Reactive Sputtering of Tantalum Nitrides for Diffusion Barrier Layers

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Abstract – The objective of this project is to develop a robust process to deposit Tantalum nitride barrier layer for copper metallization. TaN films were reactively sputtered in a twin cathode AC inverted cylindrical magnetron configuration using the IonTech Cyclone sputtering system. The dependence of thickness, resistivity and phase changes as a function of N_2 flow rate was studied. A designed experimental approach was used to optimize resistivity and the phases formed. A 10 sccm N_2 flow (with 99 sccm Ar) deposited at 4 mTorr and 2 kW pressure gave an amorphous bcc-phase Ta(N) with a low resistivity of about 220 μΩcm. Further analysis would be done to study the barrier properties, after depositing copper and doing electrical, structural and chemical characterization.

1. INTRODUCTION

A. Copper Metallization

As device dimensions are being scaled down to deep submicron, the metallization technology is becoming increasingly important. Copper is a promising interconnect material because of its low electrical resistivity and high resistance to electromigration as compared to the commonly used aluminum and its alloys. However, Cu is a fast diffuser in Si and SiO_2. The presence of Cu-Si precipitates in critical regions strongly affects the reverse leakage current of p-n junctions. It degrades the device performance by introducing deep electronic levels into the Si bandgap leading to reduction in the minority carrier life [1]. Also, there are no suitable CVD processes for Cu deposition. It oxidizes easily because of the ability to have self-passivation. It does not undergo anisotripoic etching, and cannot be etched by the normal RIE techniques. Cu also has poor adhesion to the dielectric layers.

B. Need for barrier layer

To eliminate the diffusion into the substrate, a layer diffusion barrier material which has less grain boundaries, good adhesion to Si and SiO_2, high thermal and electrical stability with respect to Cu is necessary. Various transition and refractory metals and their alloys, nitrides, silicides and oxides have been studied as potential barriers, and Tantalum Nitride compounds have been found to be promising candidates. A good diffusion barrier should have minimum interaction with copper so that it does not affect the resistance of the copper interconnect. TaN has a very high melting point (3087°C).It is thermodynamically stable with respect to Cu and has good adhesion to Si and SiO_2. TaN has a dense microstructure, shows good resistance to heavy mobility of Cu in Si and has electrical stability at high temps (upto 750°C).[1]

The objective of this project is to investigate the barrier properties of Ta and its nitrides for Cu metallization at RIT.

2. EXPERIMENTAL AND RESULTS

A. Experimental

The substrates were prepared from Si wafers on which 1000°A of oxide was grown in the Bruce furnace. They were patterned into horizontal stripes of alternate layers of Si and SiO_2 using a Kasper aligner. This would enable us to study the properties of TaN on both Si and SiO_2, and also use the four-point probe to measure sheet resistance on the TaN deposited on the SiO_2 regions, by providing an insulating substrate.

The TaN films were reactively sputtered in an AC twin cathode inverted magnetron configuration of the Ion Tech Cyclone sputtering system. The Ion Tech Cyclone is a fully automated system with short cycle times and high deposition rates. The AC inverted magnetron configuration has remarkable improvements over the RF and DC configurations. There is excellent target utilization and uniform deposition of even complex shapes.

A 7.5" Ta target was used, and the base pressure of the chamber was 5 x 10^{-6} Torr, and the working pressure was about 5.2 x10^{-3} Torr. A hysteresis plot was first obtained for nitrogen flow in the range of 0 to 50 sccm by increasing and decreasing the N_2 flow respectively and measuring the voltage of the target without using any substrate. The deposition was done at 2 kW forward power and a total pressure of 8 mTorr for 5 min. The gas mixture consisted of Ar at 99sccm. In the operating range, no hysteresis was observed as seen in figure 1. This is because of the high pumping speed of 1600 l/s obtained by a turbopump. There is no poisoning of the target, and the films were deposited in the high rate metal sputtering

regime. The films were then deposited under the same conditions, while the N_2 flow rate was varied from 0 to 40sccm.

