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Void formation by thermal stress concentration at twin interfaces in Cu thin films

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A void formation mechanism was investigated in an electroplated copper thin film on Ta/SiO$_2$/Si. Microstructural observation after thermal cycling indicated that void formation occurred at intersecting points or terminating corners of annealing twins. The calculated stress distribution was compared with experimental results of the void formation tendency. An excellent correlation was found between void formation sites and stress concentration sites. Electron diffraction analysis revealed that most twin interfaces in Cu thin films are incoherent {322} planes. The stress concentration drives diffusion along incoherent twin interfaces of {322} and leads to void formation at twin interfaces and corners. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1399021]

The advancement in integrated circuits requires much faster computing speed and higher cell density than conventional devices. In order to meet constantly renewing requirements, the gate length is reduced to less than 0.2 μm, with the aim of 0.1 μm in the next several years. Therefore, interconnect reliability has become a key issue to ensure device quality and performance. The reduction of the gate length has also raised the problem of resistance–capacitance delay. In order to overcome these challenges, Cu has been selected as a new interconnect material in place of conventional Al alloys. One of the major interconnect reliability problems is stress migration, namely, the formation of voids and hillocks that occurs under thermal stress conditions during thermal processing up to a temperature of approximately 700 K.

Stress migration failure was not originally expected for Cu because of its lower diffusivity than Al. However Borgesen *et al.* observed stress voiding in passivated Cu thin films during annealing at 673 K for 1 h.[1] Since this report of voiding in Cu thin films, most work has focused on understanding plastic deformation mechanisms during thermal cycling.[2–5] However, the stress values in the work reported were microscopic stresses averaged over the entire film area. Since vacancy flow and subsequent void growth are driven by the stress gradient, knowledge of localized stress distribution is essential in understanding the stress voiding behavior. To date, only a few groups have reported on voiding. Nucci, Keller and co-workers[6–9] investigated a grain boundary structure in order to find a possible relation between the grain-boundary misorientation angle and the voiding tendency. Although their results may provide useful information about the location of fast diffusion paths for supplying vacancies for void growth, detailed information about the driving force has not been understood clearly. In the present work, a stress-voiding mechanism was investigated in electroplated Cu thin films by relating the void formation tendency with the localized stress distribution around voids.

Copper thin films of 900 nm in thickness were deposited by electroplating on Ta(20 nm)/SiO$_2$(1700 nm)/Si(300 μm) substrates. The Ta layer was sputter deposited as a diffusion barrier to prevent intermixing between Cu and Si at elevated temperatures. The samples were subjected to thermal cycling at a heating and a cooling rate of 3.3 K/min in a temperature range between room temperature and 723 K.

The morphology of the film surface was observed by a scanning electron microscope (SEM) after thermal cycling. A film surface before thermal cycling is smooth, without any noticeable features. Figure 1 shows a SEM secondary-electron image of the film surface after the thermal cycle. Figure 1 shows the twin formation in the dark banded contrast and void formation in a black dotted contrast. Notice that voids were formed not only along grain boundaries but

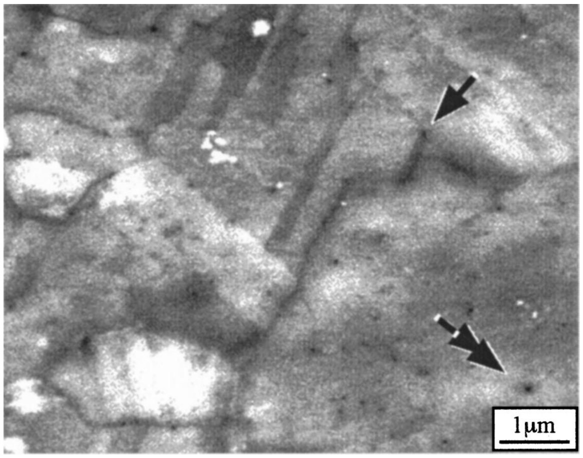

FIG. 1. SEM image after thermal cycling. A single arrow indicates void formation along the grain boundary. A double arrow indicates void formation in the grain interior.

