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Conductivity improvements of Atomic Layer Deposited Ta_3N_5

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INTRODUCTION

Thin TaN is frequently used in work function metal (WFM) stacks for CMOS devices. Current technological approaches like replacement metal gate (RMG) requires TaN to be very conformal with mono-layer thickness control. This can be achieved by using atomic layer deposition (ALD). Using $TaCl_5$ instead metal-organic precursors avoids the incorporation of carbon in the film and induces only a few atomic percent of chlorine contamination. Unfortunately, the reduction of $Ta(5^+)$ in the $TaCl_5$ molecule is not sufficient to obtain the desired cubic TaN phase. Instead, Ta_3N_5 with an orthorhombic crystal structure is formed. [1] This phase is often described as the dielectric phase because of the high sheet resistance.[2,3] However, the resistivity has been observed to decrease with increasing deposition temperatures, which is not explained in literature. In this work the resistivity of $TaCl_5$ based ALD Ta_3N_5 is evaluated in detail. Correlation with crystallinity and the interaction with aluminum from the gate trench fill is investigated.

EXPERIMENTAL

ALD of Ta_3N_5 is performed at 400 – 550 ^oC, using separated, saturated pulses of $TaCl_5$ and NH_3. For cubic TaN PDMAT and NH_3 was used. Mass measurements, ellipsometry and XRR are used to check the thickness and uniformity of the deposited films. With grazing incidence (GI) XRD the crystallinity of the material is investigated.

RESULTS

For all deposition temperatures (T_{dep}) the sheet resistance of Ta_3N_5 up to thicknesses of ca. 10 nm remains too high to be measured. Broad peaks in the GIXRD spectrum indicates a disordered bottom layer, still carrying the signature of the Ta_3N_5 phase. Beyond 10 nm thickness, the sheet conductance starts to increase linearly with film thickness. Etch-back measurements indicate the conductivity to originate from the top layer and increases for higher temperatures. For thicker films, a detailed signature of the orthorhombic phase appears distinctly in the GIXRD spectrum, superposed on the spectrum of the disordered bottom layer. At all T_{dep}, the film remains in the orthorhombic Ta_3N_5 phase (see fig. 1 and 2), but additional peaks at 22.1^o and 36.7 ^{o} appear. Those features become more distinct with increasing T_{dep} (fig. 2). When 38 nm Ta_3N_5 films deposited at 400 ^oC are annealed at 500 ^oC for 4h, these same two peaks are also observed together with a large decrease in sheet resistance. Moreover, the back ground of the disordered layer disappears. Annealing both TaN and Ta_3N_5 films with Al layers on top decreases the resistivity significantly (fig 3). GIXRD spectra for both films are showing much more intensive and sharper peaks (fig. 2), indicating an improved crystallinity for both the cubic TaN and the orthorhombic Ta_3N_5 phase. SIMS measurements show the diffusion of Al into TaN, however the concentration is too low to be measured with XPS and thus rule out the presence of the formation of a TaN-Al alloy.

DISCUSSION AND CONCLUSION

When Tantalum nitride is deposited with $TaCl_5$, the first 10 nm is disordered, but of a Ta_3N_5 signature. Both explain the very high resistivity. This is in contrast with PDMAT, which also shows a similar disorder, but clearly involving cubic TaN phase which is conductive. In further growth beyond 10 nm, Ta_3N_5 becomes more crystalline. With higher T_{dep} or annealing at 500 ^oC new peaks appear in the XRD spectrum. Those additional peaks do not originate from Ta_4N_5, Ta_5N_6 or the cubic TaN phase. Instead, they might be forbidden reflections that appear due to symmetry breaking induced by stress or the formation of vacancies caused by further crystallization of the Ta_3N_5 film. This can also explain resistivity improvements of Ta_3N_5. Annealing with Al enhances this crystallization effect correlation with conductivity improvement which is also observed in PDMAT based TaN. The disorder of the bottom layer is removed by Al anneal, improving the conductance of Ta_3N_5 films of a few nm's thick. This allows the replacement of cubic TaN in WFM stacks in combination with Al gate trench fill. The use of $TaCl_5$ improves the compatibility with $TiCl_4$ based TiN ALD and integration into WFM stacks of CMOS devices.

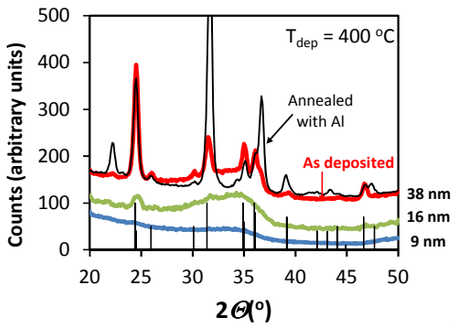

Fig. 1, GIXRD to Ta_3N_5 deposited at 400 ^oC. The 38 nm film is shown before and after Al assisted anneal.

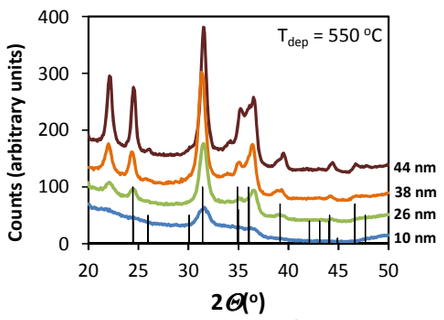

Fig. 2, GIXRD oft Ta_3N_5 deposited at 550 ^oC

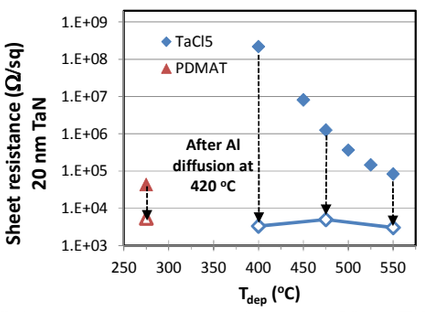

Fig. 3, improvement of sheet resistance on 20 nm TaN and Ta_3N_5 layers by Al assisted anneal at 420 ^oC for 20 minutes.

[1] L. Hiltunen *et al*., Thin Solid Films 166, 149 (1988).
[2] M. Ritala *et al*., Chem. Matter. 11, 1712 (1999).
[3] H. Kim, J. Vac. Sci. Technol. B 21, 2231 (2003).