Micro-Texture Dependence of Stress-induced Migration of Electroplated Copper Thin Film Interconnections Used for 3D Integration

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***Abstract*— Effect of the micro texture of electroplated copper thin film interconnections on stress-induced migration was investigated experimentally and theoretically. The micro texture of electroplated copper thin films changed drastically as a function of the annealing temperature after the electroplating. However, stress-induced migration was activated even though the thin film interconnection was kept at room temperature after annealing. As a result, voids and hillocks appeared on the thin film interconnection. This is because high residual stress was caused by shrinkage of the thin film interconnection due to the densification caused by recrystallization. Molecular dynamics simulations showed that the diffusivity of copper atoms along grain boundaries with low crystallinity was enhanced significantly by high tensile residual stress. Therefore, the grain boundary diffusion accelerated by tensile residual stress is the main reason for the formation of hillocks and voids in the thin film interconnection after annealing.**

Keywords*— *Reliability, Electroplated copper thin film interconnection, Stress-induced migration

I. INTRODUCTION

Electroplated copper thin films have started to be applied to not only interconnections in printed wiring boards but also thin-film interconnections and through-silicon vias (TSVs) in semiconductor devices because of their low electrical resistivity and high thermal conductivity. However, there still remain some problems in the practical use of electroplated copper thin-film interconnections. One of them is that both electrical and mechanical properties of the electroplated copper thin film vary drastically depending on its electroplating conditions and thermal hysteresis after electroplating. For example, brittleness [1] and a high electrical resistivity [2] often appeared in the electroplated copper thin film, and in some cases, the lifetime under electro migration (EM) tests was incredibly shorter than that expected [3]. The reason for the variation of the electrical and mechanical properties can be attributed to the unique micro-texture of electroplated copper thin films that mainly consist of fine columnar grains with porous grain boundaries [4]. The columnar grain structure induces the cooperative grain boundary sliding phenomenon and the porous grain boundary is an important source of electron scattering and a bypass for diffusion. The porous grain boundaries also decreases the thermal conductivity of the thin film interconnection, and some porous grain boundaries with high electrical resistivity cause the localized Joule heating and resulting open failures due to local fusion.

Thus, the crystallographic quality (crystallinity) of grain boundaries in electroplated copper thin films plays an important role in the mechanical and electrical properties and the resulting reliability. High temperature annealing that can improve the crystallinity of the film is one of the effective methods for improving the long-term reliability of thin film interconnections. However, even though the crystallinity and electrical properties were improved markedly by annealing, it was also observed that stress-induced migration was activated substantially in the annealed interconnection. The crystallinity of the annealed interconnection degrades markedly by stress-induced migration and therefore, it is necessary to clarify the dominant factors of the stress-induced migration and to establish the design guideline for highly reliable copper interconnections in order to assure the long term reliability of electronic products. In this study, the effect of the change of crystallinity and micro texture of electroplated copper thin films by annealing on stress-induced migration was investigated experimentally and theoretically.

II. STRESS-INDUCED MIGRATION IN ANNEALED COPPER THIN FILM INTERCONNECTION

A. Measurement of the residual stress in the annealed films

The stress-induced migration in the electroplated copper thin-film interconnection should be caused by high tensile residual stress existing in the film after annealing. The electroplated copper films tend to shrink because of the densification due to recrystallization in the films upon annealing. However, the volumetric shrinkage of the electroplated copper thin-film interconnection was constrained by the surrounding silicone dioxide used for isolation in the interconnection structure and, therefore, a high tensile residual stress existed in the interconnection. Thus, the residual stress of the electroplated copper thin film was measured after electroplating and annealing. Self-made electroplated copper

