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Characterization of Tungsten Carbide as Diffusion Barrier for Cu Metallization

Shui Jinn Wang¹, Hao Yi Tsai¹ and S. C. Sun,²¹Microelectronics Lab., Dept. of Electrical Engineering,
National Cheng Kung University, Tainan, Taiwan

Tel & Fax: 886-62345482 e-mail: sjwang@eembox.ee.ncku.edu.tw

²R&D, Wafertech, Camas, WA 98607, USA

1. Introduction

Based on its superiority in low resistivity ($\sim 1.67 \mu \Omega$ cm) and electromigration resistance, copper has played a crucial role in advanced IC metallization technology. Unfortunately, Cu is quite mobile in Si at elevated temperature, and its presence in Si creates trap levels that are detrious to device operation. Refractory metal nitride such as WN and TaN have been widely studied to establish thermally stable metallization schemes with low resistivity [1, 2]. However, to the authors' knowledge, little related information of refractory metal carbide as diffusion barrier in Cu metallization has been reported. In this paper, sputtered tungsten carbide (WC_x) films were investigated for the first time as an alternative diffusion barrier in preventing Cu diffusion. In addition to SEM, XRD, XPS, AES and SIMS analysis, the thermal stability of WC_x films was also examined via leakage current measurement by employing a $Cu/WC_x/Si(p^+n)$ structure. It is found that the WC_x films is still metallurgically stable after a 550 °C-annealing process for 30 min. The failure mechanism of the WC_x films will be reported.

2. Experiments

In this work, deposition of WC films were carried out by DC magnetron sputtering using a water-cooled WC (50:50 weight percent) target with 99.5% purity in pure Ar atmosphere. The applied DC power was 200W and deposition rate was measured to be around 0.3Å/s. The sputtered WC_x films were evaluated by electrical measurements performed on a shallow implanted p^+n diode with $Cu(200nm)/WC_x(60nm)/Si(p^+n)$ contact structures. Furthermore, X-ray diffraction (XRD), scanning electron microscopy (SEM) and secondary ion mass spectroscopy (SIMS) analyses were employed in conjunction with the

junction leakage measurements to examine the failure mechanism.

3. Results and Discussion

Figure 1(a) shows the XRD patterns of the WC_x/Si structures before and after 600°C~850°C annealing. As shown in this figure, no significant peak is observed for the as-deposited sample, it implies the as-deposited WC_x film is composed of very small grains or is essentially an amorphous phase. After 600°C~650°C annealing, there was no obvious change in the XRD pattern as compared with the as-deposited one. However, after 700°C~850°C annealing, tungsten silicides W_5Si_3 were observed, it indicates that strong interaction occurs between the WC_x layer and Si substrate at such high temperatures.

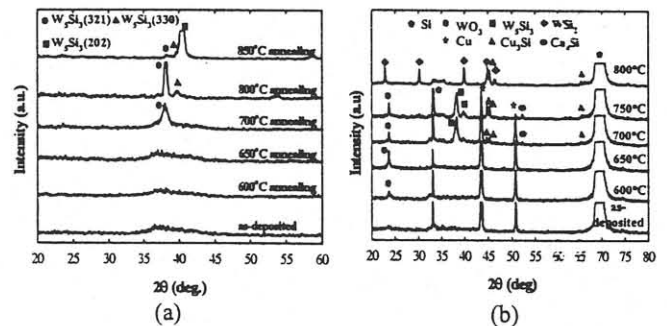


Fig. 1 (a)X-Ray pattern of $WC_x(60nm)/Si$ structure vs. annealing temperature (b)X-Ray pattern of $Cu(200nm)/WC_x(60nm)/Si$ structure vs. annealing temperature.

Figure 1(b) shows the XRD analysis of the annealed $Cu/WC_x/Si$ samples. It is seen that only Cu and Si peaks appear in the as-deposited sample. This confirms that WC_x barrier layer is with an amorphous structure. It is also evident that the amorphous structure keeps unchanged up to 650°C, however, Cu_3Si , W_5Si_3 and WO_3 phase were observed on the 700°C-annealed sample. The appearance of

Cu₃Si indicates that Cu has penetrated the WC_x layer and intermixed with the underlying silicon.

Figure 2 shows the SEM images of Cu/WC_x(60nm):p⁺n diode structure after thermal annealing. The Cu overlayer was stripped by a diluted HNO₃ solution. As was evident in Fig. 2(b), the surface micrograph of the sample annealed at 500°C exhibits no obvious damage. However, as annealing temperature was increased up to 550°C, the WC_x surface became slightly damaged (Fig. 2(c)). After 600°C annealing, as shown in Fig. 2(d), bright particles assigned to be Cu₃Si were observed. It suggests that a strong reaction between Cu and Si has happen and the barrier film might have lost its integrity. Similar phenomenon was also observed by Tsai *et al.*[3] using TaN as diffusion barriers.

