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Electrical properties of Ta_2O_5 films deposited on ZnO

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Abstract. **High dielectric constant (high-*k*) Ta_2O_5 films have been deposited on ZnO/*p*-Si substrate by microwave plasma at 150°C. Structure and composition of the ZnO/*p*-Si films have been investigated by X-ray diffraction (XRD), atomic force microscopy (AFM), scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS) for chemical composition. The electrical properties of the Ta_2O_5/ZnO/*p*-Si metal insulator semiconductor (MIS) structures were studied using high frequency capacitance–voltage (*C*–*V*), conductance–voltage (*G*–*V*) and current–voltage (*I*–*V*) characteristics. Charged trapping properties have been studied by measuring the gate voltage shift due to trapped charge generation under Fowler–Nordheim (*F*–*N*) constant current stressing.**

Keywords. **ZnO; Ta_2O_5; rf magnetron sputtering; microwave plasma; PECVD; high-*k*.**

1. Introduction

Zinc oxide (ZnO) is of great interest as a suitable material for high temperature, high power electronic devices either as the active material or as a suitable substrate for epitaxial growth of group III-nitride compounds (Look *et al* 1998). With its large, direct band gap ≈ 3·4 eV and wurtzite crystal structure, ZnO is similar to GaN. Due to its relatively close match in lattice constants, it may be used as a substrate for GaN and AlN epitaxy. As a consequence, there is renewed interest in the properties of ZnO relevant for microelectronic device applications. ZnO thin films have been prepared by a wide variety of techniques, including sputtering, spray-pyrolysis and electrodeposition (Izaki and Omi 1996; Noh 2003). In particular, the rf sputter method has advantages over other processes because of its simplicity.

To continue the scaling trend of MOS technology, the anticipated high gate leakage current in ultrathin thermal oxide must be suppressed. The development of ULSI storage capacitors requires also investigation of new materials with a much higher dielectric constant than the SiO_2 based layers and a sufficiently low leakage current for a favourable memory operation. Among many high dielectric constant insulators (TiO_2, HfO_2, ZrO_2, Al_2O_3, La_2O_3, Pr_2O_3), tantalum pentoxide (Ta_2O_5) shows high-*k* (25), and it seems to be the most promising candidate for high density DRAMs because of its high dielectric constant, thermal stability and adequate breakdown voltage (Cappellani *et al* 1999; Nandi *et al* 2002).

In this paper, we report the plasma enhanced chemical vapour deposition (PECVD) of Ta_2O_5 layers on rf-sputtered undoped ZnO films. The chemical and electrical properties of Ta_2O_5/ZnO/*p*-Si are also investigated.

2. Experimental

The metal–insulator–semiconductor (MIS) capacitors used in this study were fabricated on undoped ZnO (100 nm) thin film deposited on *p*-Si (100) at 450°C using rf magnetron sputtering of sintered commercial 2-inch ZnO target (purity > 99·99%). Only argon gas was introduced as a plasma gas up to 10 mTorr. In the XRD pattern (figure 1) a major peak of the preferential orientation along the (103) and minor one related to (002) of the undoped ZnO films were observed. It indicates that ZnO films are polycrystalline structures. Figure 2 shows the atomic force micrograph of ZnO film. The scan was taken on a 20 × 20 μm area. The statistical information of the topography of the ZnO films as observed from the height histogram of the AFM image are: rms surface roughness (Z_{rms}), and average roughness (Z_{av}) were found to be 62·1 Å and 23·6 Å, respectively. An SEM image of the cross-sectional view of ZnO/*p*-Si film (figure 3) shows columnar growth which indicates an orientation parallel *c*-axis (002) (Water and Chu 2002).

