



Synthesis and Characterisation of Ta₂O₅ Thin Films For Microelectronics Application

KEYWORDS

Tantalum PentaOxide, C-V Analysis, DC Sputtering

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ABSTRACT Amorphous tantalum oxide thin films were deposited by reactive sputtering of tantalum target onto silicon substrates. Oxygen flow rate has been varied to obtain thin films with different densities. The thin films were analysed by X-RAY diffraction and atomic force microscopy (AFM). We present the data of deposition rate and refractive index of amorphous tantalum oxide as a function of oxygen flow rate. Also the C-V characteristics of the as deposited amorphous tantalum oxide is compared with that of annealed tantalum oxide film. The I-V measurements are taken by I-V model set and the value of leakage current is found to vary in the range $[6.0 \times 10^{-4} \text{ A} - 2.3 \times 10^{-4} \text{ A}]$ for corresponding values of electric field density $[0-4 \text{ MV/cm}]$ in case of as deposited film, whereas it ranges from $[4.8 \times 10^{-4} - 1.8 \times 10^{-4} \text{ A}]$ in case of annealed film for similar range of electric field density.

INTRODUCTION

The industry's demand for greater integrated circuit functionality and performance at lower cost requires an increased circuit density, which has translated into a higher density of transistor on a wafer [1]. This rapid shrinking of the transistor feature size has forced the gate dielectric thickness to also decrease rapidly. This clearly presents a significant challenge for the continued use of SiO₂ as gate dielectric. [2-6] Many gate materials are under considerations as potential replacements for SiO₂ such as metal oxides of 3rd group and 4th group elements. The gate dielectric may indeed be the key structural element in the MOSFET. It must have low levels of fixed charge ($\sim 5 \times 10^{10}/\text{cm}^2$) and interface states ($\sim 5 \times 10^{10}/\text{cm}^2\text{-eV}$) and must remain reliable after years of high field stressing (~ 10 years). In the present work tantalum oxide has been selected for detailed study due to its potential properties i.e high dielectric constant of 25 and significant band gap of 4.4eV. Tantalum pentaoxide has emerged as one of the most promising candidate in terms of its chemical and thermal stability. But the choice alone of suitable metal oxide with high dielectric constant is not sufficient to overcome the scaling challenges. The various deposition techniques and the conditions under which the thin films are deposited plays important role in deciding the structural and electrical properties of the deposited films. This paper discusses to crystallize the tantalum oxide thin films by varying the oxygen flow rate, to avoid the annealing of these films at high temperature which largely degrades the structural properties of the deposited films. Tantalum pentaoxide is widely used as an electrolytic capacitor dielectric. [Lin et al 1999]. The various techniques are anodization [7], ion plating [8,9], magnetron sputtering [10,11], laser ablation [12,13], atomic layer deposition, of the various depositions techniques reactive has been employed to deposit the tantalum oxide films have been investigated using Keithly 590 CV analyser and I-V set model (Keithly 595). Effect of O₂ flow rate on deposition rate and refractive index has also been studied.

EXPERIMENT

The silicon wafers were chemically cleaned, by the standard RCA procedure, and subsequently etched in diluted HF solution, to remove the native SiO₂ layer. All the films were deposited onto p-type (100) single crystalline silicon substrates in the 1-10 Ω cm resistivity range. Tantalum oxide films were deposited by reactive sputtering of a tantalum (Ti) target, in mixed argon (Ar) and oxygen atmosphere. The flow rate of Ar was maintained constant at 50 sccm while flow rate of oxygen was varied at kept at 5, 7 sccm, 10 sccm and 15 sccm for different composition of the film. The total pressure during

the deposition in the chamber was kept at 100 mtorr. The sputtering power was 100 watt. The thickness of the films as measured using AMBIOS stylus surface profiler was found to be 80nm. MOS capacitors were formed by thermal evaporation of aluminium through shadow mask having circular openings of 1 mm diameter.

