

Full Length Article

Quantitative studies of electric field intensity on atom diffusion of Cu/Ta/Si stacks during annealing

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ABSTRACT

It has been shown that enhanced electric field intensity (0–4.0 kV/cm) has an obvious effect on accelerating atom diffusion in Cu/Ta/Si interconnect stacks at 650 °C. The theoretical deduction proves that diffusion coefficient is accelerated proportional to an acceleration factor $(1 + a \cdot \alpha^{E/0.8})^2$. The analysis indicates that the accelerating effect is mainly attributed to the perturbation of the electric state of the defects and enhanced vacancy and dislocation densities.

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1. Introduction

To prevent the formation of copper silicide and the consequent failure of integrated circuits (ICs), a thin barrier with high thermal stability, good interface adhesion and low electrical resistivity is strongly demanded [1–5]. It has been extensively reported that refractory metals such as practically used Ti, Ta and their nitrides can be used as a perfect barrier in Cu metallization [6–10]. As device sizes reduce, the resistance-capacitance time delay (R-C delay), electromigration (EM) and service environment became a major significant issue in integrated circuits (ICs) [2,11].

Recent studies mainly focus on the effect of temperature on barrier properties, but other complicated service environment related to its performance, such as stress, electric and magnetic fields, has been overlooked [9,12]. Generally, complicated service environment might also affect the mobility of atoms, vacancies and dislocations during annealing. Conrad et al. found that the major factor responsible for increase in sintering rate with both AC and DC electric field is the retardation of grain growth of zirconia by the field [13]. Zuo et al. reported that external high magnetic field promoted formation of rod-like microstructure in Cu-Ag alloy [14]. In previous work, it was discovered that external electric field accelerated interface diffusion of Cu interconnect during annealing

[10,15–17]. Thus, it is important to know how the atom diffusion in Cu interconnect evolves in complex service conditions.

In fast ICs, the working temperature can be quite high with the participation of electric field that accompany small distances close to sharp features inside modern IC [18]. Therefore, we present a comparative study on the Cu/Ta/Si structure with different electric field intensities at 650 °C. The diffusion coefficient as a function of electric field intensity can reveal important information on the nature of the intrinsic mechanism for atom diffusion by combined action of temperature and electric field.

2. Experimental details

Cu film and barrier layer Ta film were deposited on single crystal Si (111) wafers by DC magnetron sputtering. The substrate wafers were cleaned separately by ultrasonically in acetone and ethanol, respectively. After drying with ultrahigh purity N₂ gas, the substrate was immediately loaded into the sputtering system. The background pressure of the sputtering chamber was 2.0×10^{-4} Pa. Before the deposition of Ta and Cu layer, the Ta (99.95%) and Cu (99.99%) targets were pre-sputtered for 10 min to remove the surface contaminants. First, a 50 ± 2 nm Ta layer was deposited on Si (111) substrate with an Ar gas deposition pressure of 1.1 Pa and a target power of 60 W. Cu thin film with thickness of 300 ± 10 nm was subsequently deposited in situ on the top of Ta layer at room temperature with an Ar gas pressure of 1.1 Pa and a target power of 100 W without opening the chamber. After deposition, the stacks were annealed in the vacuum chamber for 30 min at 650 °C with various electric field intensities (E) ranging from 0 to 4.0 kV/cm

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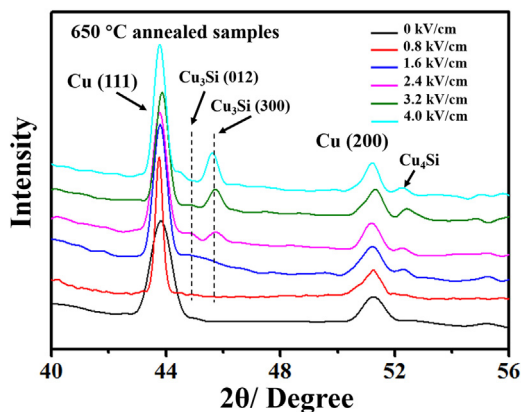


Fig. 1. (Color online) XRD patterns of the Cu/Ta/Si stacks annealed at 650 °C with different electric field intensities.

at a pressure of 1×10^{-4} Pa. The specimens were connected to the anode. The distance between sample and negative electrode was maintained at 5 mm, so that the electric field intensity can be changed by adjusting the high voltage. Hence, the electric field distribution maintained steady during the experiment. More details about the deposition and thermal treatment system employed in this work are available in previous research [10,15–18].

The microstructure of the annealed Cu films was characterized by x-ray diffraction (XRD) with Cu $K\alpha$ radiation source. Transmission electron microscopy (TEM) and energy dispersive x-ray spectroscopy (EDX) in scanning-transmission electron microscopy (STEM) mode measurements were carried out on JEM2100F. The composition evolution of the stacks was carried out by means of X-ray photoelectron spectroscopy (XPS, Thermo Fisher, K-alpha). An ion gun was used to etch the material for a period of time before being turned off whilst XPS spectra were acquired. The etch-rate of the ion-gun can be precisely controlled by Ar ion beam energy and etch time. By combining a sequence of ion gun etch cycles, a depth profile of the stacks in terms of XPS quantities can be obtained from the surface to Cu/Ta/Si interfaces.

