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Surface chemical states, electrical and carrier transport properties of Au/ZrO_2/n-GaN MIS junction with a high-k ZrO_2 as an insulating layer

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ABSTRACT

High-k zirconium oxide (ZrO_2) thin insulating layer is deposited on n-type GaN and explored its chemical properties by XPS technique. XPS core level spectra confirms that the formation of ZrO_2 thin film on the n-GaN substrate. Later, the Au/ZrO_2/n-GaN MIS junction is constructed with a ZrO_2 as insulating layer and correlated its electrical properties with the Au/n-GaN MS junction. Results present that a high barrier height (0.94 eV) is obtained for the MIS junction compared with the MS junction (0.73 eV), suggesting the barrier height is altered by the ZrO_2 insulating layer. The estimated interface state density (N_{SS}) of the MIS junction is lower compared with the MS junction, revealing that the high-k ZrO_2 thin insulating layer decreased N_{SS}. Results confirmed that the reverse leakage current mechanism is governed by a Poole-Frenkel emission in both MS and MIS junctions.

1. Introduction

III-nitride semiconductor materials, specially gallium nitride (GaN), have attracted significantly in the fabrication of high power, high frequency and high temperature devices such as metal/oxide/semiconductor field effect transistors (MOSFETS) [1], heterojunction field effect transistors (HFET's) [2] and high electron mobility transistors (HEMT's) [3]. However, metal/semiconductor (MS) junctions in these devices may suffer from high leakage-current and low break-down voltage, which limits the device performance, reliability and stability. This could restrain by employing a thin insulator/interlayer between the metal and semiconductor. The formation of high-quality Schottky junctions with low-leakage current and low ideality factor by insertion of a thin insulator/interlayer in the middle of the metal and semiconductor is challenging task. Hence, the detailed investigations are prerequisite on the formation of a thin insulator/interlayer in the middle of the metal and semiconductor to achieve high barrier height with low ideality factor and good thermal stability. Therefore, it is stimulating to form a thin insulator/interlayer on n-type GaN and explored its characteristics are yet to be scientific challenge. Various research groups have reported on the formation of high-k dielectric materials on GaN as insulating layer between the metal and GaN substrate, and probed their characteristics [4–13]. For instance, Kuzumik et al. [13] reported that the leakage current of the Al/ZrO_2/n-GaN metal/oxide/semiconductor (MOS) was substantially reduced compared to the Au/Ni/n-GaN Schottky contact. Ye et al. [14] demonstrated that the reverse gate leakage current was four orders of magnitude lower for ZrO_2/AlGaN/GaN metal-insulator-semiconductor HEMTs compared to the Schottky barrier HEMTs. Ye et al. [15] investigated the band alignment between Ga-face GaN and ZrO_2 by using X-ray photoelectron spectroscopy measurements. Hatano et al. [16] showed the improved operation stability in AlGaN/GaN HEMTs with an Al_2O_3/ZrO_2 bilayer gate dielectric. Zheng et al. [17] fabricated the ZrO_2/n-GaN metal-oxidesemiconductor capacitors, reported that a low leakage current density was 3×10^{-9} A/cm^2 at 1 V.

Mainly, the present work is intended for preparation and characterization of the Au/ZrO_2/n-GaN metal/insulator/semiconductor (MIS) junction using pulsed laser deposition (PLD) of a thin zirconium oxide (ZrO_2) film as an insulating layer between the Au and n-type GaN substrate. Exploitation of GaN MIS with a thin dielectric film as insulator is one of the effective method to reduce the high leakage current with the enhancement of device performance. High-k dielectric materials can provide the comparatively large response at smaller electric fields. The high-k materials can also be employed for future gate dielectric to achievement of higher ultra large scale integration (ULSIs) with high efficiency and low power consumption. In this work, zirconium oxide (ZrO_2) is selected since it is an attractive candidate for new gate oxide layer due to its quite high-k dielectric contact (~25), large band gap (5.2–7.8 eV), large break down field (15–20 MV/cm), elevated melting point, small thermal conductivity at high temperature, good thermal stability, high mechanical strength, superior chemical strength and high corrosion resistance [18,19]. Moreover, ZrO_2

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provides a suitable value of band offset with GaN (valence band offset ≃1.6 eV, conduction band offset ≃1.1 eV [20]. Due to the excellent properties of ZrO_2, first we deposited ZrO_2 thin film on n-type GaN and characterized its chemical composition and surface morphology. Then, we fabricated the Au/ZrO_2/n-GaN metal/insulator/semiconductor (MIS) junction with the ZrO_2 as an insulating layer and investigated its electrical and reverse current transport properties. Also, the electrical and current transport properties of MIS junction are correlated with the conventional Au/n-GaN Schottky junction.