The capacitance voltage studies were performed using Keithley 590 CV analyzer. The glancing-of-incidence XRD measurements were performed in order to obtain the Tantalum oxide thin films microstructure and phase compositions. The crystal phase structure was analyzed with a XPERT-PRO diffractometer from Panalytical, equipped by a Gionometer PW3050/60 working with Cu Kα radiation of wavelength $\lambda = 1.54060 \text{ \AA}$. The Gionometer scan was performed at the scan rate of $0.01^\circ \text{ sec}^{-1}$. Diffraction peaks related to crystalline phases of tantalum oxide are selected with in this region. The voltage was set at 45 kV with 40 mA flux. The microstructure was analyzed by Atomic Force Microscope (AFM), model Pro 47, NT MDT. The AFM was operated in non contact mode. We register the root mean square (rms) value (standard deviation of the measured height values, i.e, the standard deviation of the elongation of the AFM cantilever tip) as a measure of the surface roughness. A commercial rotating-polariser, rotating-compensator, Fourier-transform based variable angle of incidence ellipsometer was used to measure the refractive index.

RESULT AND DISCUSSION

1. Structural Analysis

Figure 1 represents X- diffraction patterns of Ta₂O₅ thin films. The X-RD pattern shows that the thin film at oxygen rate is amorphous in nature' since no peaks appears in the spectrum. Two or more peaks occurs corresponding to (001) (201) plane Ta₂O₅ indicating that amorphous thin films could be crystallized by varying the oxygen flow. Usually the substrate temperature higher than 700 °C is necessary to obtain crystalline Ta₂O₅ thin film, or a post annealing at higher temperature for as deposited films is required to improve the crystallinity based on high diffusing energy of Ta in the crystal lattice of Ta₂O₅ but in the present work crystallinity enhancement could be attributed to the variation of oxygen flow rate.

Figure 1 :X-RD Pattern

The grain size of Ta₂O₅ thin film can be calculated using Scherrer function $D = .89\lambda / \beta_{1/2} \text{Cos}\theta$ Where D is average grain size, β is full width at half maximum (FWHM) of Ta₂O₅ X-RD spectrum, θ is Bragg's angle, λ is the wavelength of X-ray, and k is Scherrer constant. Here the value of k is 0.94. It is clearly visible that the grain size changes from 110 nm for

7 sccm oxygen to 75 nm for 15 sccm oxygen. Table 2 shows the variation of root square

Table 1:(Variation of deposition rate, and refractive index with oxygen flow rate)

Oxygen flow rate(sccm)	Deposition rate(nm/min)	Refractive index
5%	9.2	2.3
7%	8.2	2.30
10%	6.1	2.31
15%	3.3	2.4

roughness and average roughness of the tantalum oxide films with different oxygen flow rate. From this data it is clearly visible that R_{rms} and R_a values increases with increase in oxygen flow rate. This increase may be due to the fact that presence of oxygen act as impurities in the film and it reduces the movement of tantalum on the surface and hence the roughness increases.

Table 2 : (variation of grain size, root square roughness, and average roughness with oxygen flow rate)

Oxygen flow rate(sccm)	Grain size (nm)	R_a (nm)	R_{rms} (nm)
7%	110	5.1	4.3
10%	95	7.2	6.2
15%	75	8.4	8.3

2. Deposition Rate And Refractive Index

The deposition rate and refractive index for the deposited tantalum oxide films has been studied as a function of oxygen flow rate. The results have been listed in table 1. With the increase in oxygen flow rate, the probability of the reaction between tantalum and oxygen increases forming oxide and sputtering with tantalum is difficult then with tantalum metal and hence the deposition rate decreases. The refractive index values obtained are with the help of ellipsometer are found to increase with increase with increase in oxygen flow rate and are also found to vary from theoretical values of refractive index i.e 2.42 and 2.53 with change in oxygen content.

3. Electrical characteristics

The I-V data obtained using I-V model set (keithly 595) has been shown in fig.2 for as deposited film (at oxygen flow rate 10 sccm) and the annealed film. It is found that the value of leakage current reduces with annealing. Its value ranges from $(6.0 \times 10^{-4}A - 2.3 \times 10^{-4}A)$ for Corresponding values of Electric field density (0 to 4 MV/cm) in case of as deposited film, whereas it ranges from $(4.8 \times 10^{-4} - 1.8 \times 10^{-4})$ in case of annealed film for similar range of Electric field density.