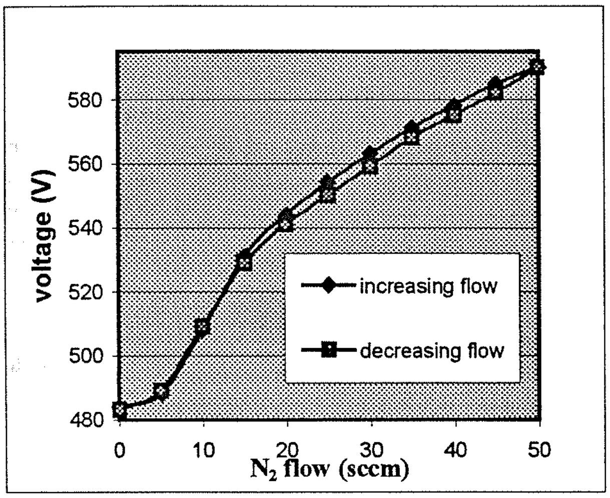

Figure 1: Hysteresis behavior of TaN

The thickness of the films was measured using a Tencor AlphaStep profilometer. Steps were made by marking a line on the wafers prior to deposition with a sharpie pen, and then rubbing it off after the deposition using acetone. Sheet resistance was measured by a four-point probe. The x-ray diffraction Analysis was done on Rigaku x-ray diffractometer with Cu K_α radiation. The adhesion of the films to the substrate was tested using a tape test.

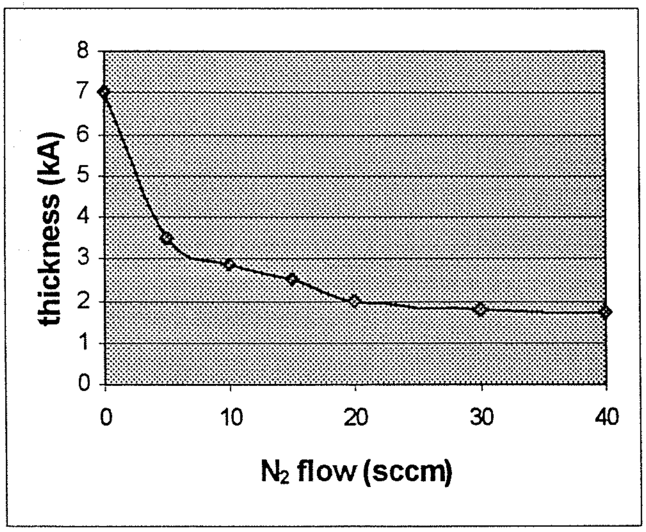

Figure 2: Dependence of thickness on N_2 flow

B. Results and Discussion

The resistivity of the pure Ta film is about 720 μΩ cm. As the nitrogen in the film is increased to 5% there is a decrease in resistivity to 430 μΩ cm. Increasing the N_2 content further to 20%, causes a gradual increase to 1200 μΩ cm. The deposition rate was high at low levels of nitrogen, but there was a sharp decrease in deposition rate with nitrogen. At higher levels of N_2 there is a steep increase in resistivity due to low deposition rate and high sheet resistance. This is seen in figures 2 and 3.