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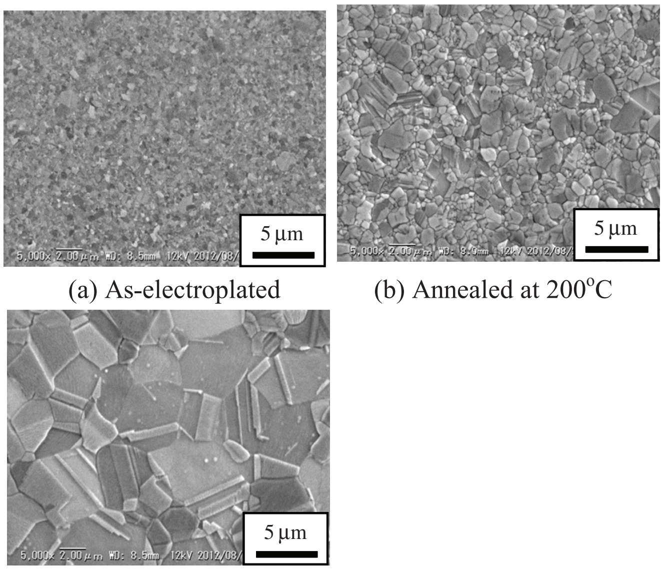
thin films were used for the measurement. Test samples for measuring the residual stress were prepared by the electroplating of copper thin film on a Si substrate. Electroplating conditions were as follows. The composition of the plating bath was controlled by diluting 80 g of CuO powder and 186 g of H_2SO_4 into 1000 ml of purified water. The current density during the electroplating of thin film interconnections is varied from 10 mA/cm^2 to 100 mA/cm^2. In addition, some films were annealed in pure argon gas at temperatures from 100^{o}C to 400^{o}C for 3 h. The thickness of the films was fixed at 8 µm. The change of the surface morphology of the films as a function of the annealing temperature is shown in Fig. 1. The as-electroplated film mainly consisted of columnar grains as shown in Fig. 1 (a). On the other hand, the average grain size of the films annealed at temperatures higher than 200^{o}C increased drastically as shown in Figs. 1 (b) and 1 (c). The average grain size increased monotonically with the increase of the annealing temperature and subsequently, the annealed films mainly consisted of large polycrystalline grains.

Measurement method of the residual stress in thin films used in this study was that proposed by G. G. Stony (8). The residual stress in thin films is calculated based on elastic deformation of a substrate after deposition of thin film. Assuming that the residual stress in the deposited or annealed film was uniform, the residual stress in the film was calculated from the measured change in the radius of the substrate R, as expressed by Eq. (1).

$$\sigma = \frac{E_s t_s^2}{(1-\nu_s)6 t_f R} \qquad (1)$$

where Es is Young's modulus of the substrate, ν_s is the Poisson ratio of the substrate, t_s and t_f are the thicknesses of the substrate and the deposited film, respectively. In this study, the curvature R was measured parallel to the <110> crystallographic direction of Si, which was used as the substrate by using a laser displacement meter. Thus, Es is 170 GPa, and ν_s is 0.07 in this study.

The measured result was shown in Fig. 2. The residual stress of the annealed films changed drastically depending on the annealing temperature. As was described before, electroplated copper thin films shrink during high temperature annealing owing to the densification caused by recrystallization. When the shrinkage of the films is constrained by their surrounding structures, high tensile stress remains in the films after annealing. The grain coarsening by recrystallization of the film started to occur at temperatures around 200^{o}C, as shown in Fig. 1. The average grain size increased with increasing the annealing temperature, and thus, the residual stress increased monotonically with increasing the annealing temperature and it reached 250 MPa after annealing at 400^{o}C. Since this value is much higher than the yield stress of about 90 MPa in the electroplated copper film annealed at 400^{o}C [5], this residual stress was significantly high to cause the stress-induced migration of copper atoms. Thus, the stress-induced migration caused by high tensile residual stress occurs in the annealed electroplated copper thin-film interconnection even at room temperature, which induces the degradation of the long-term reliability of the interconnection.



(a) As-electroplated (b) Annealed at 200^{o}C (c) Annealed at 400^{o}C

Fig. 1. SEM images of the change of the surface morphology of the films as a function of the annealing temperature