After standard cleaning of the ZnO/*p*-Si substrate, Ta_2O_5 were deposited using metallo–organic tantalum pentaethoxide [$Ta(OC_2H_5)_5$] by microwave (700 watt, 2·45 GHz)

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plasma cavity discharge system at a pressure of 500 m Torr and temperature of 150°C. Tantalum pentaethoxide [$Ta(OC_2H_5)_5$] kept in a bubbler at 150°C was used and O_2 was used as the carrier gas. The film composition was analysed by X-ray photoelectron spectroscopy. The XPS measurements were performed with a VG Microtech system equipped with a concentric hemispherical analyser (CHA). All XPS spectra were obtained using non-monochromatized Mg K_a (hn = 1253·6 eV) radiation at an angle 30° between the analyser axis and the sample normal. The core levels of O 1*s*, Zn 2*p* and Ta 4*f* spectra of the Ta_2O_5/ZnO/*p*-Si are shown in figure 4. Figure 4a shows the measured O 1*s* peak, which can be deconvoluted into two subpeaks at 531·8 eV and 529·7 eV, assigned to –OH and Zn–O bonding, respectively (Dalchiele *et al* 2001). The peaks of Zn 2*p* (figure 4b) are found to be at 1044·8 eV and 1021·7 eV for Zn $2p_{1/2}$ and Zn $2p_{3/2}$, respectively, with a separation of 23·1 eV between the two peaks which is due to the Zn 2*p* state (Wagner *et al* 1979). The observed Zn $2p_{3/2}$ peak at 1021·7 eV is a typical characteristic of the Zn^{+2} in ZnO (Komuro *et al* 2000). The Ta 4*f* XPS peak (figure 4c) is deconvoluted into two subpeaks. The two peaks are located at 28·7 eV and 26·8 eV with energy separation of 1·9 eV for Ta $4f_{5/2}$ and Ta $4f_{7/2}$ state, respectively. The Ta 4*f* peaks shift 0·6 eV towards higher binding energy (BE), attributed to increasing the oxygen content of the tantalum oxide. The Ta $4f_{7/2}$ peak position at 26·8 eV is typical of Ta^{+5} chemical state in Ta_2O_5 (Atanassova *et al* 1995).

The thickness of Ta_2O_5 film (~ 110 Å) was determined using a single wavelength (6328 Å) ellipsometer (Model Gaertner L-117). The electrical properties of the deposited films (studied using MIS capacitors with an Al gate

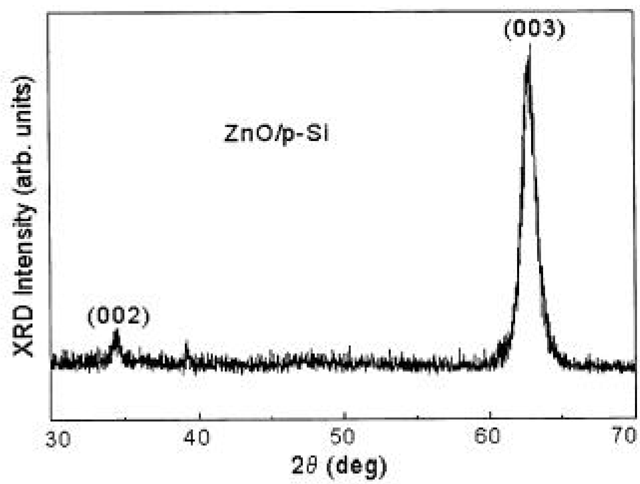


Figure 1. X-ray diffraction pattern of ZnO thin films.

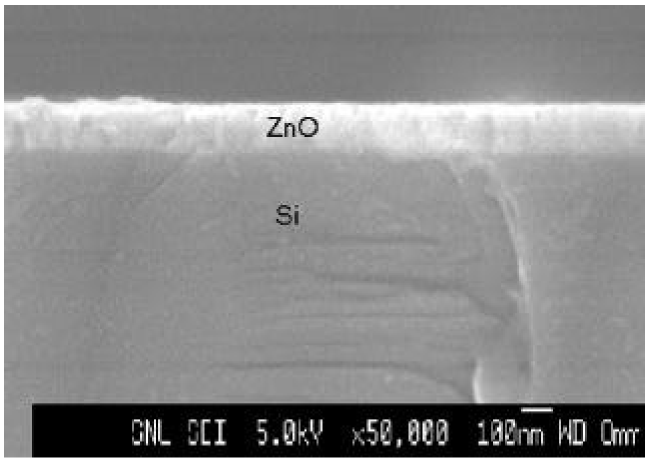
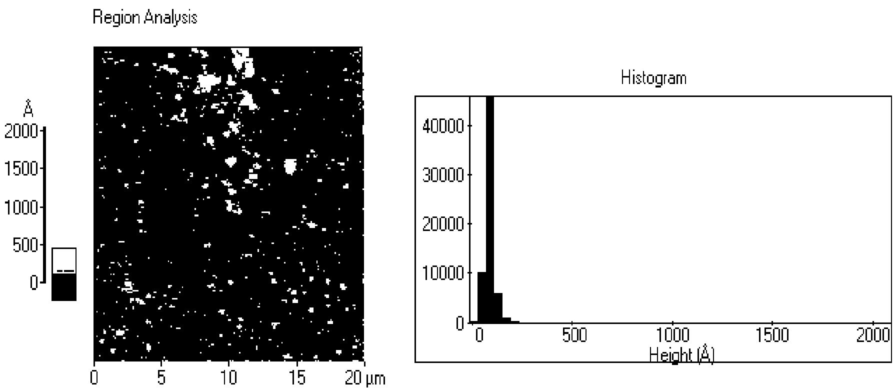