2. Experimental process

In this work, 2 µm thick Si-doped n-GaN wafers (carrier concentration about $\sim 4.07 \times 10^{17}\,cm^{-3}$) were developed by a metal organic chemical vapor deposition (MOCVD) on c-plane Al_2O_3 sapphire substrate were employed. The cleaning process of n-GaN wafer was followed as stated in the reference [13]. Using an e-beam evaporation system, Ti/Al (30 nm/100 nm thick) layers were deposited on a half part of the n-GaN substrate and annealed at 650 °C for 3 min using a rapid thermal annealed (RTA) system in nitrogen ambient to yield ohmic contact. Afterwards, the n-GaN substrate was dipped in a solution of HCL:DI [1:1] for 30 s, blown dry with N_2 gas. Subsequently, ZrO_2 films were formed on other half part of the n-GaN substrate after covering the ohmic contact by pulsed laser deposition (PLD) system (Quanta Systems SPA, Italy) at a pressure of 3×10^{-6} torr. The thickness of ZrO_2 film was estimated to be 40 nm by profilometer. At last, using a 0.7 mm diameter stainless steel mask, 20 nm thick Au Schottky junctions were formed on the ZrO_2 thin film by an e-beam evaporation system at a pressure of 5×10^{-6} mbar. In order to correlate the electrical properties of the Au/ZrO_2/n-GaN MIS junction, the Au/n-GaN metal/semiconductor (MS) junction was also prepared on the same GaN substrate as a reference junction. Surface chemical analysis of ZrO_2 films was investigated by X-ray photoemission spectroscopy (XPS). Energy-dispersive X-ray spectroscopy (EDAX) was also used to find the chemical composition of the ZrO_2 thin films on n-GaN substrate. Atomic force microscopy (AFM) was applied to characterize the surface morphology of ZrO_2 thin films. Finally, the electrical properties of the fabricated Au/ZrO_2/n-GaN MIS junction and Au/n-GaN Schottky junction (reference junction) were investigated by a Keithley source measurement unit (Model No: 2400) and automated deep level transient spectrometer (DLS-83D) in the dark, respectively.

3. Results and discussion

The X-ray photoemission spectroscopy (XPS) analysis was employed to confirm the surface elemental compositions and chemical states of deposited ZrO_2 thin films. Fig. 1(a) illustrates the XPS survey spectrum of the ZrO_2 films. The spectrum clearly reveals the predominant presence of Zr, O and C. The XPS spectrum of Zr 3d is shown in Fig. 1(b). As can be seen in Fig. 1(b), the binding energy of Zr $3d_{5/2}$ and Zr $3d_{3/2}$ double peaks is noted at 183.2 eV and 185.6 eV, respectively, indicates Zr $3d_{5/2}$ and Zr $3d_{3/2}$ peaks are correspond to Zr-O bond [21,22]. Also, the separation binding energy of Zr $3d_{5/2}$ and Zr $3d_{3/2}$ peaks is 2.4 eV, which suggests the Zr in Zr^{4+} states in ZrO_2 films [23]. The O 1s spectrum of ZrO_2 is shown in Fig. 1(c). The O 1*s* peak is noted at binding energy of 530.6 eV, indicating O 1*s* originates from ZrO_2. Moreover, the distribution of the elements at the ZrO_2/n-GaN interface, the XPS depth profile was applied. The XPS depth profile of deposited ZrO_2 film on n-type GaN is depicted in Fig. 1(d). The depth profile demonstrates the sharp interface, which indicates the Zr, O, Ga and N layers are well defined. But, a little quantity of Ga out-diffused into the ZrO_2 oxide layer, demonstrating Ga-O interfacial phases are created at the interface.

The energy-dispersive X-ray spectroscopy (EDAX) was employed to find the chemical composition of deposited ZrO_2 on n-type GaN. Fig. 2(a) depicts the EDAX spectrum of ZrO_2 on n-GaN and the corresponding percentage of the elements, respectively. The EDAX spectrum clearly exhibits the existence of Zr, O, Ga and N elements. The constituent elements percentage extracted from EDAX results as represented in the inset of Fig. 2(a). Further, the EDAX results confirm that no other foreign elements existence in the deposited ZrO_2 film. The XPS and EDAX analysis demonstrate that the ZrO_2 film is developed on n-type GaN. Fig. 2(b) illustrates the atomic force microscopy (AFM) images of the ZrO_2 film on n-GaN wafer. The AFM analysis reveals that the surface roughness of the ZrO_2 film is significantly smooth with a root mean square (rms) roughness of 1.264 nm, which indicates the formation of a uniform layer of ZrO_2 on n-GaN surface.

