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PhD Student / Regular Participant:	Regular Participant

Experimental band alignment of Ta_2O_5/GaN for MIS-HEMT applications

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1. Introduction

GaN Metal Insulator Semiconductor High Electron Mobility Transistors (MIS-HEMTs) have been used extensively for high frequency, high power and low noise applications [1,2]. A layer of GaOx can be formed on the GaN surface by reaction with oxygen even at room temperature. Surface-related defect states associated with the GaOx layer result in large leakage current and severe current collapse at high frequency, inhibiting device performance. Recently, the insertion of a dielectric layer for surface passivation has been reported to mitigate the issues above [1,3,4]. Ta_2O_5 shows good interface qualities with GaN and also has a high dielectric constant (~25) [5], leading to improved transconductance (g_m). An increase of the 2DEG carrier concentration of AlGaN/GaN structures passivated with a thin Ta_2O_5 film (2–4 nm) has been reported [3]. Larger g_m has been reported for devices incorporating Ta_2O_5 compared to HfO_2 passivated HEMTs, with comparable gate leakage currents [4]. This paper provides experimental evidence of band alignment between Ta_2O_5/GaN using the techniques X-ray Photoelectron Spectroscopy (XPS) and Variable Angle Spectroscopic Ellipsometry (VASE). Note that only theoretical values of the valence (VBO~1.1 eV) and conduction band offsets (CBO~0.1 eV) derived using the method of charge neutrality levels have been reported previously for this system [6].

2. Sample preparation and cleaning procedure

The Ta_2O_5 films of nominal 3 nm and 10 nm thickness were deposited by RF magnetron sputtering at 5 mT. Prior to the deposition of Ta_2O_5, surface cleaning was carried out to minimize C and O contaminants on the GaN with ultrasonic rinses in acetone for 10 minutes followed by methanol for a further 10 minutes. [7]. Then the sample was dipped in 3 different etchants separately: 30% NH_4OH, 20% $(NH_4)_2S$, and 37% HCl solution followed by a rinse in deionized water. As can be seen from Fig. 1a, the HCl treatment gave the lowest O 1s intensity, and was used to pretreat the GaN surface prior to Ta_2O_5 deposition. There is an indication of Cl on the surface (Fig. 1b), possibly in the form of gallium chloride likely due to a Ga-rich surface [8].

3. Results and discussion

The VASE fitting for the wavelength region (240-1700 nm) was done using a parametric model [9]; the fitting of experimental ellipsometric Ψ and Δ angles for the GaN substrate is shown in Fig. 2. The Ta_2O_5 film properties were fitted using the Tauc-Lorentz model, with resulting thicknesses of 2.8 and 10.6 (±0.1) nm for the interfacial and bulk Ta_2O_5 samples. The resulting dielectric function spectra, ε_1 and ε_2, for GaN and Ta_2O_5, are shown in Figs. 3a and 3b respectively. The band gap obtained from ε_2 spectra using linear extrapolation of the leading edge to the baseline is 3.34±0.1 eV for GaN (Fig. 3a) and 4.40±0.15 eV (Fig. 3b) for Ta_2O_5. The obtained values are in close agreement with literature [10-11]. The valence band offset was calculated using Kraut's method [12]:

$$VBO = \delta_{SUB} - \delta_{OXIDE} + \delta_{INT} \qquad (1)$$

where δ_{SUB} refers to the binding energy difference of Ga 3d XPS core level (CL) and valence band maximum (VBM) for GaN substrate (Fig. 4a), δ_{OXIDE} of Ta 4f CL and VBM for Ta_2O_5 bulk sample (Fig. 4b), and δ_{INT} of Ga 3d and Ta 4f CLs for interfacial Ta_2O_5 sample (Fig. 4c). The value of VBO from the data in Fig. 4 is 0.71 ± 0.2 eV, which with the band gap extracted by VASE gives CBO = 0.35 ± 0.2 eV, illustrated schematically in Fig. 5.

4. Conclusion

This paper experimentally demonstrates the band alignment of Ta_2O_5 prepared by RF sputtering on ex-situ HCl treated GaN surface. The HCl treatment is compared to NH_4OH and $(NH_4)_2S$ and shows the lowest contaminants on the GaN surface. The VBO of Ta_2O_5/GaN is found to be 0.71 ± 0.2 eV from the XPS and Kraut's method, while CBO is derived using the band gaps of GaN (3.34 eV) and Ta_2O_5 (4.4 eV) and found to be 0.35 ± 0.2 eV. The results have importance for developing future GaN based MIS-HEMTs.

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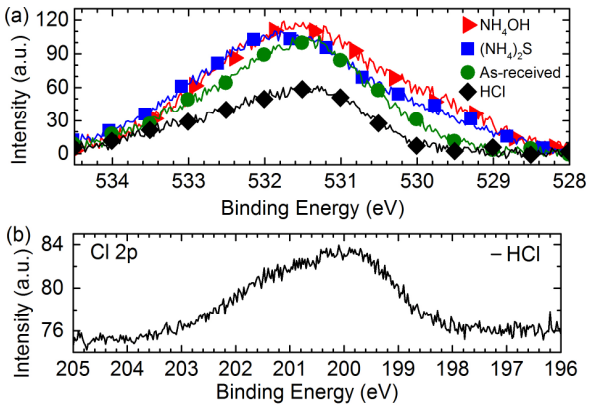

Fig.1: (a) Background subtracted O 1s CL XPS peaks from different cleaning treatments. The HCl treatment shows the lowest intensity. (b) Cl 2p CL XPS spectrum of the GaN surface cleaned by HCl treatment.

