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Thin and Low-Resistivity Tantalum Nitride Diffusion Barrier and Giant-Grain Copper Interconnects for Advanced ULSI Metallization

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1. Introduction

Copper interconnect is the most promising metallization scheme for the next generation high-speed ULSI. This is because copper exhibits lower resistivity and higher electro/stress-migration resistance than conventional Al-based materials [1]. However, copper atoms easily diffuse into silicon device and act as efficient recombination centers and spoil device performance. In order to adopt copper interconnects for ULSI, it is essential to develop highly reliable diffusion barrier [2]. Various kinds of materials such as Ta, TaSiN, TiN, TaN, and WN have been investigated for copper diffusion barriers [3-6]. The purpose of this paper is to demonstrate for the first time that reverse-bias current of n^+p junctions with Ta_2N diffusion barrier does not increase after 700°C annealing for 30min and that the grain size of copper films actually affects the diffusion performance of the thin Ta_2N layer.

2. Experiments

Ta_xN_y films were formed by reactive sputtering by Ar/N_2 plasma. N_2 was mixed in the range of 0%-7%. Ta_xN_y films were deposited using a UHV (background pressure ~10^{-10} Torr) RF-DC coupled mode bias sputtering system by a low energy ion bombardment process [7-8]. Total gas pressure was 10 mTorr. Before loading, substrates were cleaned in a dilute HF solution and rinsed by UPW. Copper films were also deposited by UHV RF-DC coupled mode bias sputtering system with precisely controlling ion energy and ion flux. To evaluate quality of Ta_xN_y films, Ta_xN_y samples were analyzed by four-point probe sheet resistance measurement and X-ray diffraction. In order to evaluate barrier performance n^+p junctions were fabricated with copper electrode. The area and the depth of junctions are 1mm×1mm and about 500nm. Contact hole area is 940μm ×940μm or 20μm×20μm. Samples were annealed in Ar ambient in the range of 500°C-700°C for 30 min. 50nm and 10nm thick diffusion barriers were evaluated.

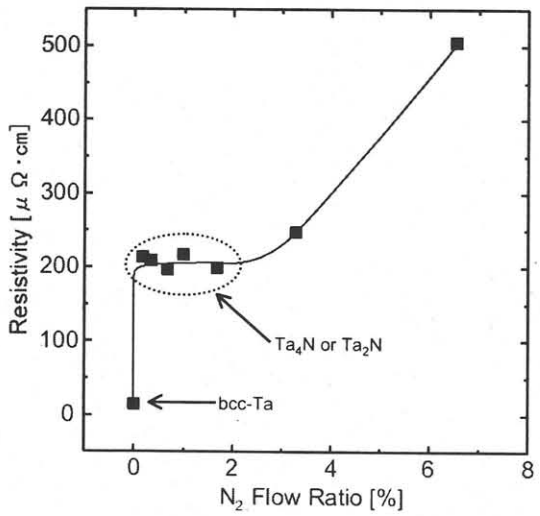

Fig. 1 Registivity of Ta_xN_y films as a function of N_2 flow ratio

3. Results and Discussion

Fig. 1 shows the resistivity of Ta_xN_y films as a function of N_2 flow rate. More than 2% N_2 addition causes increase in resistivity. At 0.16%-1.6% N_2 flow ratio, Ta_xN_y films exhibits ~200μΩ·cm. Table I shows crystalline phases of Ta_xN_y films evaluated by X-ray diffraction pattern. Every films exhibit a single crystalline phase. These three films ware sputtered in the same condition except N_2 flow ratio. When N_2 flow ratio 0% bcc-Ta was formed. Ta_4N and Ta_2N were formed by adding 0.16% and 1.6% N_2 respectively.

Fig. 2 shows reverse-bias current densities of n^+p junction at 5V reverse-bias with these 50-nm-thick Ta_xN_y diffusion barrier layers after 500°C, 600°C, and 700°C annealing for 30min. A broken line means current density of the control n^+p junction with aluminum electrode. The control n^+p junction exhibits ~10^{-10} A/cm^2 at 5V reverse-bias. It is low and sensitive enough to detect a small amount of copper diffusion. In bcc-Ta and Ta_4N diffusion barrier samples reverse-bias current increases with annealing temperature increasing. However Ta_2N diffusion barrier sample prevented increasing of reverse-bias current after 700°C annealing. The thickness of these foregoing diffusion barriers is 50nm and contact area is 940μm×940μm. Ta_2N diffusion barrier in 50-nm-thick performs as a good diffusion barrier. However 10-nm-thick Ta_2N diffusion barrier can not prevent copper atom diffusion perfectly. Contact holes and vias volume continues to shrink in size. Therefore thinner diffusion barrier is desirable. Thick diffusion barrier narrows contact area for copper and makes more difficult to fill and makes contact resistance higher.