To examine the effect of high-k dielectric ZrO_2 thin film on the electronic parameters of Au/n-GaN MS Schottky junction, we fabricated the Au/ZrO_2/n-GaN MIS junction with ZrO_2 as an insulating layer in the middle of the Au metal and n-GaN semiconductor. The measured forward and reverse bias current-voltage (I-V) characteristics of MS and MIS junctions are depicted in Fig. 3. The inset of Fig. 3 illustrate the fabricated schematic structure of the Au/ZrO_2/n-GaN MIS junction. The MS and MIS junctions exhibit an excellent rectifying nature with the rectification ratio of 1.8×10^4 and 2.2×10^5, respectively. The measured reverse leakage currents are 2.301×10^{-8} A and 5.566×10^{-11} A at -1 V for the MS and MIS junctions, respectively. Measurements confirm a significant reduction in the reverse leakage current by about three orders of magnitude for the MIS junction as compared with that of the conventional MS junction. This suggests the electrical properties of MIS junction are improved after a insertion of high-k dielectric ZrO_2 thin insulating layer between Au and n-GaN layers. Assuming the thermionic emission (TE) theory [24], the barrier height (BH) and ideality factor of Au/n-GaN MS and Au/ZrO_2/n-GaN MIS are extracted from I -V characteristics. Using the slope and intercept of the lnI-V plot, the ideality factor and BHs are obtained for the MS and MIS junctions. In the present work, twenty Au/n-GaN MS and Au/ZrO_2/n-GaN MIS junctions are prepared identically on the same GaN substrate. The extracted BH and ideality factor values varied from 0.67 eV to 0.76 eV and 1.2 to 1.6 for the MS, and 0.91 eV to 0.95 eV and 1.5 to 2.3 for the MIS junctions, respectively.

Further, the results reveal that the ideality factor and BHs are varied from junction to junction although they are prepared in the same manner. Investigations demonstrate that potential barriers at the metal/semiconductor interfaces sturdily depend on the applied voltage apart from the image force effect for ideal contacts. Thus, it is indispensable to attain the average values [25,26] of barrier heights and ideality factors of the MS and MIS junctions by way of statistical distribution analysis. Fig. 4(a) and (b) demonstrate the statistical distribution of the BHs and ideality factors for the twenty fabricated Au/n-GaN MS and Au/ ZrO_2/n-GaN MIS junctions extracted from the I-V data. The extracted BHs and ideality factors experimentally are fitted by the Gaussian function. According to Fig. 4(a) the statistical results gives an average BH value of 0.73 eV with a standard departure of 0.00563 eV, and an average ideality factor of 1.38 with a standard departure of 0.016 for the MS junction. Moreover, from Fig. 4(b), the statistical analysis of data provides an average barrier height value of 0.94 eV with a standard departure of 0.0016 eV and an average ideality factor of 2.13 with a standard departure of 0.033 for the MIS junction. Results showed that the difference between the average barrier height of Au/n-GaN MS and Au/ZrO_2/n-GaN MIS junctions is 0.21 eV, which is due to the occurrence of ZrO_2 insulating layer at the Au/n-GaN interface. The standard departure of the BH of Au/ZrO_2/n-GaN MIS junction is more than the Au/n-GaN MS junction. This may be associated with the excess of divergence in thickness of the ZrO_2 layer developed on the n-GaN substrate. Further, the extracted average barrier height of MIS junction is larger than MS junction. This may be due to rise in negative charge at the junction, which occurs because of electron traps localized at the GaN interface which are associated to Ga vacancies formed near to the surface during the creation of the insulating layer [9,12,13,27,28]. Evaluation results indicate that the ideality factor values are larger than one for both MS and MIS junctions. This may be because of the image force lowering, interface states at the interface and barrier inhomogeneities. Another reason, the insulating layer may be formed non-uniform at the metal and semiconductor interface. Higher ideality factors may also be due to the occurrence of surplus current and recombination current via interface states between the interlayer and semiconductor [29,30].