3. Results and discussion

The phase evolutions of 650 °C annealed samples with different electric field intensities are shown in Fig. 1. The 2θ diffraction peaks found at 43.4°, 50.6° correspond to Cu(111), Cu(200), respectively. Initially, no peaks corresponding to copper silicide were observed for 650 °C annealed-only sample as well as the one with $E = 0.8$ kV/cm. A small Cu₄Si peak can be observed at $2\theta = 52.3^\circ$ with $E = 1.6$ kV/cm, Cu₃Si (012) and Cu₃Si (300) were detected in the samples with $E = 2.4$ –4.0 kV/cm. Cu₃Si (300) peak became stronger, however Cu₃Si (012) peak became weaker with enhanced electric field intensity, which can be mainly due to (300) preferred orientation is energetically more favorable due to the enhanced electric field intensity [15].

Fig. 2 displays the cross sectional TEM images of Cu/Ta/Si stacks annealed at 650 °C with different electric field intensities. It reveals that no evident columnar grains of Ta were presented for the 650 °C annealed Cu/Ta/Si stacks, as shown in Fig. 2a. The thickness of the Ta layer was ~50 nm, as predicted by the deposition rate. The Ta/Si interface was abrupt and flat in the inset of Fig. 2a. The interconnect structure of the samples with $E = 0.8$ and 1.6 kV/cm was unchanged compared with 650 °C annealed sample and no considerable formation of copper silicide was observed in Fig. 2b and c. Nevertheless, the Cu/Ta interface was destroyed by electric field intensity as it increased from 2.4 to 4.0 kV/cm as arrowed in Fig. 2d–f. When the E increased to 2.4 kV/cm, Ta layer no longer retained its lateral integrity, as depicted in Fig. 2d. For the sample with $E = 3.2$ kV/cm, ~12 nm Ta layer was destroyed by Cu diffusion, as seen in Fig. 2e. When E was as high as 4.0 kV/cm, ~23 nm Ta layer was completely destroyed, as shown in Fig. 2f.

In order to observe the interface diffusion, STEM-EDX line scanning was used to determine the atomic distribution for Cu/Ta/Si stacks after annealing at 650 °C with different electric field intensities, as shown in Fig. 3. The approximate interfaces of Cu/Ta/Si stacks are indicated by black dashed lines in Fig. 3a. For 650 °C annealed stack in Fig. 3a, the interfaces can be clearly identified, suggesting a well-defined interface structure. Ta and Si signals were homogeneously distributed in the Ta barrier region. Cu intensity gradually decreased as the scan came into Cu/Ta interface and then

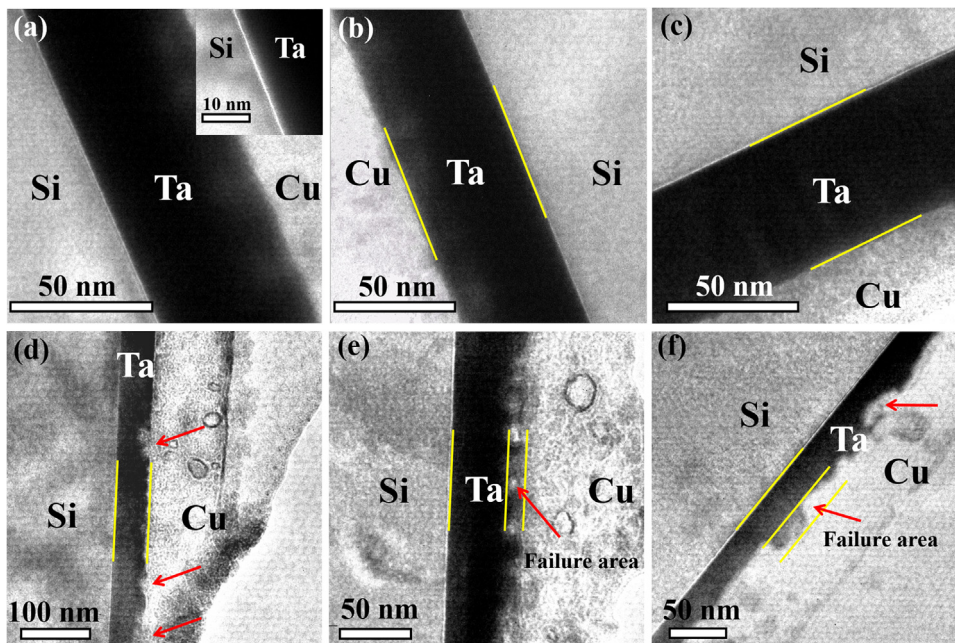


Fig. 2. (Color online) Cross sectional TEM images of Cu/Ta/Si stacks annealed at 650 °C with electric field intensity (a) 0 kV/cm, the inset shows the high magnification image of Ta/Si interface, (b) 0.8 kV/cm, (c) 1.6 kV/cm, (d) 2.4 kV/cm, (e) 3.2 kV/cm, (f) 4.0 kV/cm.

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