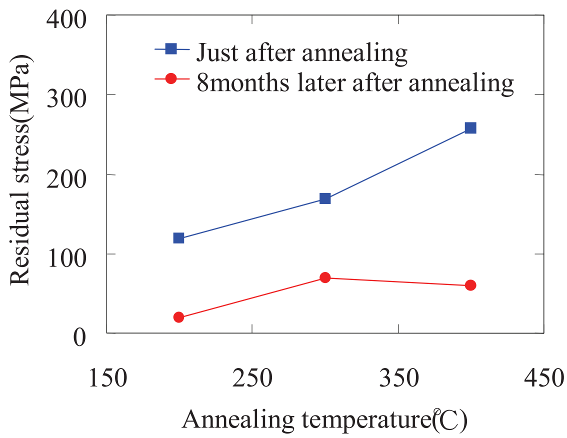


Fig. 2. Residual stress in the films as a function of annealing temperature

B. Stress-induced migration in the annelaed interconnection

The change of the surface morphology of the electroplated copper thin film interconnection after annealing was investigated. The interconnections used in this investigation were made by using the popular damascene process. First, 1.5-µm thick SiO_2 layer was deposited on a Si wafer by Plasma-CVD. Next, the SiO_2 layer was locally etched off to make thin trenches whose depth was 1.0 µm. The width of the interconnection was 8 µm. Ta (50 nm) / Cu (150 nm) layer was deposited by sputtering. The trench was filled with copper by electroplating. Finally, the excess copper layer was mechanically-polished to make isolated interconnections. After the fabrication of the interconnection, the interconnection was annealed at 400^{o}C for 3 h in Ar gas. All samples were kept at room temperature without any loading during the stress-induced migration test.

Figure 3 shows the change of the surface morphology of the interconnections during the stress-induced migration test. Hillocks appeared without current loading on the surface of the annealed interconnections 72 hours later at even room temperature after the annealing, as shown in Fig. 3(b). The degradation of the surface morphology continued to proceed and the number of hillocks and voids increased continuously. Large hillocks grew for about 6 months, as shown in Fig. 3(c). During the degradation process, it was observed that the residual stress in the interconnections was relaxed and decreased lower than the yield stress eight months after annealing, as shown in Fig. 2. On the other hand, no hillocks and voids were observed in the film without annealing during one year, as shown in Fig. 3(d). Therefore, the stress-induced migration was caused by high tensile residual stress which occurred in the film after annealing. This result suggests that the electroplated film is degraded without any application of electrical current after the annealing by the stress-induced migration.

III. MOLECULAR DYNAMICS SIMULATIONS OF STRESS-INDUCED MIGRATION IN ANNEALED COPPER FILMS

In order to investigate the effect of change of crystallinity by annealing on the stress-induced migration, molecular dynamics (MD) simulations were applied to analyze the diffusion behavior of copper atoms. Figure 4 shows the simulation models of copper thin films annealed at different temperatures. The structures of the annealed copper thin film models were prepared by quenching a melted Cu structure and annealing at 673 K, 873 K and 1073 K for 1000 ps after the quenching under fixed volume condition (no fluctuation of the lengths of the unit cell during the simulation). The fine grain structure of the film with high concentration of vacancies was modeled after the quenching and the grain coarsening by the recrystallization occurred during the annealing, as shown in Fig. 4. Two different structures were obtained after the annealing calculation at 1073 K by changing initial velocity of atoms, as shown in Fig. 4(d) and (e). Simulation models shown in Fig. 4(d) and (e) are referred to as model A and model B, respectively. Lengths of the unit cell in x-, y- and z-axis were 400.4, 231.2 and 12.58 Å, respectively. These lengths were equilibrium values evaluated from MD simulation of bulk (single) copper crystal model where (111) planes parallel to xy plane at 300 K. The volumetric atomic density of the models was fixed at 95% of bulk Cu density at 300 K for simulating electroplated copper thin films with porous grain boundaries.

After the annealing calculation, the MD simulations were carried out for 3,000 ps under the fixed volume condition at 300 K for evaluating the diffusion constants of cooper atoms in the annealed film. The diffusion constants of atoms were calculated from the slope of the mean square displacement (MSD) with time. The embedded atom method (EAM) potential [6] of LAMMPS code [7] was used for all simulations. Total number of atom was 92340 atoms. All of the simulations were carried out with 1 fs MD time step and a periodic boundary condition was adopted in all directions.

