Nanostructured Ta-Si-N Thin Films as Diffusion Barriers Between Cu and SiO₂

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In order to reduce the RC delay of interconnects in integrated circuits, copper has replaced aluminum as the conducting material for sub-0.15 μ m integrated circuits owing to its lower resistivity. However, copper exhibits a substantial diffusivity in SiO₂. Therefore, a stable barrier is necessary to prevent the undesired diffusion between Cu and the SiO₂ dielectrics. Many materials have been investigated as diffusion barriers for Cu metallizations. Among them, Ta-Si-N alloys have shown superior performances. In this work, the thermal stability and interdiffusion behavior of three Cu/Ta-Si-N/SiO₂ systems with various compositions for the Ta-Si-N barriers are studied in parallel and their differences will be explored.

Ta-Si-N barriers of different compositions, 50 nm in thickness, were deposited on SiO₂ (280 nm) covered Si wafers by co-sputtering. Between Ta-Si-N and SiO₂, a thin Ta interlayer was interposed to improve the adhesion. Compositions of Ta-Si-N films were determined by Rutherford backscattering spectrometry (RBS). Cu films (200 nm) were then sputtered on Ta-Si-N. After deposition, Cu/Ta-Si-N/Ta/SiO₂ samples were annealed in vacuum $(2\times10^{-5} \text{ Torr})$ at temperature ranging from 500 to 900°C for 30 min. The crystalline structure and elemental depth distribution of all samples (before after annealing) were investigated by using glancing incident angle X-ray diffraction (GIAXRD) and RBS, respectively.

Table 1 shows the composition, average grain size (estimated from the FWHM of the X-ray diffraction peak), resistivity and crystallization temperature of three Ta-Si-N films (denoted as "A", "B" and "C"). The high Si content in film C results in the smallest grain size and high resistivity. However, the crystallization temperature of film B is higher than that of A and C films.

Fig. 1 shows the sheet resistances of Cu/Ta-Si-N(A, B, C)/Ta/SiO₂ samples as a function of annealing temperature. It is clear that sample with barrier C shows the least stable sheet resistance upon annealing. The GIAXRD spectra of three Cu/Ta-Si-N/Ta/SiO₂ samples after annealing at 800°C are shown in Fig. 2. Diffraction peaks other than Cu peaks are seen in the sample with barrier A. Those are diffraction peaks of Ta_2N phase. Some small diffraction peaks, which are associated with TaSi_x phase, are also observed in the sample with barrier C. GIAXRD spectra of 900°C annealed Cu/Ta-Si-N/Ta/ SiO₂ samples indicate that all three Ta-Si-N barriers are crystallized after annealing at 900°C.Therefore, with the Cu overlayer, Ta-Si-N films crystallize at lower temperatures as compared to the films without the Cu overlaver.

Fig. 3 shows the RBS spectra of the Cu/Ta-Si-N(C) /Ta/SiO₂ ample, as deposited and after annealing at 800°C. From the spectra, one can see that both Ta and Si in the Ta-Si-N barrier had diffused across the Cu layer, to the sample surface after annealing at 800°C. Also, the tail of the Cu profile indicates that Cu atoms had diffused into the barrier layer. In contrast, the Cu/Ta-Si-N/Ta/SiO₂ multilayer structures with barriers A and B did not show

such interdiffusion after annealing at 800° C. The increase of sheet resistance of Cu/Ta-Si-N(C)/Ta/SiO₂ upon annealing thus should be attributed to the interdiffusion between Ta-Si-N(C) and Cu.

From the experiment results, one can find that the stability of Ta-Si-N barrier is strongly dependent on its composition. The composition should relate with the chemical bonding configurations so that the thermal stability of Ta-Si-N is affected. The original grain size and crystallization temperature of the Ta-Si-N layer may also relate with the composition, but they will not be the major factors to determine its barrier performance.

Table 1 Composition, average grain size, resistivity and crystallization temperature of three Ta-Si-N films.

Sample	Ta:Si:N	Average	Resistivity	Crystallization
		grain size	(µΩ-cm)	temperature
Α	53: 3:44	2 nm	261	900 °C
В	53:11:36	1.5 nm	259	1000 °C
С	29:32:39	1 nm	1046	900 °C



Fig. 1 Dependence of sheet resistance of Cu/Ta-Si-N/Ta/SiO₂ samples on the annealing temperatures.







Fig. 3 RBS spectra of the Cu/Ta-Si-N(C)/Ta/SiO₂ sample, as deposited and after annealing at 800° C.