Figure 3. Cross-sectional SEM view of the rf sputtered ZnO film deposited on *p*-Si.



Region	Rp-v	Rms rough	Ave rough	Prj area
[A]	0.208 um	62.1 Å	23.6 Å	400. μ²

Figure 2. Two-dimensional AFM image of the ZnO film.

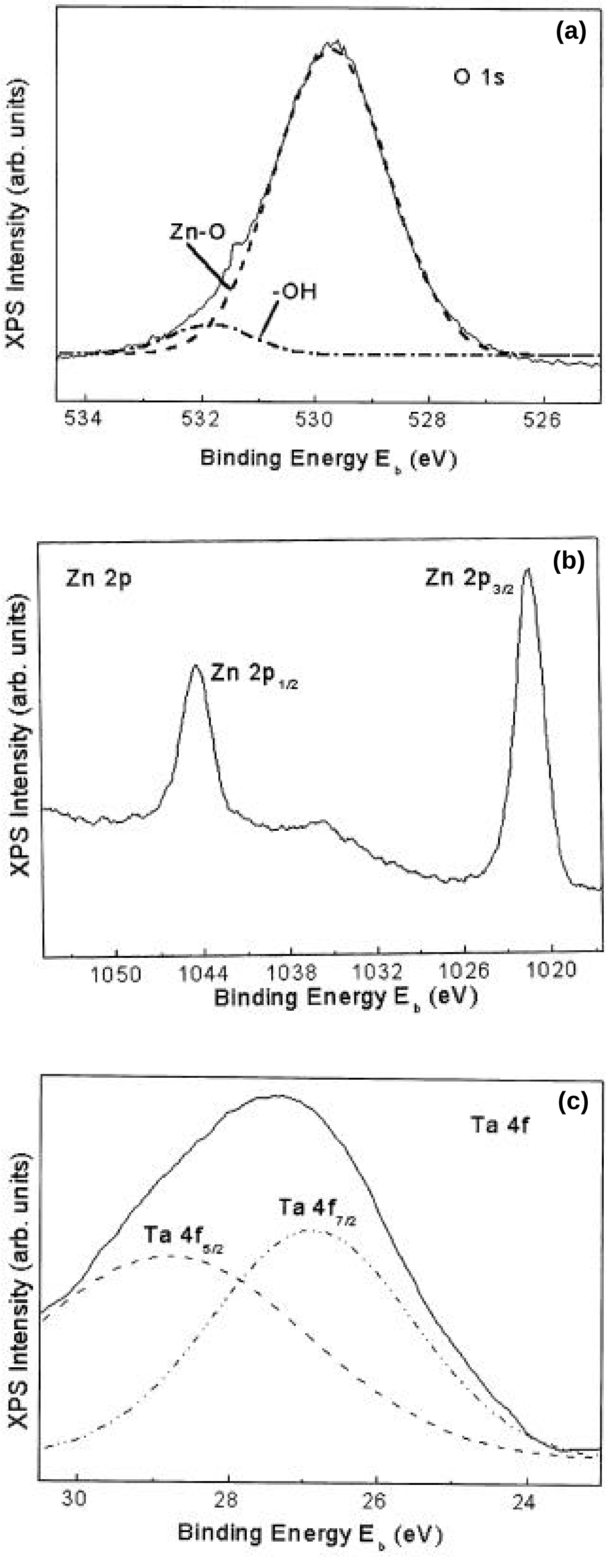


Figure 4. X-ray photoelectron spectroscopy results of the (**a**) O 1*s*, (**b**) Zn 2*p* and (**c**) Ta 4*f* peaks of Ta_2O_5/ZnO/Si films.

which has area: $1{\cdot}96 \times 10^{-3}$ cm^2) were characterized by high-frequency capacitance–voltage (*C–V*), conductance–voltage (*G–V*) and constant current stressing characteristics. The measurements were performed using both HP-4061A semiconductor test system and HP-4145B DC parameter analyser.

