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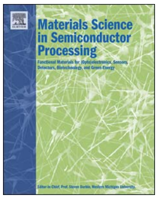

Influence of substrate bias voltage on crystallographic structure, optical and electronic properties of Al/$(Ta_2O_5)_{0.85}(TiO_2)_{0.15}$/p-Si MIS Schottky barrier diodes fabricated by dc magnetron sputtering

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ABSTRACT

Thin films of $(Ta_2O_5)_{0.85}(TiO_2)_{0.15}$ were prepared on p-Si and quartz substrates by reactive magnetron sputtering and the influence of substrate bias voltage (V_b) on their structural and electrical properties was studied. The crystal structure of the prepared films was elucidated by X-ray diffraction (XRD) studies. The structure of the as deposited films was found to be amorphous and the surface roughness of the films was found to be low. The crystallinity of the films was observed to be improved by increasing the substrate bias voltage. The XPS results revealed that the composition of the films were nearly stoichiometric with V_b at 0 V and −150 V. The optical properties of the films at various substrate bias voltages were also studied. The optical band gap of the films formed at various V_b values from 0 to −150 V decreased from 4.49 to 4.39 eV as revealed from the optical transmission spectra. The fabricated Al/$(Ta_2O_5)_{0.85}(TiO_2)_{0.15}$/p-Si metal-insulator-semiconductor (MIS) Schottky diodes leakage currents at −1.5 V decreased from 4.65×10^{-6} A (unbiased) to 3.73×10^{-8} A (V_b = −100 V). On the other hand, the sample biased at V_b= −150 V exhibited an increase in leakage current (2.99×10^{-4} A) when compared to all other prepared samples. Furthermore, the electrical parameters such as Schottky barrier height and ideality factor were calculated for the Al/$(Ta_2O_5)_{0.85}(TiO_2)_{0.15}$/p-Si MIS Schottky structure and systematically investigated as a function of substrate bias voltage using current-voltage (*I-V*) and capacitance-voltage (*C-V*) characteristics.

1. Introduction

Si has numerous industrial uses and is the prime constituent element in majority of semiconductor devices, most prominently integrated circuits, and microchips [1]. Over the last three decades, much attention has been given to the fabrication of metal contacts to Si semiconductors (Schottky barrier diodes). In addition, the steadfast performance and simple fabrication process of metal-semiconductor (MS) junctions on Si have allowed them to be used in a wide variety of applications such as microwave devices, field effect transistors (FETs), photodetectors, and solar cells [2], etc. However, the electrical characteristics of Schottky diodes are governed by interface conditions between metal and semiconductor. The first report on the influence of the interface layer on the electrical properties of Schottky diodes was explained by analyzing barrier heights as a function of the metal work function by Cowley and S.M. Sze [3]. For many decades, SiO_2 has been the principle dielectric material in the semiconductor electronic industry due to its excellent compatibility with silicon semiconductors. Though, the main drawback of SiO_2 is its high power consumption and large leakage currents [4], limiting its technological applications. For example, the improved performance of complementary metal-oxide-semiconductor (CMOS) transistors requires the substitution of the SiO_2 gate oxide with high k-materials. Thus, several interfacial insulator layers such as TiO_2 [5], Ta_2O_5 [6], HfO_2 [7], SnO_2 [8], Si_3N_4 [9] and bilayer CeO_2/TiO_2 [10] etc., have been used as an interfacial layer to replace the existing SiO_2 based gate dielectrics. Ta_2O_5 thin films find a wide variety of applications in areas such as optoelectronic devices as catalysts [11], electrochemistry, where they are used as proton conductors [12], microelectronics as gate insulators (as a high-k dielectric material) [13,14] and optics as a high refractive index low loss coating