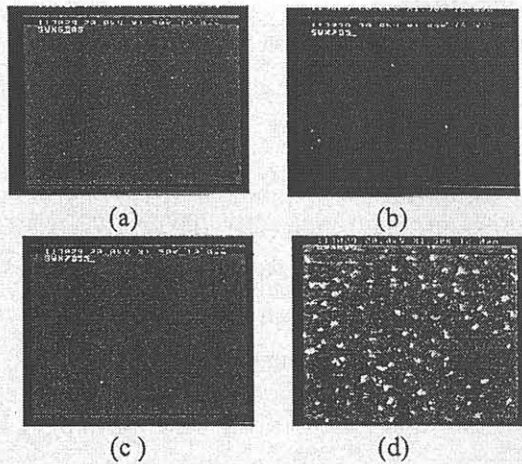


Fig. 2 SEM images of Cu/WC_x(60nm)/p⁺n diode (a) as-deposited and annealed at (b)500°C, (c)550°C and (d)600°C.

Figure 3 illustrates the distribution of leakage current density of annealed Cu/WC_x/p⁺n structure under a reverse bias of 5V. Leakage current remains stable up 550oC annealing (Figs. 3(b)). However, after 600oC annealing, a severe degradation of the Cu/WC_x/p⁺n diode occurred and the leakage current density was above 10⁻⁶A/cm² (Fig.34(c))

Figure 4 shows the SIMS depth profiles of Cu/WC_x(60nm)/p⁺n junction diode under 500°C~600°C annealing. As shown in Figs. 4(a) and 4(b), no sign of copper diffusion through the barrier layer into Si substrate was observed for the 500°C and 550°C annealing cases. However, for the 600°C-annealed sample, strong

interdiffusion of copper into Si substrate was observed.

4. Conclusion

The sputter-deposited WC film was investigated as a diffusion barrier for Cu metallization. The Cu/WC_x Si(pn) structure was found being metallurgically stable after 550°C annealing. Experimental results suggest that the incorporation of carbon in tungsten is very benefit in improving the thermal stability of the barrier metal for Cu metallization. According to XRD, SEM and SIMS analyses, the failure of WC_x layer was found mainly due to the diffusion of Cu along the localized defects of WC_x barrier layer into underlying silicon.

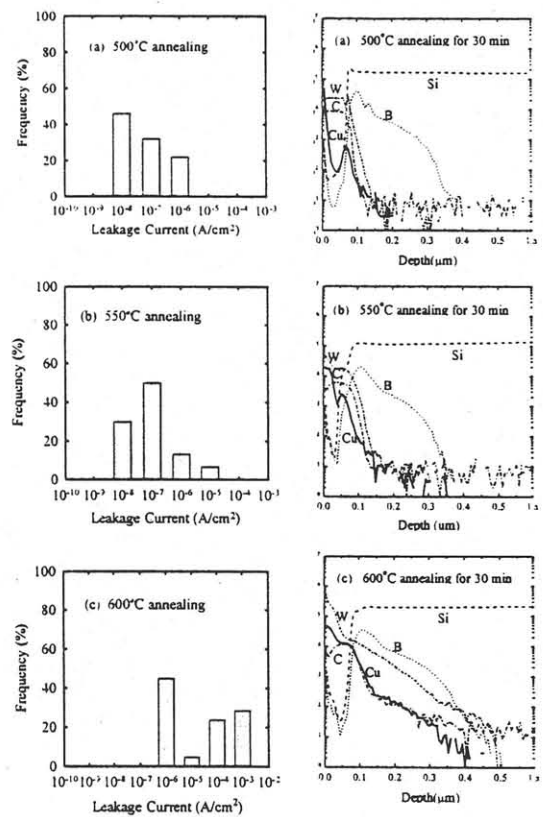


Fig. 3(upper-left) Leakage current distribution of Cu/WC_x/p⁺n after (a) 500 °C, (b) 550 °C, and (c) 600°C annealing.

Fig. 4(upper-right) SIMS depth profile of Cu/WC_x p⁺n structure annealed at (a)500°C, (b)550°C and (c)600°C.

References

- [1] Holloway et al. J.Appl. Phys. 71, 5433 (1992)
- [2] Uekubo et al. Thin Solid Films 286, 170 (1996)
- [3] Tsai et al. J. Appl. Phys. 79, 6932 (1996)