3. Electrical characterization

The *C–V* characteristics measured at different frequencies (0·1–1 MHz) is shown in figure 5. In the *C–V* curves a frequency dispersion is observed in the depletion region. The flat band voltage shift due to change in the measuring frequency indicates the generation of interface charge or traps. However, no frequency dispersion is observed in the accumulation and inversion regions. The fixed oxide charge density (Q_f/q) was found to be $2{\cdot}4 \times 10^{11}$ cm^{-2} and the interface trap density (D_{it}) at midgap, calculated using Hill's method (Hill and Coleman 1980) was found to be $1{\cdot}22 \times 10^{12}$ cm^{-2} eV^{-1}.

Figure 6 shows a high frequency (1 MHz) *C–V* characteristics of the Ta_2O_5 films with different stressing times (300 s and 600 s) at a constant current stressing of $J_0 = -2{\cdot}5$ mA/cm^2. A negative voltage shift in the high frequency *C–V* characteristics indicates the presence of positive charges in the film. The charge trapping behaviour of the sample, observed by continuously monitoring the change in gate voltage (DV_g) required to maintain a constant current of $-5{\cdot}0$ mA/cm^2 under gate injection is shown in figure 7.

The trapped charge density (Q_t) has been measured using the bidirectional *I–V* technique (Liu *et al* 1991). In this technique, a voltage shift is measured after a charge injection by *F–N* constant current stressing is completed. The gate current depends on the barrier height and on the

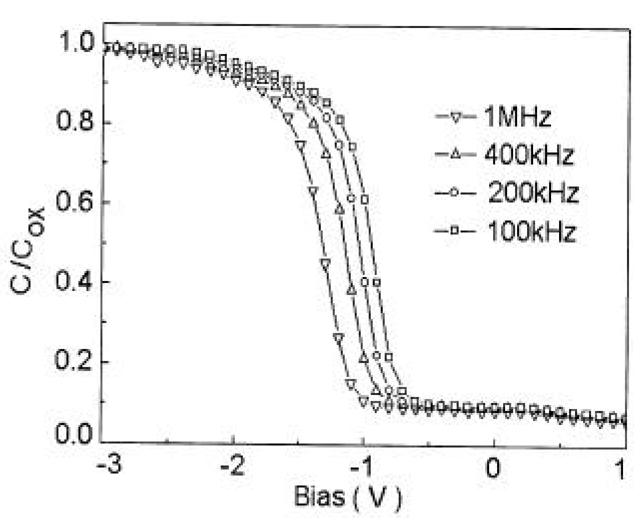


Figure 5. *C–V* characteristics at different frequencies for Ta_2O_5/ZnO/*p*-Si MIS structures.

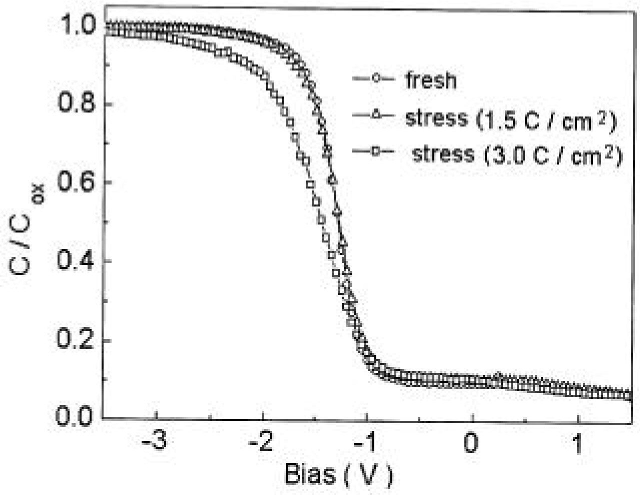


Figure 6. High frequency (1 MHz) *C–V* characteristics of MIS structures: before and after stressing.