Figure 5 shows change of pressures in the copper thin film structures during the simulation at 300 K. In this figure, tensile stress in the film has negative value of pressure. The pressure of the films changed drastically depending on the annealing temperature and then, the magnitude of tensile stress increased with increasing the annealing temperature. When the copper thin film was annealed, the copper film structure intended to

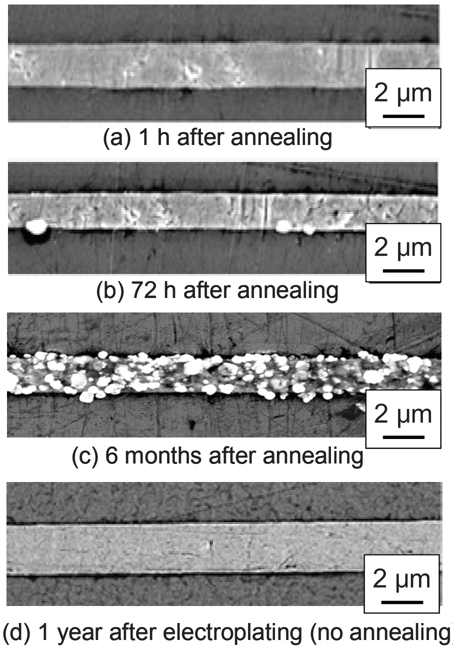


Fig. 3. Change of the surface morphology of the annealed electroplated copper thin film interconnection caused by stress-induced migration

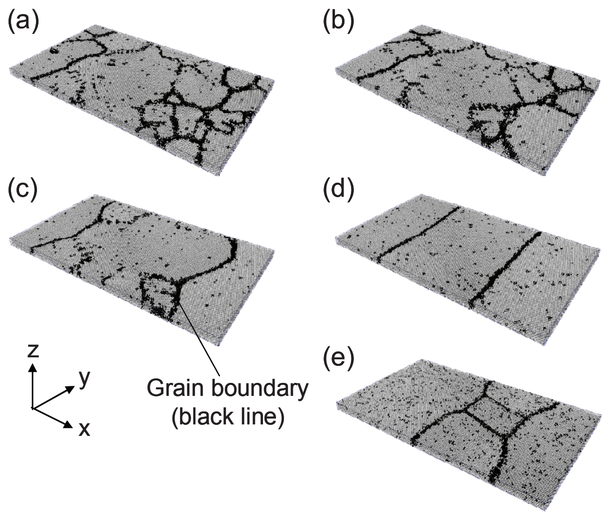


Fig. 4. Simulation models of copper thin films, (a) after quenching (without annealing), (b) annealed at 673 K, (c) annealed at 873 K, (d) and (e) annealed at 1073 K. Black color indicates the region of grain boudnaries.

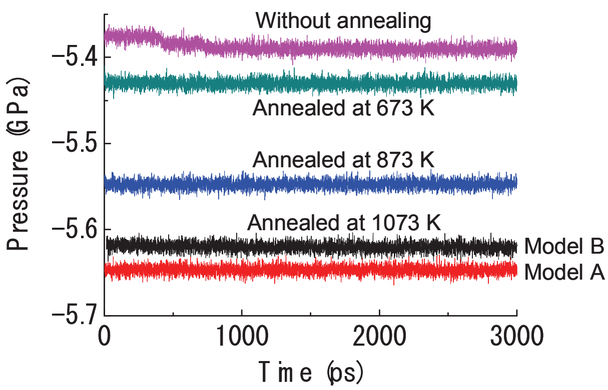


Fig. 5. Change of pressures in the copper thin films without and with annealing during the simulation at 300 K

shrink because of the atomic rearrangement and grain growth in the film. The grain size was found to be increased with increase of the annealing temperature, as shown in Fig. 4. However, the volumetric shrinkage of the copper film was constrained. Therefore, high tensile residual stress in annealed electroplated copper films with large grains is caused by the constraint of the shrinkage due to the recrystallization.

