Effect of the crystallinity of a grain boundary on the self-diffusion of copper in thin-film interconnections

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Abstract
In this study, the effect of the crystallinity and the characteristics of grain boundaries on the grain boundary diffusion was investigated experimentally. The crystallinity and characteristics of the grain boundaries were evaluated by using an EBSD (Electron Back-scattered Diffraction) method. The atomic diffusion of the grain boundary was also observed as the change of the surface morphology of interconnections by SPM (Scanning Probe Microscopy). It was found that the main diffusion paths during EM (Electro Migration) was random grain boundaries. The grain boundaries with low quality, regardless of crystallographic orientation, were also the main atomic diffusion paths.

1. Introduction
Miniaturization of electric devices has been continued for improving their performance [1]. The size reduction of interconnections should increase their resistance, and thus, degrades the performance of the devices due to the increase in signal delay and Joule heating. In addition, the current density through interconnections has been increasing for increasing operating speed of the devices. The increase of the current density in interconnections has the fracture risk by EM (Electromigration). Electromigration is defined as atomic diffusion induced by momentum exchange due to collision of component atoms in interconnections with high speed electrons. Copper is applied to thin film interconnections, because copper has excellent physical properties such as high thermal and electrical conductivities and high melting point, comparing with the conventional interconnection materials such as aluminum. Since the copper thin film interconnections are manufactured by electroplating, the electroplated copper thin films tend to have porous grain boundaries because of large mismatch in lattice constant between copper and a seed layer material such as tantalum. It is well known that the porous grain boundaries are important source of electron scattering and bypass for atomic diffusion. Thus, the resistivity of the electroplated copper thin films is usually higher than that of bulk copper [2, 3], and the degradation of their crystallinity is accelerated by grain boundary diffusion under EM and SM (stress-induced migration) [4-7]. Therefore, it is necessary to suppress the grain boundary diffusion for improving the resistance to the migrations and thus, the long-term reliability of the interconnections. In this study, the crystallinity of grain boundary and atomic diffusion were investigated experimentally. The quality of the electroplated copper thin film interconnection was degraded by EM test. The change of microtexture around grain boundaries during the EM test was observed by SPM (scanning probe microscopy). In addition, the change of the crystallinity of the copper thin film was evaluated before and after the EM test, using the IQ (Image Quality) value obtained by EBSD (Electron Back-Scatter Diffraction) method [8,9]. Considering the relation between the changes of microtexture and IQ value, the dominant factor for controlling the grain boundary diffusion was investigated in detail from the viewpoint of the order of atom arrangement in the interconnections.

2. Sample preparation and EM test
Figure 1 shows a schematic structure of the electroplated copper thin film interconnection fabricated for the evaluation. There were electrode pads at both ends and 11 pads for detecting the local resistance. The pitch of the 11 pads was 200 μm. These pads were also used for deciding the position of the observation by the SPM and the evaluation by the EBSD method. In this study, the surface of the interconnection was free surface, without the passivation, to be evaluated by EBSD method and the SPM. Thus, the surface diffusion of the interconnections should be accelerated comparing with that of the interconnections covered by passivation films. This sample was fabricated by the damascene process. First, 1.5 μm SiO₂ layer was deposited on Si wafer by Plasma CVD (Chemical Vapor Deposition). Secondly, the SiO₂ wafer was etched off locally to make trenches, depth was 1.0μm. Next, 150 nm Ta (tantalum) barrier layer and 50 nm Cu seed layer were continuously deposited on the by PVD (Physical Vapor Deposition). Then, the trench was filled by electroplated copper thin film at the current density of 10 mA/cm². The electroplating condition was as follows. The plating bath

![Diagram of interconnection structure](image)
3. Effect of the crystallinity of the interconnection on the grain boundary diffusion

It is known that the surface morphology of the interconnection changes during the EM test. Thus, the change of the surface morphology of the copper thin film interconnection was observed before and after the EM test.

The EM test was performed under the current density of 7 MA/cm² for an hour in atmosphere. The stage temperature was fixed at 30°C and the change of the electrical resistance of the interconnection was measured at every 1s and the surface temperature was also measured using a digital thermography. The resistance was measured by a four-probe method. Figure 2 shows the change of the electrical resistance of the interconnection during the EM test. The horizontal axis shows the time from the beginning of the test. The vertical axis shows the resistance of the interconnection. This figure indicates that the resistance increased monotonically with time due to EM. Figure 3 shows the distribution of the surface temperature of the interconnection during the EM test. The horizontal axis indicates the distance from the position (c) in Fig. 1. The vertical axis indicates the surface temperature. This figure indicates that the temperature at the center of the interconnection was higher than that at both ends by about 60°C, and the maximum temperature reached about 240°C.

Consisted of 80 g of CuO powder and 186 g of H₂SO₄ into 1000 ml of purified water. After that, the sample was annealed at 400 °C for 30 minutes. Finally, the surplus copper layer was eliminated by CMP (Chemical Mechanical Polishing).

