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Structural and electrical properties of Ta_2O_5 thin films prepared by photo-induced CVD

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Abstract. **Tantalum oxide (Ta_2O_5) films and Al/Ta_2O_5/Si MOS capacitors were prepared at various powers by ultraviolet photo-inducing hot filament chemical vapour deposition (HFCVD). Effects of ultraviolet light powers on the structure and electrical properties of Ta_2O_5 thin films were studied using X-ray diffraction (XRD) and atomic force microscopy (AFM). The dielectric constant, leakage current density and breakdown electric field of the samples were studied by the capacitance–voltage (C–V) and current–voltage (*I–V*) measurements of the Al/Ta_2O_5/Si MOS capacitors. Results show that the Ta_2O_5 thin films grown without inducement of UV light belong to amorphous phase, whereas the samples grown with inducement of UV-light belong to δ-Ta_2O_5 phase. The dielectric constant and leakage current density of the Ta_2O_5 thin films increase with increasing powers of the UV- lamps. Effects of UV-lamp powers on the structural and electrical properties were discussed.**

Keywords. **Chemical vapour deposition processes; oxides; dielectric material; MOS capacitor.**

1. Introduction

High-dielectric-constant (high-*k*) materials, such as HfO_2, Ta_2O_5 and Er_2O_3, are now being intensively studied in view of their use in further generations of integrated circuits as a replacement for the currently dominant SiO_2 (Atanassova and Paskaleva 2007; Losurdo *et al* 2007). Specifically, Ta_2O_5 thin film was identified to be exceptionally appropriate for applications in high-density dynamic-random-access memories (DRAMs), as well as in metal–oxide–semiconductor field-effect transistors (MOSFETs) and transparent optical coatings (Huang *et al* 2002; Jolly *et al* 2003; Lee and Jan 2005) due to its potential properties, such as a wide bandgap, high dielectric constant and high refractive index (Jain *et al* 2005). Recently, many low temperature processing techniques employed to prepare these films have been studied. The photo-induced chemical vapour deposition processes (Kim *et al* 2005) are very promising since the processed surface is not subjected to damaging ionic brombardment which can occur in plasma assisted systems, compared to other preparation methods such as MOCVD (Jolly *et al* 2003), reactive magnetron sputtering (Jain *et al* 2005), pulse laser deposition (PLD) (Watanabe *et al* 1993). In this paper, Ta_2O_5 thin films were prepared by UV light photo-induced hot filament CVD with various powers of UV lamp. Effects of UV-lamp power on the structural and electrical properties of Ta_2O_5 films were studied.

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2. Materials and methods

The Ta_2O_5 thin films were deposited onto *n*-Si wafers by photo-inducing hot filament CVD. Figure 1 shows a schematic diagram of the photo-induced CVD reactor designed for these experiments. A tantalum filament (99·99%) was used as hot filament. The hot filament temperature was maintained at 2200°C. At the same time, Ta was also used as metal source for preparing Ta_2O_5 thin films. O_2 and Ar mixture with a flow ratio of 1:3 was used as reaction gas. The chamber was pumped down to 5×10^{-3} Pa and backfilled with Ar and O_2 mixture to a pressure of 8 Pa. The samples were prepared with the power of the UV-lamp of 0, 60, 120 and 180 W, respectively. The power of the UV lamp was changed by adjusting voltage and current of electrical source. The substrate temperature of 500°C and substrate bias voltage of −100 V were used. *n*-Si wafers (100) were used as substrates, which were ultrasonically cleaned sequentially in acetone, alcohol for 10 min each, and then dipped in dilute HF (1%) to remove the native oxide. After being rinsed in deionized water and blown dry using high purity nitrogen gas, the substrates were immediately placed into the processing chamber. The thicknesses of thin films determined using an Ambios XP-2 α-step meter were 0·25, 1·05, 1·41 and 1·5 μm, corresponding to samples deposited at the power of UV lamps of 0, 60, 120 and 180 W, respectively. The structure of the thin films was analyzed with D/max-IIIA XRD with a scanning accuracy of 0·02° and wavelength of X-ray of 1·54056 Å. The surface morphology of thin films was observed using the Standard Nanoscope AFM system in air. The Al/Ta_2O_5/Si MOS capacitors were made. Al electrodes

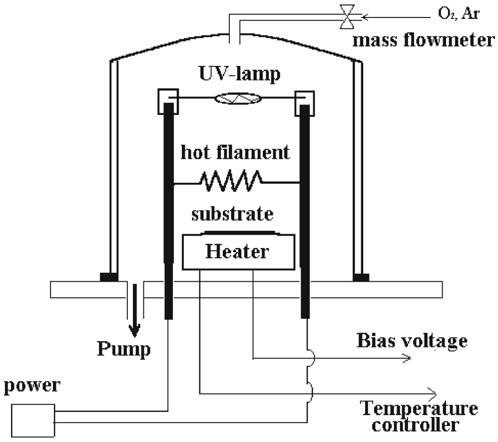

Figure 1. A schematic of photo-induced HFCVD deposition set-up.