Observed high residual stress caused by the constraint of the shrinkage of copper thin films is considered to be a dominant factor in the stress-induced migration of electroplated copper interconnections because the electroplated copper interconnections are constrained by surrounded silicone dioxide used for isolation in the interconnection structure. Figure 6 shows the example of atomic displacement vectors in the annealed copper film during the simulation at 300 K. Copper atoms around the grain boundaries, especially high angle grain boundaries, moved significantly even at 300 K. This result indicates that the stress-induced migration is mainly dominated by the diffusion of atoms along grain boundaries. In addition, the crystallinity of grain boundaries also dominates the stress-induced migration because random atomic configuration around the grain boundary with low crystallinity accelerates the atomic diffusion significantly. Figure 7 shows MSD of copper atoms in the films annealed at different temperatures. The MSD value in the film annealed at 1073 K increased sharply compared to that in other films. Calculated diffusion constant in the film annealed at 1073 K (1.2×10^{-8} cm^2/s in model A) was about 4 times larger than that in the film annealed at 673 K (0.27×10^{-8} cm^2/s). These results indicate that the diffusivity of copper atoms along grain boundaries with low crystallinity such as random and porous (low atomic density) grain boundaries is enhanced significantly even at room temperature by high tensile residual stress. This grain boundary diffusion is the main reason for the formation of voids in the interconnections. Since the amplitude of the stress developed due to the densification strongly depends on the initial density and texture of the thin film, the improvement of the crystallinity of the film just after electroplating is indispensable for improving the long-term reliability of the electroplated copper thin film interconnections.

IV. Conclusion

In this study, the change of the micro-texture and surface morphology of the electroplated copper film interconnections caused by the stress-induced migration was observed. It was found that the average grain size increased drastically by high temperature annealing. However, the tensile residual stress of the films increased with increasing annealing temperature. Since electroplated copper thin films shrink during high temperature annealing owing to the densification caused by recrystallization, high tensile stress remains in the films after annealing when the shrinkage of the films is constrained by their surrounding structures. After annealing at 400°C, voids and hillocks grew on the film interconnection during the storage of the interconnection even at room temperature without any loading. MD simulations showed that the diffusivity of copper atoms along grain boundaries with low crystallinity was enhanced significantly by high tensile residual stress. Therefore, the grain boundary diffusion accelerated by tensile residual stress is the main reason for the formation of hillocks and voids in the film interconnection. It is, therefore, very important to control the micro texture and crystallinity of electroplated copper thin film interconnections to assure the reliability of electronic products.

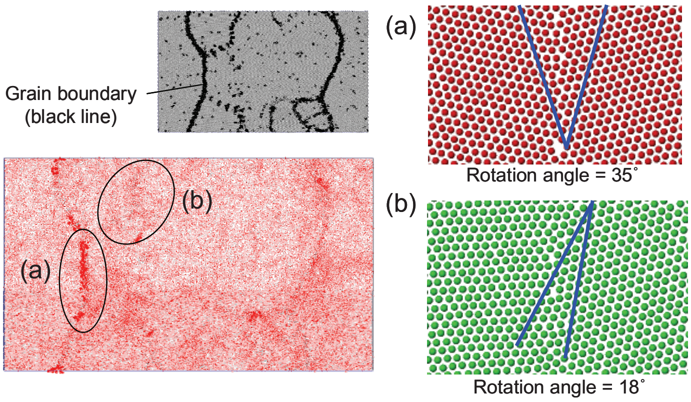


Fig. 6. Atomic displacement vectors in the copper film annealed at 873 K and atomic configurations around grain boundaries (a) and (b).

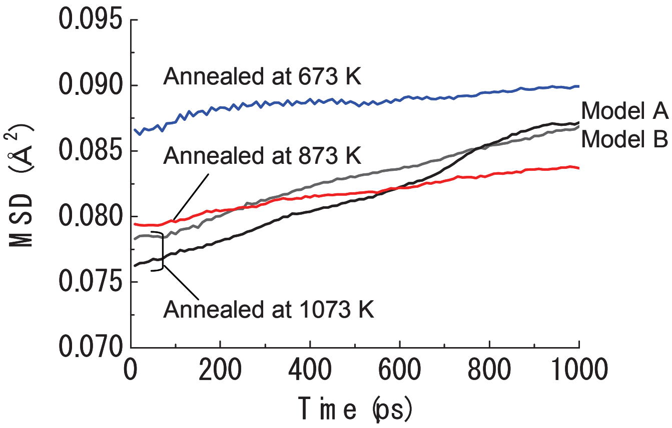


Fig. 7. Mean square displacements (MSD) of copper atoms in the annealed copper films

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