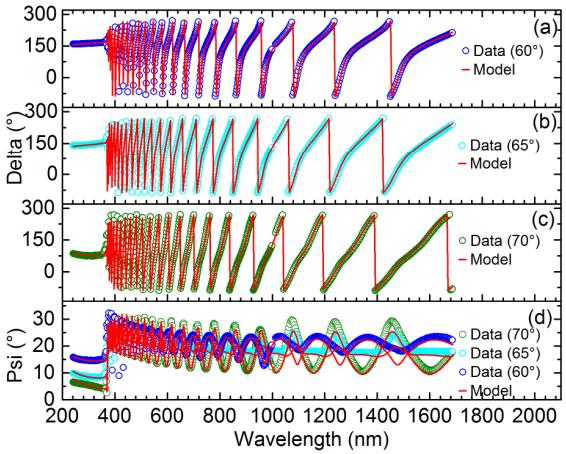

Fig.2: VASE data for the GaN sample (circle) and the best multiple-layer model (red line) in the wavelength range of 240–1700 nm; Δ fit at: (a) 60˚, (b) 65˚, (c) 70˚, (d) Ψ fit at the three SE angles (60-75˚).

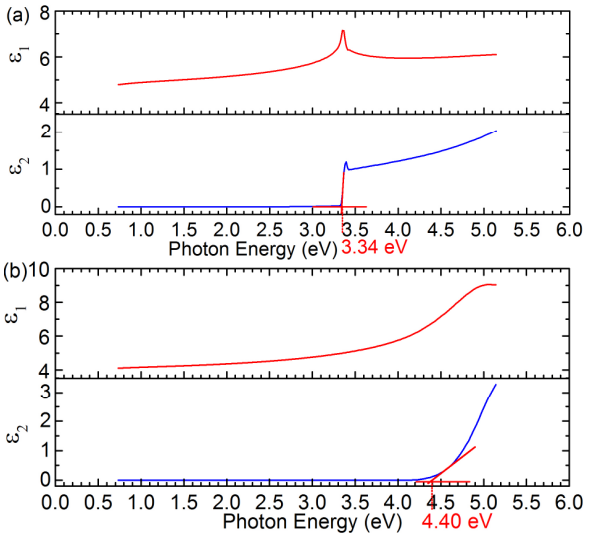

Fig.3: Photon energy dependence of parametric dielectric function, ε_1 and ε_2, for (a) as-received GaN substrate and (b) 10 nm (nominal) RF magnetron sputtered Ta_2O_5.

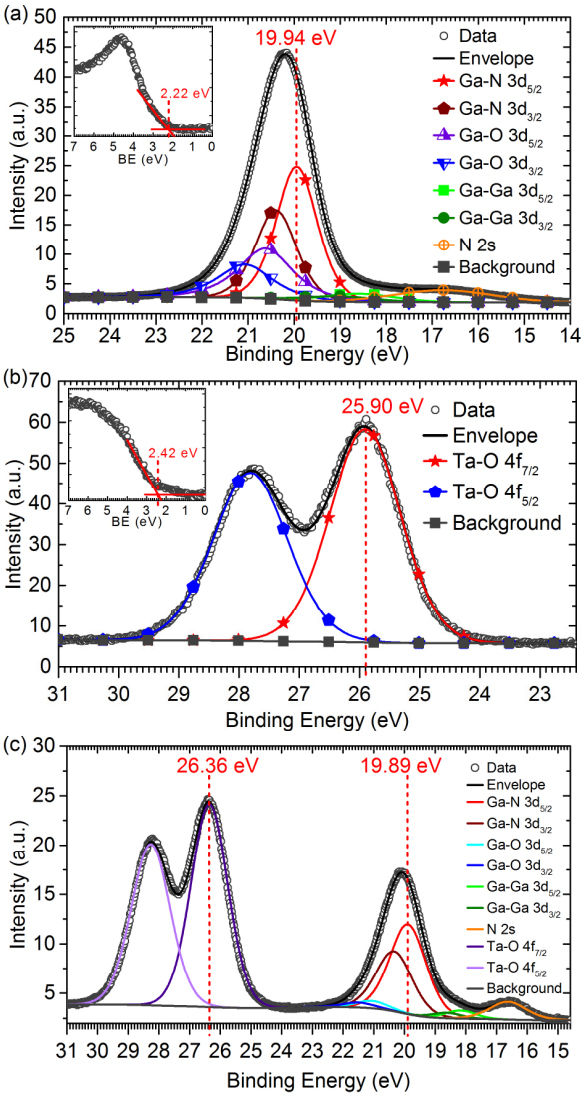

Fig.4: The XPS spectra of: (a) Ga 3d CL for GaN substrate. The spectrum is fitted by 7 components. (b) Ta 4f CL for bulk Ta_2O_5 sample. The insets in (a)-(b) show the VBM estimation from valence band leading edge linear fitting. (c) The XPS spectrum of Ga 3d and Ta 4f CLs for interfacial Ta_2O_5/GaN sample showing the difference between the CLs.

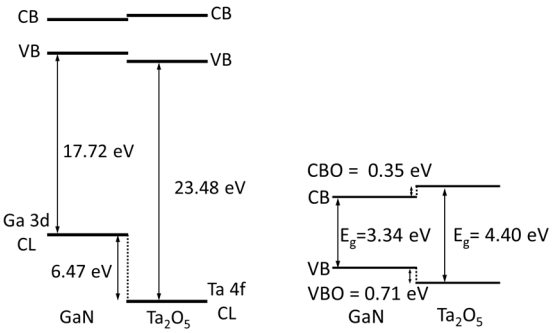

Fig.5: Band diagrams of experimentally derived band alignment for the Ta_2O_5/GaN interface; (left) Kraut's method for VBO measurement, and (right) CBO derived using band gap energies by VASE.