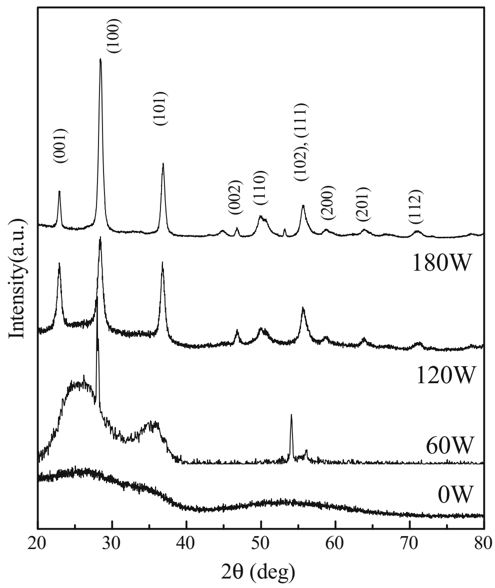

Figure 2. XRD spectra of samples deposited at various powers of UV-lamp.

with a diameter of 1 mm were evaporated through a shadow mask onto the Ta_2O_5 thin films. The *C–V* characteristics were measured by using a Keithley 590 *C–V* meter.

3. Results and discussion

3.1 *Structure of Ta_2O_5 thin films*

XRD patterns of samples deposited at various powers of UV lamp were measured and typical results are shown in figure 2. The XRD results indicate that the Ta_2O_5 thin films deposited without UV light are amorphous. However, for the samples deposited at the power of UV-lamp of 120 W and 180 W, crystallization of Ta_2O_5 films is observed, as evidenced by these characteristic peaks of (100), (101), (001) and (111) of δ-Ta_2O_5 thin films. The grain size of Ta_2O_5 thin films can be estimated according to the Scherrer function:

$$D = k\lambda/\beta \cos\theta, \tag{1}$$

where D is the average grain size, β the full width at half maximum intensity (FWHM) of the Ta_2O_5 XRD spectrum, θ the Bragg angle, λ the wavelength of X-ray and k the Scherrer constant. Here k is 0·94. The results as shown in table 1 reveal that the UV light can induce thin films of crystallization. It is possible to get the crystalline Ta_2O_5 thin films under a low substrate temperature when the thin films grow with UV light inducement. The UV light has three functions: (i) turning oxygen to ozone and enhancing chemical reaction activity; (ii) enhancing the diffusivity of the deposited atoms and (iii) decreasing nucleation energy of thin films.

3.2 *Surface morphology of Ta_2O_5 thin films*

The surface morphology of Ta_2O_5 thin films has been obtained using a Standard Nanoscope III AFM system. The three-dimensional image and root-mean-square (RMS) roughness were used to investigate the surface microstructure of these samples. Typical contact mode AFM images (1×1 μm) of Ta_2O_5 thin films deposited at various powers of UV-lamp are shown in figure 3. The AFM images have been obtained in at least five different regions for each sample and they are found to be similar. Figure 3 indicates that the microstructure of samples depends on the power of UV-lamp. Thin films grown without inducement of UV light belong to amorphous state, whereas thin films grown with inducement of UV-light belong to crystalline phase. The grain size of sample increases with increasing UV-lamp power, which is in agreement with XRD results. The improvement in the electrical property and grain size of thin films is attributed to the UV-generated active oxygen species O (D-1) which strongly oxidizes any suboxides to form more stoichiometric oxides on removing certain defects and oxygen vacancies. The UV-generated active oxygen species are readily adsorbed onto the surface and then diffuse into thin film to react with oxygen vacancies. The optical and electrical properties of thin films were strongly affected by the O/Ta atomic ratio.

Table 1. Grain size of Ta_2O_5 thin films determined from XRD spectrum with Scherrer function.