In order to form copper layer, various deposition methods have been proposed such as CVD, electro-plating

Table I Crystalline phases of Ta_xN_y films evaluated with X-ray diffraction pattern

N_2 flow ratio	0 %	0.16%	1.6%
Crystalline phase	bcc-Ta (110)	Ta_4N (111)	Ta_2N (101)

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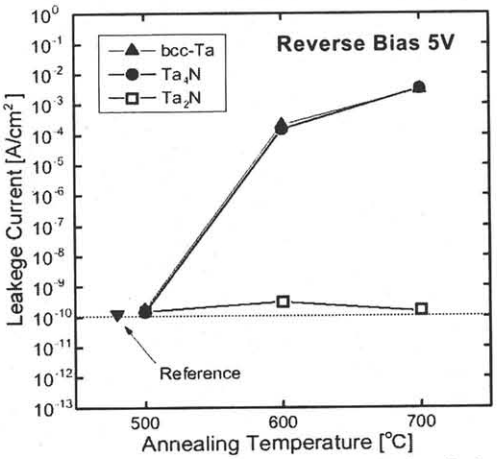

Fig. 2 Reverse-bias current densities of n^+p diodes with various Ta_xN_y diffusion barriers at the reverse bias voltage of 5V (contact hole size: 940μm×940μm)(thickness of Ta_xN_y films: 50nm)

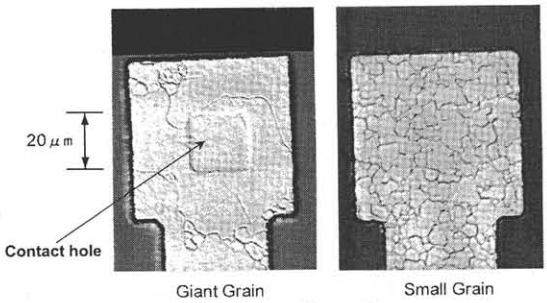

Fig. 3 Two different copper electrodes

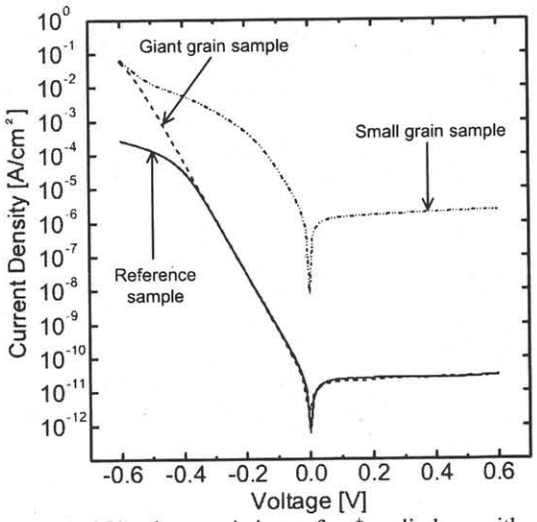

Fig. 4 J-V characteristics of n^+p diodes with 10nm thickness Ta_2N diffusion barrier and small or giant grain copper electrode (contact hole size: 20μm×20μm)(thickness of Ta_2N films: 10nm)(annealing temperature: 700°C)

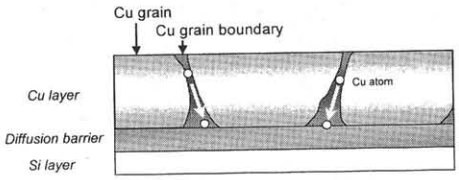

Fig. 5 The relation between copper grain size and copper atom diffusion

and directional sputtering. However, it is not clear how the quality of the copper layer affects the diffusivity of copper atoms. We demonstrate that, for the first time, copper grain size seriously influences copper diffusivity. Fig. 3 shows a micrograph of two different copper electrodes. One has a small grain (foregoing sample)(average grain size: 5μm), and the other has a giant grain (average grain size: 40μm). Fig. 4 shows J-V characteristics of n^+p junction with 10-nm-thick Ta_2N diffusion barrier and with small or giant grain copper electrode. Junctions with giant grain copper electrode and 20μm×20μm contact hole keep the same J-V characteristic as reference sample after 700°C annealing. The Difference of J-V characteristics in high forward-bias current region, between reference sample and giant grain sample, means lowered contact resistance by silicidation at the interface between Ta_2N and n^+ silicon [6]. However n^+p junctions with 940μm×940μm contact hole and with giant grain copper electrode could not prevent copper diffusion perfectly. Fig. 5 shows the relation between copper grain size and copper atom diffusion. To penetrate diffusion barrier and diffuse into silicon layer, copper atom have to cross interface between copper layer and diffusion barrier layer. Copper grain boundary can be fast diffusion path for copper atoms. Therefore copper grain boundary on diffusion barrier can be a primary penetration point. This is because copper atoms which composite crystal are fixed tightly than those on the grain boundary of copper. Ta_xN_y is a poly-crystalline film. Therefore copper atoms diffuse through grain boundary of Ta_xN_y. If the grain size of Ta_xN_y films primary determines copper diffusivity, n^+p junctions with small and giant grain copper electrode must exhibit the same J-V characteristic. However they exhibit different J-V characteristic as show in Fig. 5. Moreover the fact that only n^+p junctions with 20μm ×20μm contact hole can prevent copper diffusion suggests that copper grain size has a great influence upon copper diffusivity. It is confirmed that copper grain size as well as the performance of diffusion barrier is the important factors to prevent copper diffusion.

4. Conclusions

It is demonstrated that 10-nm-thick Ta_2N diffusion barrier and giant grain (average grain size: 40μm) copper interconnect can suppress increasing in reverse-bias current of 700°C-annealed n^+p junctions with 20μm×20μm contact hole. Ta_2N diffusion barrier also exhibits resistivity of ~200μΩ·cm, which is comparatively lower than the other diffusion barriers for its barrier performance.

References

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