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material [15]. In practical use, Ta_2O_5 films as gate dielectrics have shown large leakage currents and numerous methods have been proposed for reducing this drawback. TiO_2 is found to be thermodynamically unstable when in direct contact with silicon resulting in the formation of a titanium silicide and SiO_2 interfacial layer [10]. Cava et al. [16] attained higher dielectric constant values ranging from 35 to 126 by incorporating 8 mol% TiO_2 into bulk Ta_2O_5. TiO_2 doped Ta_2O_5 thin films can be produced using several techniques such as metal organic decomposition [17], sol-gel technique [18], remote plasma atomic layer deposition [19] and DC/RF sputtering [20,21]. The advantages of sputter deposition over other methods are a resulting composition close to that of the source material, efficiency in growth such as low losses, and the production of high quality coatings, which are typically compact, porous-free, and have better adhesion on the substrate. Recently, Raja et al. [22] developed Ag/n-WO_{3-x}/p-Si diodes and reported the influence of the oxygen content on the electrical properties and microstructure based on the thermionic emission mechanism with a laterally inhomogeneous Gaussian distribution prevailing at the WO_3/Ag interface. Very recently, Chong et al. [10] investigated the electrical and physical properties of Si/CeO_2/TiO_2 bilayer gate stacks and reported that a 600 °C annealed CeO_2/TiO_2 sample exhibited a dielectric constant of 18, compared to a value of 17.1 for a pure CeO_2 deposited sample. Furthermore, they reported that the produced rare earth oxides can be employed as a gate dielectric exhibiting an ideal k-value and considerable reduction in the leakage current.

In our earlier work [23], we have fabricated Al/$(Ta_2O_5)_{1-x}(TiO_2)_x$/p-Si metal-insulator-semiconductor (MIS) structures and reported the effects of compositional variation on the electrical and structural properties of $(Ta_2O_5)_{1-x}(TiO_2)_x$ films ranging from $x = 0$ to $x = 0.18$. In addition, we observed improved electrical parameters such as leakage currents, barrier height and capacitance for $(Ta_2O_5)_{1-x}(TiO_2)_x$ films at the composition $x = 0.15$. The present work describe the significance of substrate bias(V_b) on the electrical, optical, and structural properties of $(Ta_2O_5)_{1-x}(TiO_2)_x$ films at the composition $x = 0.15$ using optical transmittance/reflection, X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), atomic force microscopy (AFM), current-voltage (*I-V*), and capacitance-voltage (*C-V*) techniques.

2. Experimental

Thin films of $(Ta_2O_5)_{0.85}(TiO_2)_{0.15}$ were deposited on quartz (for investigating optical properties) and p-Si (100) (for investigating structural and electrical properties) substrates using reactive magnetron sputtering. A mosaic target was used to prepare the $(Ta_2O_5)_{0.85}(TiO_2)_{0.15}$ thin films, created by mounting small pieces of titanium (99.9% purity) on a 4″ diameter Tantalum (99.9% purity) metallic target. The numbers of titanium pieces were used to produce the required stoichiometric films by covering different areas on the tantalum target. The negative bias (V_b) voltage ranging from 0 to -150 V was applied to the silicon and quartz substrates and the target power was kept constant at 200 W.The total pressure in the deposition chamber was pumped down to 3×10^{-4} Pa by a combination of rotary and diffusion pumps, the oxygen partial pressure maintained in the chamber was 5×10^{-2} Pa and the sputtering pressure was maintained at 0.5 Pa. Initially, the Si substrates were cleaned in deionized water and ultrasonically degreased for 20 min. Further, to remove any native oxides on the silicon substrates, the Si wafers were dipped in 5% HF solution for 10 min and cleaned ultrasonically. Finally, they were ultrasonicated for 5 min in deionized water and dried with nitrogen gas. Prior to deposition, the substrate was pre-sputtered for 10 min to remove any surface contaminants such as silicon dioxide. Usually, for crystalline Ta_2O_5 thin films, a high substrate temperature or post-deposition annealing is required. By applying a suitable bias voltage to the substrate, the crystallinity is observed to be improved even at low temperatures. This might be beneficial to control the growth of the SiO_2 interfacial layer, which is useful for metal-oxide-semiconductor (MOS) devices with improved electrical properties.