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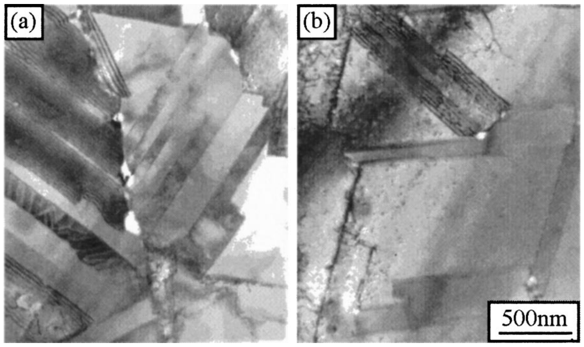

FIG. 2. TEM images after thermal cycling. Twin formation is observed at intersections of twins with a grain boundary in (a) and with other twins in (b).

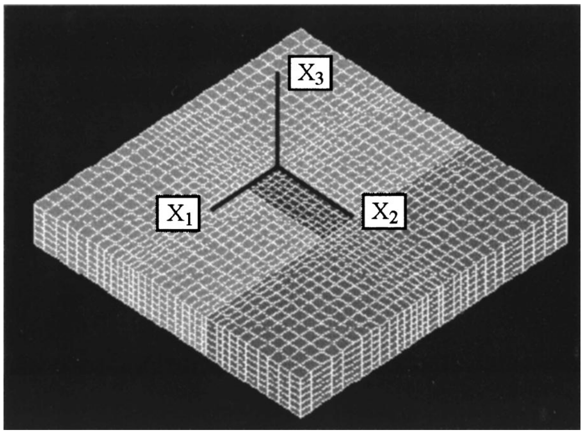

FIG. 3. Schematic of a three-dimensional FEM mesh and arrangement of the *x*, *y*, *z* coordinate system.

also in the grain interior. In conventional Al thin films, voids are formed by diffusion creep at grain boundary triple junctions and at grain boundaries.[10,11] So it is peculiar in the Cu thin film that voids formed in the grain interior.

Microstructural observation by a transmission electron microscope (TEM) was carried out to identify the void location and to relate any microstructural features with void formation. Figures 2(a) and 2(b) show TEM images of voided regions after thermal cycling. In both Figs. 2(a) and 2(b), voids are formed at intersecting points of twins. In Fig. 2(a), voids are observed along a grain boundary where twin interfaces intersect the boundary. In Fig. 2(b), voids are observed in the grain interior where twin interfaces intersect other twins.

The results obtained suggest a correlation between the void formation tendency and twin formation. This correlation can be explained as follows. Annealing twins are formed during heating in Cu thin films. The crystallographic orientations are different between the twins and the parent phase. Then, under isotropic thermal strain, large elastic anisotropy of Cu would induce differences in thermal stress between the twins and the parent phase. This difference may cause stress concentration at twin interfaces, corners, and intersections. The stress concentration, then, acts as a driving force for void formation. However analytical calculation of the stress concentration by including crystallographic information is a very difficult task. In this work, a numerical procedure is employed, as shown next.

The localized stress distribution was calculated using a finite element method (FEM) computer code, called MARC.[12] Since void formation is expected under tensile stress during cooling process, thermal tensile strain is applied theoretically by changing the temperature by -100 K from an initial state of zero strain. In reality, this procedure corresponds to decreasing the temperature by 100 from 723 K, at which the experimental film stress is found to be zero. The calculation was performed in an elastic limit without any consideration of plastic deformation. Since TEM observation revealed little dislocation activity, dislocation relaxation of the calculated stress distribution is not likely to happen. Thus, the calculation under the elastic assumption is valid in considering a possible relation between the stress distribution and the void formation tendency. Figure 3 shows a three-dimensional (3D) FEM mesh including a twin, a matrix, and a grain boundary. The effects of the underlying substrate are taken into consideration by fixing the displacement value at the Cu bottom plane to zero and by replacing the thermal expansion coefficient of the film by a differential coefficient, $\alpha_{\mathrm{Cu}}-\alpha_{\mathrm{Si}}$. The stress at the film top surface and the side surface is also set to zero. In order to simulate the actual microstructure of the film, experimental results were incorporated into the FEM calculation using an analysis of Kikuchi patterns. The Kikuchi patterns allowed us to identify the configuration of the cubic principal axes of the twins and the matrix phase with respect to the orthogonal coordinate of a FEM mesh pattern. The rotation matrix was then obtained to convert the cubic coordinate to the FEM coordinate. Using this rotation matrix, the elastic stiffness tensor of each grain was expressed in terms of the FEM coordinate.[13] The stress