Power (W)	Grain size from (100) peak (nm)	Grain size from (101) peak (nm)
0	Amorphous	Amorphous
60	-	40
120	132	142
180	149	153

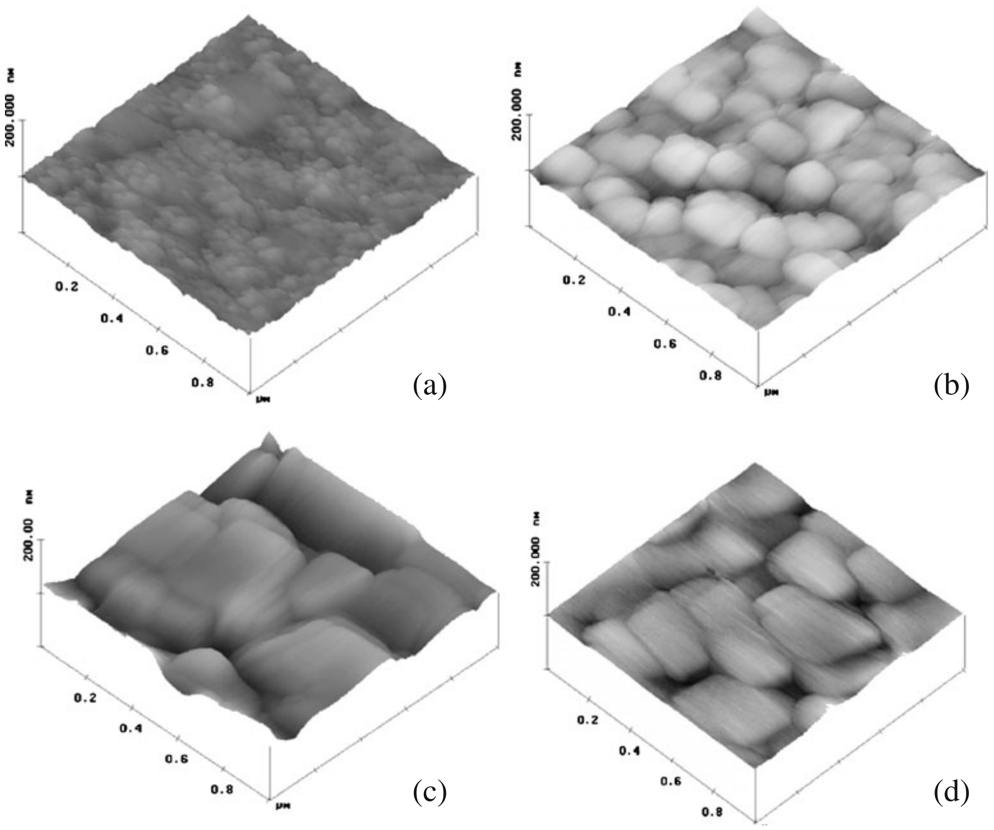

Figure 3. Contact-mode AFM images of Ta_2O_5 thin films deposited at various powers of UV-lamp: (**a**) 0 W, (**b**) 60 W, (**c**) 120 W and (**d**) 180 W.

3.3 *Electrical properties of Al/Ta_2O_5/Si MOS capacitors*

Figures 4 and 5 are the *C–V* and *I–V* characteristic curves of the Al/Ta_2O_5/Si MOS capacitors, respectively. The threshold voltage, dielectric constant, leakage current and breakdown field strength of Ta_2O_5 thin films can be determined from these curves. For applied voltage $V > 0$ V, the Si surface is in accumulation. Therefore, this structure behaves as a parallel plate capacitor, and the dielectrics constant of the Ta_2O_5 dielectric layer in capacitors can be calculated from the following equation

$$C\,(acc) \approx C_O = \frac{\varepsilon_{ef}\varepsilon_0 A_G}{T_{ox}}, \tag{2}$$

where A_G is area of the gate electrode, ε_{ef} the relative dielectrics constant of the Ta_2O_5 thin films and T_{ox} the thickness of Ta_2O_5 thin films, respectively. Table 2 shows calculated results of the relative dielectric constant of Ta_2O_5 thin films deposited at various powers of UV-lamp. The maximum dielectrics constant of crystalline Ta_2O_5 thin films deposited at 180 W is 29. For applied voltage V < 0 V, a depletion region forms in the Si substrate, in which there is no mobile charge. The capacitance is a series combination of the oxide capacitance and the junction capacitance, the total capacitance is

$$C(dep) = \frac{C_o C_s}{C_S + C_o} = \frac{C_O}{1 + \frac{\varepsilon_{ef} W}{\varepsilon_s T_{ox}}}, \tag{3}$$

where ε_s is the dielectrics constant of Si, W the depletion region depth. When the capacitance, C (dep) achieved the minimal value of C_{min}, the MOS capacitor is in an inversion mode. The capacitance is

$$C_{min} = C(inv) = \frac{C_o C_s}{C_S + C_S} = \frac{C_O}{1 + \frac{\varepsilon_{ef} W_T}{\varepsilon_s T_{ox}}}, \tag{4}$$

W_T is the maximum depletion width. The capacitance is independent of the voltage at high frequencies in the inversion mode. The voltage corresponding to a depletion mode changing to an inversion mode is defined as the threshold voltage, V_T.

