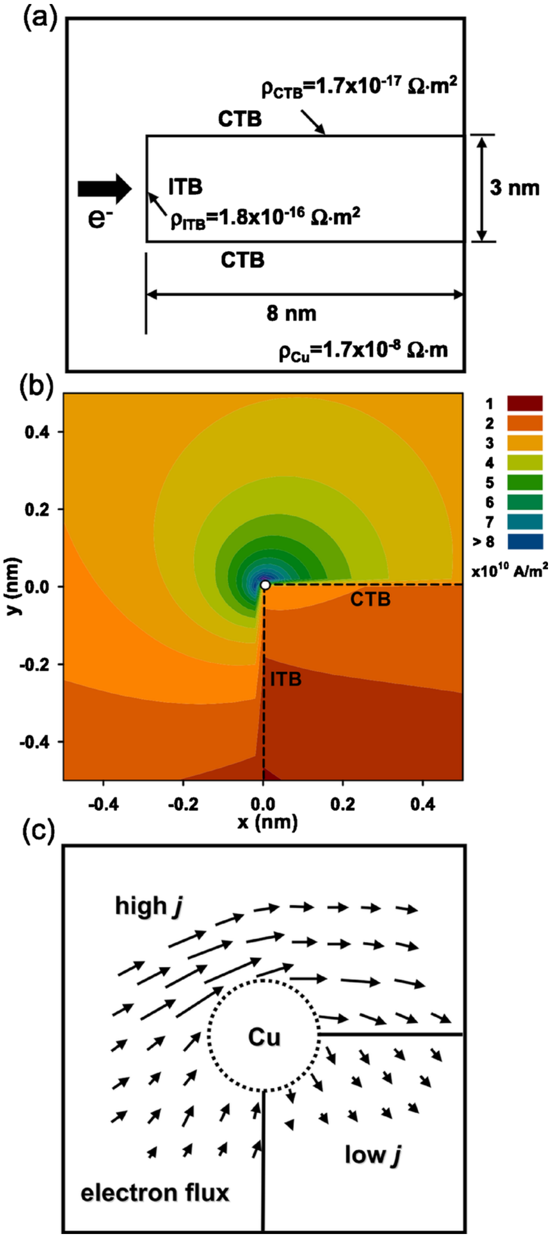

FIG. 3. (Color online) Electrical simulation of current distribution in a twin-structured Cu crystal. (a) Geometric and material parameters of the simulated twin-structured Cu crystal. (b) Simulated current-density distribution near the ITB/CTB junction in the Cu crystal with an averaged current density of 2×10^{10} $\mathrm{A/m^2}$. (c) Schematic diagram of electron flux around a Cu atom located at the ITB/CTB junction.

Because of disrupted lattice periodicity ITBs are expected to cause higher resistance to electron flow than normal crystal lattices. By assuming ITB resistivity, ρ_{ITB}, to be electrical resistance per unit boundary area, Cu atoms in ITBs are subjected to an excess resistance $\Delta R=(\rho_{\mathrm{ITB}}/A-\rho_{\mathrm{Cu}}d_{\mathrm{ITB}}/A)$ over those in normal crystal lattices, where ρ_{Cu}, d_{ITB}, and A represent Cu electrical resistivity, ITB thickness, and cross-section area of Cu atoms, respectively. If the effective charge of Cu atoms is $Z^{*}e$, we can estimate the excess electrical potential energy associated with the Cu atoms in ITBs under a current density of j to be

$$P=(Z^{*}e)(jA\Delta R)=Z^{*}ej(\rho_{\mathrm{ITB}}-\rho_{\mathrm{Cu}}d_{\mathrm{ITB}}). \tag{1}$$

When a current-density gradient exists near ITBs, a driving force occurs in order to minimize the excess potential energy as follows:

$$F = -\nabla P = -Z^{*}e(\rho_{\mathrm{ITB}} - \rho_{\mathrm{Cu}}d_{\mathrm{ITB}})\nabla j. \qquad (2)$$

The driving force shall "reform" the ITB in the way of lowering spatial nonuniformity of current density. For example, a current crowding that occurs at the ITB/CTB junction will introduce a current-gradient force acting on the atoms at the junction. Indeed, a similar current-gradient driven vacancy diffusion mechanism has also been proposed to explain the location of void formation in a multilevel structure of Al and Cu interconnects.[11] To evaluate the current crowding and the gradient force near ITB/CTB junctions, an electrical simulation of twin-structured Cu has been conducted using the FLEXPDE™ software. Discontinuous boundary conditions have been considered in the simulation by assigning appropriate contact resistivity values to the ITB and CTBs. We assume ρ_{ITB} to be 1.8×10^{-16} $\Omega\mathrm{m}^2$ that is about half of the specific resistivity of GBs in Cu.[12] On the other hand, a boundary resistivity of 1.7×10^{-17} $\Omega\mathrm{m}^2$ seems to be a reasonable estimate for ρ_{CTB}.[3] Figure 3(a) shows the geometric and material parameters of the simulated twin-structured Cu crystal with an averaged current density of 2×10^{10} $\mathrm{A/m}^2$ The current-density distribution near the ITB/CTB junction is highly nonuniform due to crowding effect, as shown in Fig. 3(b). If we assume a Cu atom of a diameter 0.27 nm located at the ITB/CTB junction, the current density at the upper left of the Cu atom is 3×10^{10} $\mathrm{A/m}^2$, twice higher than that at the lower right of the Cu atom, as shown in Fig. 3(c). The difference of current density shall induce a force to move the atom in the direction of lower current density. The current-gradient induced force is estimated to be $\sim10^5$ eV/m according to Eq. (2) by assuming $\rho_{\mathrm{Cu}}=1.7\times10^{-8}$ Ωm, $d_{\mathrm{ITB}}=0.5$ nm, and $Z^{*}=5$.[13] It is much higher than the electron wind force $(=Z^{*}e\rho_{\mathrm{Cu}}j)\sim10^3$ eV/m induced by electromigration. Such a high level of driving force can easily shuffle the Cu atoms, leading to enhanced nucleation rate of {112} steps at the ITB/CTB junctions. It explains why the current-driven ITB migration is several orders of magnitude faster than the thermally activated ITB migration at the same temperature.

We have shown that we can move ITBs and change twinning structure in Cu by applying an electric current instead of a mechanical stress. A force generated by gradient of current density raises nucleation rate of {112} steps at ITB/CTB to facilitate ITB migration in Cu. Since ITBs in Cu can be motivated by a high density of electric current, the mechanical properties and electromigration resistance of nanotwinned Cu may change with electric current stressing, which would be an important reliability problem for nanotwinned Cu interconnects of future nanoelectronic devices.

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