Figure 4 shows SPM images of interconnection before and after the EM test at the position of (a) anode side, (b) center of the interconnection and (c) cathode side. After the EM test, the surface morphology changed drastically, and the white lines were observed along the grain boundaries. The change occurred notably at the position (b) comparing with that at the positions (a) and (c). This was because the surface temperature around the center region of the interconnection was higher than that at both ends of the interconnection as shown in Fig. 3. Figure 5 shows the distribution of the detailed surface morphology before and after the EM test on the line AB shown in Fig. 4(b). This diagram shows that the surface roughness of the interconnection increased clearly after the EM test. In addition, it was confirmed that white lines appeared on the surface of the interconnection after the EM test corresponded to the area at which the surface rose, in other words, copper atoms diffused into this area and accumulated.

To investigate the mechanism of the change of the surface morphology of the interconnection, the microtexture
of the interconnection was observed in detail by EBSD method before and after EM test. Figure 6 shows the distribution of the characteristics of grain boundaries; red lines show random grain boundaries and blue lines show CSL (Coincident Site Lattice) grain boundaries. Both grain boundaries existed randomly in the interconnection before the EM test. Figure 7 shows the comparison between SPM image shown in Figure 4(b) and the distribution of the random grain boundaries shown in Fig. 6. The distribution of random grain boundaries before the EM test agreed very well with white lines observed on the SPM image after the EM test. On the other hand, no matches were observed between the distribution of CSL boundaries and that of white lines on the SPM image. Therefore, it was concluded that the diffusion of copper atoms mainly occurred along random grain boundaries during the EM test and this local acceleration of the atomic diffusion of copper caused the increase in the surface roughness of the interconnection. This result clearly indicates that the long-term reliability of the interconnection under the high current density is dominated by the concentration of random grain boundaries in interconnections.

Figure 8 shows SIM images of the cross-sectional surface of the interconnection after the EM test. Figure 8 (a) shows the cross section of the highly damaged area, and voids were observed on the areas of random grain boundaries. Furthermore, the local elevation of the surface was observed on the area of random grain boundaries. From these results, it was concluded that the degradation of the quality of interconnection was caused by locally accelerated atomic diffusion of copper along random grain boundaries in the interconnection. The increase in the resistance was attributed in the increase in the concentration of voids in the interconnection. The change of the surface morphology of the interconnection occurred due to the local accelerated diffusion and accumulation of copper atoms caused by EM.

The IQ (Image Quality) value is the average intensity of the Kikuchi lines observed in the EBSD analysis. The quality of the Kikuchi pattern is quantitatively evaluated by the IQ value. The IQ value has strongly correlation with the diffraction intensity of the irradiated electron beam and the intensity should be dominated by the quality of atom arrangement in the observed area because the Kikuchi Lines are formed by the interaction of electron beams diffracted based on Bragg’s law. Thus, the IQ value is supposed to
evaluate quantitatively the local crystallinity, the order of atom arrangement.

Figure 9 shows the distribution of the IQ value and GB (Grain Boundary) characteristics; blue color indicates high IQ value and red color represents low IQ value. Figure 10 shows the distribution of IQ values of the CSL grain boundaries and the random grain boundaries shown in Fig. 9. The distribution of IQ value of random grain boundaries shifted to lower side comparing with that of CSL grain boundaries. But there were CSL grain boundaries of which the IQ value was lower than that of random grain boundaries. There also existed random grain boundaries with high IQ value. This result indicates that the quality of grain boundaries is not determined by their crystallographic orientation. Actually, in Fig. 7, there were regions that white lines appeared on CSL grain boundaries (area A framed by black line). Also, there were random grain boundaries on which clear white lines did not appear.

Next, local distribution of the IQ value was analyzed along the lines AB and CD in Fig. 9, and it was compared with the change of the surface morphology of the same area. Figure 11 shows the distribution of the IQ value around the CSL grain boundary before EM test (red line) and the surface morphology after the EM test (black line). The IQ value of these CSL grain boundaries showed relatively low value (under 3000), and it was confirmed that the local diffusion of these areas were accelerated and thus, the local elevation of the surface was observed on these areas. Figure 12 shows that the similar results observed around random grain boundaries. In this figure, there are two types of random grain boundaries, one is random grain boundary with low IQ value (under 3000) and the other is that with relatively high IQ value (higher than 4000). It is clearly shown that the local elevation of the surface occurred on the area of grain boundaries with low IQ value. From these results it was indicated that the grain boundary diffusion was accelerated along grain boundaries with low IQ value, in other words, grain boundaries with low crystallinity. The crystallinity is weak relationship with the crystallographic orientation of grain boundaries. The long-term reliability of interconnections, therefore, should be dominated by the concentration of the grain boundaries with low crystallinity.

4. Conclusions
The change of the surface morphology of the electroplated copper thin film interconnections before and after the EM test was observed by using SPM, and the crystallinity of grain boundaries in the interconnection was evaluated by applying an EBSD method. As a result, it was confirmed that the surface morphology of the interconnections was roughened locally and drastically due to the accelerated diffusion of copper atoms along grain boundaries with low crystallinity. The local accelerated diffusion increased the density of voids in the interconnection, and resulted in the increase of the resistance of the interconnection. The crystallinity of grain boundaries was found to have no strong relationship with their crystallographic orientation. The local acceleration occurred along both random and CSL grain boundaries with low crystallinity. It was concluded that the main atomic diffusion paths were grain boundaries with low crystallinity. Since the temperature of the interconnection during the EM test also varies depending on its resistance and the resistance of the interconnection is dominated by its crystallinity, it is important to minimize the density of grain boundaries with low crystallinity in the interconnection for improving the long-term reliability.

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References