As shown in figure 5, the leakage current density for sample deposited at various powers of UV-lamp is in a magnitude of 10^{-7} A/cm^2, where the leakage current density is defined when applied voltage is at 1 V. The breakdown field strength, E_B, can be determined from $E_B = V_B/T_{OX}$, where

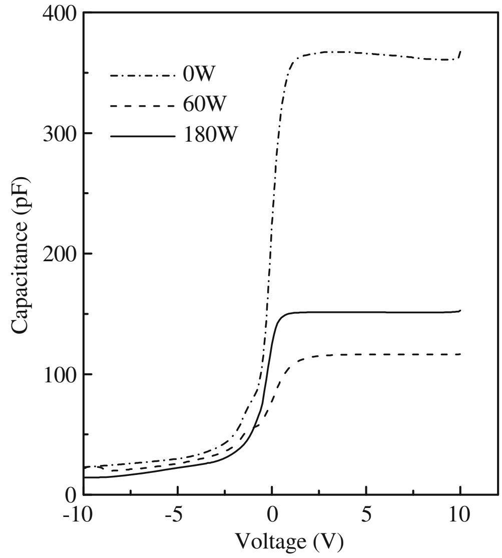

Figure 4. *C–V* curves of the Al/Ta_2O_5/Si MOS capacitors with different Ta_2O_5 dielectric layers deposited at various powers of UV-lamps.

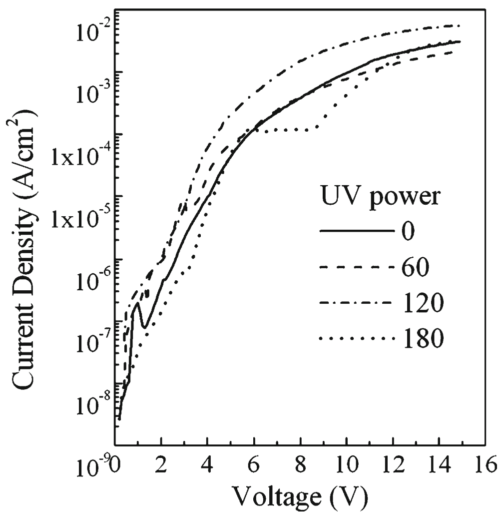

Figure 5. *I–V* curves of the Al/Ta_2O_5/Si MOS capacitors with different Ta_2O_5 dielectric layers deposited at various powers of UV-lamp.

V_B is breakdown voltage, T_{OX} the thickness of Ta_2O_5 thin films. Table 2 shows the leakage current density and the breakdown field strength of the films deposited at various UV-lamp powers.

As shown in figure 2 and table 1, the grain size and dielectric constant, relating to the microstructure and physical properties of Ta_2O_5 samples, increase with increasing UV-lamp power, while the capacitance in *C–V* curve and leakage current densities in *I–V* curve are related to the thickness of Ta_2O_5. The thickness of samples prepared at the UV-lamp power of 0, 60, 120 and 180 W, determined using an Ambios XP-2 α-step meter, are 0·25, 1·05, 1·41 and 1·5 μm, respectively. Since the capacitance and leakage current densities are inverse ratio to thickness. Therefore, the collective effect of the thickness and dielectric constant of Ta_2O_5 thin films result in the non-monotonic values of *C–V* and *I–V* curves as a function of UV-lamp.

Table 2. Electrical parameters of Ta_2O_5 thin films determined from *C–V* and *I–V* characteristics curves.

Power (W)	C_O (pF)	C_{min} (pF)	V_T (V)	ε_{ef}	$E_B \times 10^4$ (V/cm)	$J \times 10^{-7}$ (A/cm^2)
0	366	39	−2·9	13	16	1·91
60	116	35	−2·6	17	4	1·78
120	-	-	-	-	2·3	3·17
180	151	30	−2·5	29	2·8	0·34

4. Conclusions

The Ta_2O_5 thin films and Al/Ta_2O_5/Si MOS capacitors have been prepared by photo-induced hot filament CVD under an Ar and O_2 ambient. The results show that the thin films deposited without UV light are amorphous, whereas thin films grown with inducement of UV-light are crystalline δ-Ta_2O_5. The grain size of crystalline δ-Ta_2O_5 increases with increasing power of UV-lamp. The dielectrics constant and leakage current density of the δ-Ta_2O_5 thin films increase with increasing power of the UV-lamp, whereas the breakdown electric field of the samples slightly decrease with increasing power of UV-lamp.

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