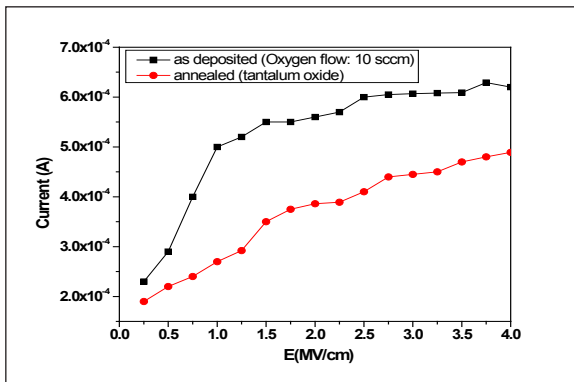


Figure 2 : Leakage current as a function of field strength

4. C- V Characteristics

The c-v measurements of the deposited film were studied using 590 cv analyser (Keithley model 590) at different oxygen flow rates as shown in the figure 3. Also the C-V character-

istics of the as deposited film are compared with that of the annealed film as shown in the figure 4.

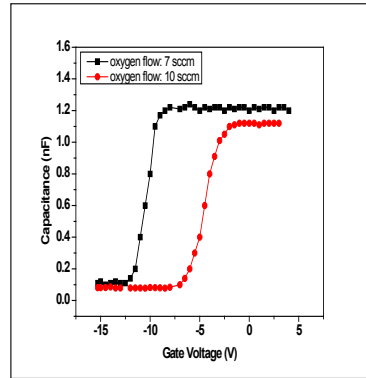


Fig 3 CV of as deposited film at different oxygen flow rate

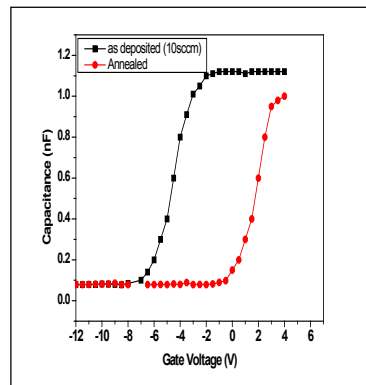


Figure 4 : CV of as deposited and annealed film

It can be appreciated that the curves for CMOS capacitors with Ta_2O_5 dielectric present higher values of capacitance when compared with a MOS capacitor with silicon dioxide as dielectric with the same thickness, indicating its higher dielectric constant value. The dielectric constant was calculated utilizing the oxide capacitance, determined from the C-V curves and the film thickness measured by ellipsometry. The dielectric constant obtained for Ta_2O_5 was 29 and for silicon dioxide was found to be 2.3.

5. CONCLUSIONS

1. We have studied the effect of oxygen flow rate on deposition rate, refractive index, I-V characteristics, C-V characteristics, average roughness and root square roughness.
2. Deposition rate of thin films is found to decrease from 9.2 nm/min to 3.3 nm/min with increase in oxygen flow rate from 5% to 15%. The refractive index values are also found to vary with oxygen flow rate.
3. Average roughness and root square roughness of tantalum oxide thin films are also found to increase with increase in oxygen flow rate, which may be due to the fact that presence of oxygen act as impurities in the film and it reduces the movement of tantalum on the surface and hence the roughness increase increases. Grain size is also found to decrease with increase in oxygen flow rate
4. The value of leakage current is found to vary in the range $[6.0 \times 10^{-4}A - 2.3 \times 10^{-4} A]$ for corresponding values of electric field density $[0-4 MV /cm]$ in case of as deposited film, whereas it reduces and ranges from $[4.8 \times 10^{-4} - 1.8 \times 10^{-4}]$ in case of annealed film for similar range of electric field density
5. Dielectric constant is found to decrease with increase in oxygen flow rate.

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