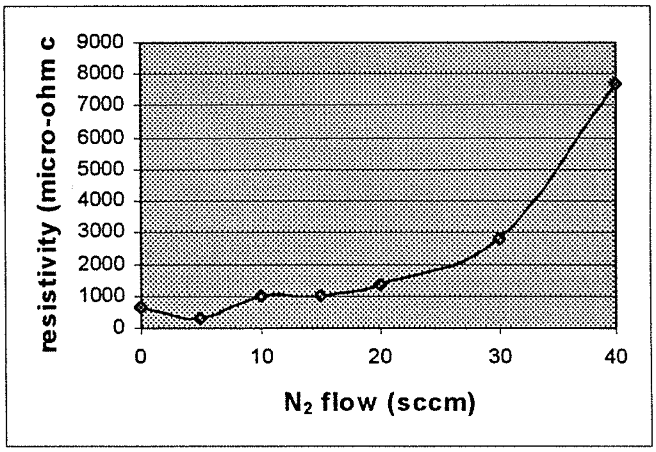

Figure 3: Dependence of resistivity on N_2 flow

This change in resistivity is explained due to the change in the crystalline structure of the TaN_x phase, which was analyzed from the XRD patterns, and compared with those observed in the literature. The pure Ta shows the (002), (202), (413) peaks of tetragonal Ta. With slight increase in N_2, bcc-Ta phase starts forming, observed by the (110) and (200) peaks [3], seen in figure 4, which explains the drop in resistivity.

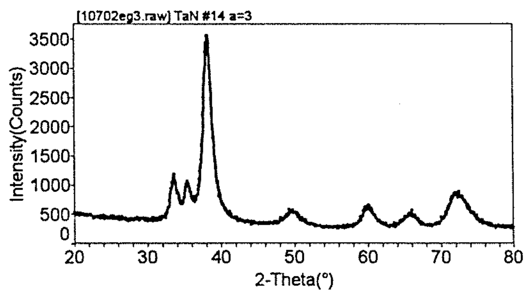

Figure 4: XRD Pattern with 5 % N_2

At higher N_2 levels of 10 –15 %, the bcc Ta(N) and at 20%Ta_2N phases are formed as seen in figure 5. The Ta_2N phase is supposed to have a good amorphous

microstructure. At 40 sccm N_2, the peaks are not sharp. Table 1 shows the various phases at different levels of N_2.

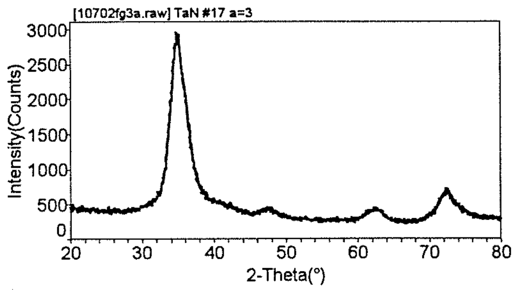

Figure 5: XRD Pattern with 20% N_2

Further analysis needs to be done to analyze the phases, which have been reported as fcc TaN. When the films were tested with a scotch tape, they did not peel off. This means the adhesion of the films to the substrate was good

Table 1: Phases of TaN [3]

N_2flow (sccm)	**Crystalline Phases**
0	Tetragonal Ta
5	TetragonalTa +bccTa(N)
10	bcc Ta(N)
15	bccTa(N) amorphous
20	bcc TaN
30	fcc TaN
40	Fcc TaN + Ta_3N_5

This interesting change in the nature of resistivity of the films was in agreement to the literature [2], but the overall resistivity was an order higher than the reported values. So a Design of Experiments methodology was used for optimization of process parameters for making the films. The following five factors were chosen to be investigated and a ½ fractional factorial experiment was run.

- N_2 flow rate : 5 and 20 sccm
- Pressure: 4 and 8 mTorr
- Power: 1 and 2 kW
- Substrate bias: 0 and 50 kV
- Time : 5 and 15 min

The responses measured were thickness, sheet resistance and resistivity. The results were analyzed using the minitab software, and after doing the Yates anova analysis, the optimum parameters obtained to get low resistivity of 220 μΩcm and good structure were 10sccm N_2, gas pressure of 4mTorr, zero bias, power of 2kW for time 15 min.

3. CONCLUSIONS

The optimum conditions for the barrier layer would be a low pressure, high power, no bias, a slightly high time deposition. Also N_2 flow of about 10 sccm N_2 gives an amorphous phase which would be a good diffusion barrier. The next phase of study includes deposition of Cu seed layer followed by electroplating of Cu on the TaN films and testing the barrier properties by doing RBS analysis. Also, other barrier materials like TaSiN, which have better barrier properties would be studied.

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