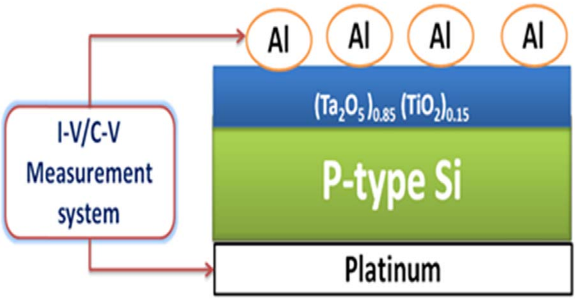

Fig. 1. The schematic diagram of the prepared Al/$(Ta_2O_5)_{0.85}(TiO_2)_{0.15}$/p-Si MIS Schottky barrier diodes.

The chemical and compositional analysis of Ta, Ti, and O were performed using a Phoibos model 100 MCD Energy X-ray photoelectron spectrometer. Crystal structure and phase purity were determined using a Seifert model 3003 TT X-ray diffractometer. The film thicknesses of all prepared samples were measured using an α-step profilometer through a sharp step produced by placing kepton plastic tape over a part of the silicon substrate prior to deposition. The measured film thickness ranged from 400 ± 10 nm to 380 ± 5 nm. Surface morphology was studied using a Digital Instrument model 3100 series atomic force microscope. Optical transmittance and reflectance properties of the films formed on quartz substrate were analyzed using a double beam spectrophotometer operated in the 200–2500 nm wavelength range. To perform *I-V* and *C-V* measurements, MOS Al/$(Ta_2O_5)_{0.85}(TiO_2)_{0.15}$/p-Si) capacitors were fabricated with a 7.8×10^{-3} cm^2 area of aluminum as the top electrode by photolithography. The schematic diagram of the prepared Al/$(Ta_2O_5)_{0.85}(TiO_2)_{0.15}$/p-Si MIS Schottky barrier diodes as shown in Fig. 1. As shown in the schematic diagram, Aluminum has been used as Schottky contact (front contact), whereas Platinum (back contact) used as Ohmic contact.

3. Results & discussion

3.1. Structural properties

The stoichiometry of deposited films were analyzed by XPS narrow scan spectra of the Ta 4f, Ti 2p and O 1s spectra of $(Ta_2O_5)_{0.85}(TiO_2)_{0.15}$ films for unbiased films was studied and reported in our earlier reports [23,24]. Fig. 2 shows the X-ray diffraction pattern obtained from the $(Ta_2O_5)_{0.85}(TiO_2)_{0.15}$ films as a function of substrate bias from 0 to −150 V. The deposited films at $V_b = 0$ V were found to be amorphous in nature. The amorphous films could be crystallized into the β - phase

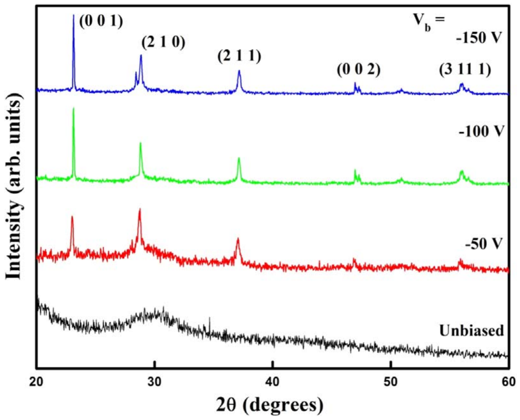

Fig. 2. X-ray diffraction profiles of $(Ta_2O_5)_{0.85}(TiO_2)_{0.15}$ thin films formed at substrate bias voltages ranging from 0 to −150 V.