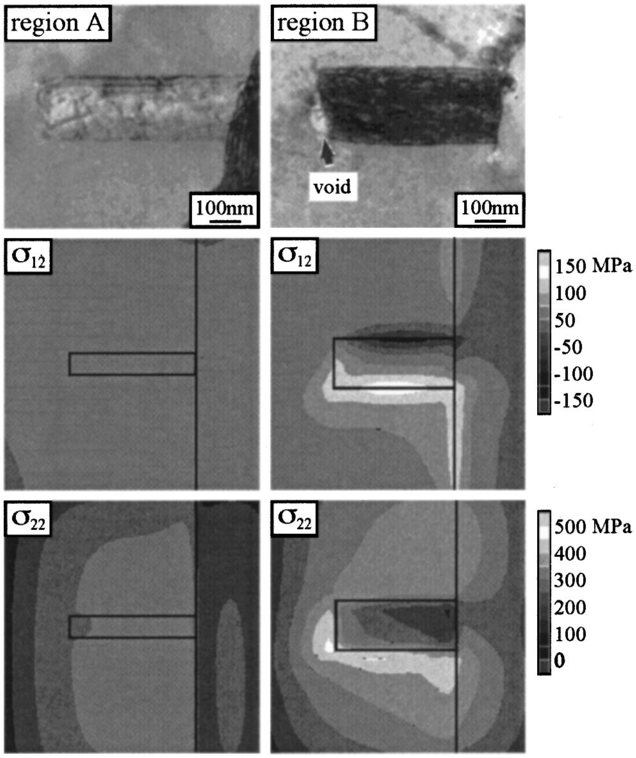

FIG. 4. TEM images and corresponding stress distribution around twins calculated by 3D FEM. Region A includes a twin without any voids. Region B includes a twin with a void.

distribution obtained was compared with the void formation tendency observed by transmission electron microscope.

Figure 4 shows an actual TEM micrograph and the calculated stress distribution of each region. Figure 4(a) indicates region A including a twin with a void, while Fig. 4(b) indicates region B including a twin without any void. The magnitude of stress is shown by the gray scale, shown on the right side of Fig. 2(b). In region A, no substantial stress concentration is observed for any stress components. On the other hand, in region B, the stress concentration of both the tensile and shear components is seen along the twin interface. The stress concentration of σ_{22} at the twin corner is more than 400 MPa. The stress concentration of σ_{12} along the twin interfaces is approximately 100 MPa both in the positive and the negative shear directions. When this stress distribution is compared with the TEM micrograph, excellent agreement is found between the stress concentration site and the void formation site.

Although not shown here, a TEM trace analysis revealed that most twins in this film have a twin interface of {322}. In bulk bicrystals of Cu, Ernst *et al.*[14] reported the structure of {322} twin interfaces. Both high resolution TEM observation and the embedded-atom-method calculation indicated that the {322} twin interfaces are incoherent planes with a disordered atomic array. Thus, the diffusivity along the observed twin interfaces is expected to be as fast as general grain boundaries.

The results obtained in the present work suggest a void formation mechanism as follows. During the heating process, annealing twins are formed in Cu thin films. Large elastic anisotropy causes stress concentration at twin interfaces and corners under isotropic thermal strain. This stress concentration could act as a driving force for vacancy diffusion. Then, the incoherent {322} twin interfaces would become a fast diffusion path, leading to void formation.

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