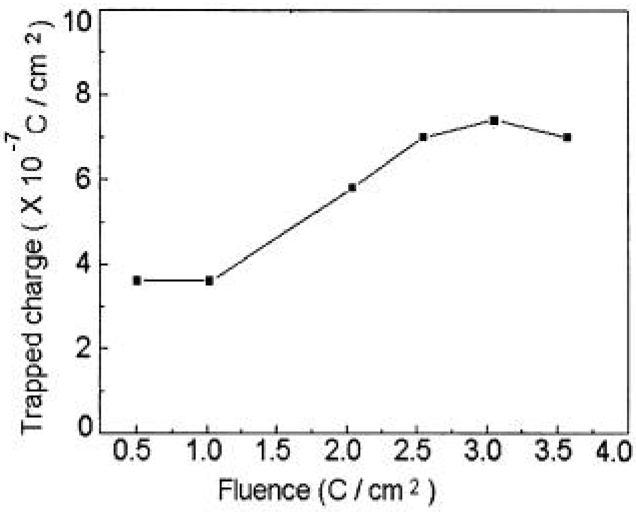


Figure 8. The density of trapped charges vs fluence under constant current injection.

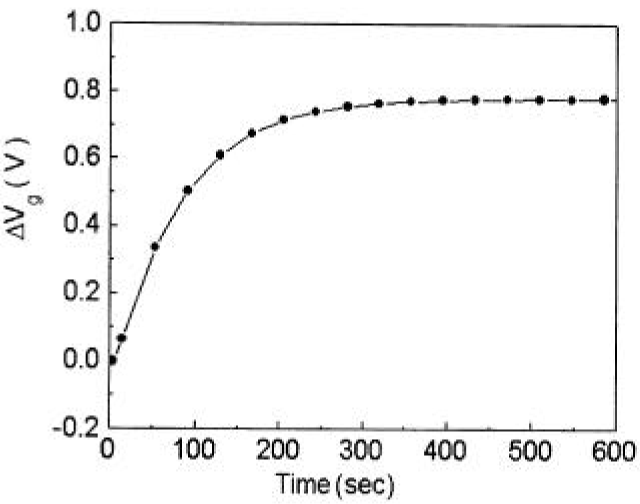


Figure 7. Gate voltage shift vs stress time under constant current stressing (– 5 mA/cm^2).

position of the potential maximum in the dielectric near the injection contact. The characteristics are sensitive to the internal field and the space charge in the oxide which, in turn, affect the barrier height and the position of the potential maximum near the interface. The trapped charge (Q_t) is given by (DiMaria *et al* 1993)

$$Q_t = [1-(\Delta V_{FN}^{-}/\Delta V_{FN}^{+})]\,\frac{e_{ox}}{t_{ox}}, \qquad (1)$$

where ΔV_{FN}^{-} and DV_{FN}^{+} are the negative and positive gate voltage shifts. The dielectric constant, e_{ox}, and thickness, t_{ox}, of the Ta_2O_5 film are 25 and 110 Å, respectively. The trapped charge distributions in Ta_2O_5 under constant gate injection, calculated from (1) is shown in figure 8. It is observed that a short stressing time leads to a low trap charge in the film compared to a longer one. The fast increase in the beginning (due to the filling of native traps and a high rate of generation of new traps) is followed by a slow evolution, mainly caused by the reduction of generation rate due to trapping.

4. Conclusions

Plasma enhanced chemical vapour deposition of Ta_2O_5 layers on rf-sputtered undoped ZnO films and the electrical properties of Ta_2O_5/ZnO/*p*-Si MIS structures have been presented. From XPS spectra of Ta_2O_5/ZnO/*p*-Si films, the peaks of Zn $2p_{3/2}$ and Ta $4f_{7/2}$ at 1021·7 eV and 26·8 eV highlight the formation of ZnO and Ta_2O_5, respectively. The fixed oxide charge density and interface state density of Ta_2O_5/ZnO structures are found to be $2{\cdot}4 \times 10^{11}$ cm^{-2} and $1{\cdot}22 \times 10^{12}$ cm^{-2} eV^{-1}, respectively.

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