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Determination of band offset in InP/YSZ hetero-junction by X-ray photoelectron spectroscopy

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ABSTRACT

Y-stabilized ZrO_2 (YSZ) was one of the familiar high dielectric constant films used in InP field effect transistors. However, the structure and optical properties of YSZ film deposited on InP substrate were rarely reported. The band offsets in InP/YSZ hetero-junction was an important parameter, which had not been measured. In the work, YSZ films were deposited on InP substrates by sputtering. The optical properties and structures of YSZ films and InP/YSZ interface were characterized. X-ray photoelectron spectroscopy was used to measure the energy discontinuity in the valence band of the InP/YSZ hetero-structure. A value of 1.4 eV was obtained with In 3d5 as the reference energy level. With the band gap of 5.8 eV for YSZ and 1.3 eV for InP, this indicated a conduction band offset of 3.1 eV in the system.

1. Introduction

As Si-based field effect transistors continue to scale down, novel channel materials in combination with high dielectric constant (K) films have been extensively explored in recent years [1]. One of the approaches is to employ the high-mobility III-V materials as channel layers [2]. InP is a good candidate material with respect to Fermi-level pinning and a higher electron saturation velocity to meet the demands for high performance and less power dissipation integrated circuits [3].

To determine the magnitude of improvement in device performance, the knowledge of accurate band offsets between InP and gate oxide is required, as sufficiently high energy barrier at the oxide interface is of critical importance [4]. The band offsets of various high K gate oxides on various III-V semiconductors have been calculated [5]. However, the factors that determine the conduction and valence band offsets for a given material system are not well understood. Predictions based on various models have historically been unreliable and band offset values should be determined experimentally [6]. The band offsets of Al_2O_3/NbAlO/Al_2O_3 [7], La_2O_3 [8], Al_2O_3 [9], HfO_2 [10], MgO [11] gate oxides between InP have been experimentally measured with the X-ray photoelectron spectroscopy (XPS) or internal photoemission methods.

ZrO_2 is one of the high K oxides commonly used in InP field effect transistors [12–14]. In there, plasma-enhanced atomic layer deposition [12], pulsed laser deposition [13] and atomic layer deposition [14] techniques were used for preparing ZrO_2 thin films. Sputtering is also a commonly used deposition technique for ZrO_2 dielectric film [15]. Sputtering deposited HfO_2 dielectric films were used in InP devices [16,17]. However, to our knowledge, the performance of ZrO_2 film deposited on InP substrate by sputtering has not been reported, and the band offsets of InP/ZrO_2 hetero-junction have not been measured.

In the paper, the optical properties, microstructures and interfacial structures of sputter deposited Y-stabilized ZrO_2 (YSZ) film on InP substrates are characterized, and the band offsets in InP/YSZ hetero-junction are measured by XPS.

2. Experimental

The single side polished intrinsic n-type InP wafers of (100) crystalline orientations with a carrier concentration of ~5×10^{15} cm^{-3} were used. The native oxide on InP were removed with 1% diluted HF solution, followed by 20% $(NH_4)_2S$ pretreatment. The YSZ films were deposited by RF sputtering using 8% Y stabilized ZrO_2 target at room temperature with the power of 120 W and a

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working pressure of 0.3 Pa in Ar ambient at base pressure of 9.0×10^{-4} Pa. A spectroscan ellipsometer was used to characterize the optical properties and film thickness of films. The microstructure, surface morphology, and interfacial structures of films were studied by a X-ray diffraction (XRD) meter, a Scanning electron microscope (SEM), and Scanning transmission electron microscopy (STEM) with Energy dispersive x-ray spectroscopy (EDS), and Transmission electron microscopy (TEM). For EDS test, the 300 kV probe had a third-order spherical aberration coefficient $C_s = 1.2$ mm. The probe forming aperture semi-angle was 9.6 mrad and the probe was under focused by 560 Å into the specimen. The probe size was estimated at 1.4 Å and the beam current was 10–20 pA. The EDS detector subtended a collection angle of 0.13 sr. The acquisition time for a single x-ray spectrum was 500 ms (corrected for dead time). The BW 3067 RoHS standard material was used for correcting the EDX data. During correcting, the standard material was tested by EDX for 10 times. Each time when the test data was within the 30% range of standard data, the teat was OK. The test error was about 3%.

To measure the band offsets of InP/YSZ hetero-junction, the samples of a blank InP substrate, a 500 nm-thick YSZ film grown on InP, and a 8 nm-thick YSZ film grown on InP (InP/YSZ hetero-junction)were characterized by a Thermo ESCALAB 250 X-ray photoelectron spectrometer with a mono-chromate Al Kα (energy 1486.6 eV) X-ray source. The X-ray spot size was 500 μm. The measurement was taking at chamber pressure of 10 mbar. The XPS spectra were collected in the condition with pass energy of 20 eV and a 0.05 eV/step for high-resolution scans. The low-energy electron flood gun (−3 V, 200 μA) was applied to compensate for charging effects due to the poor conductivity of samples. The spectra in this paper were calibrated using the absorbed C1s peak at 284.8 eV. This experiment didn't use sputtering ion beam. The spectra were fitted by using Avantage software. A Smart mode was used to calculate the background and the spectra were fitted with Gaussian-Lorenzian curve, whose shape of all peaks was assumed to be 80% Gaussian and 20% Lorentzian. A core-level (CL) photoemission-based method [18] was used to determine the valence band offset. Charge neutralization was performed with an

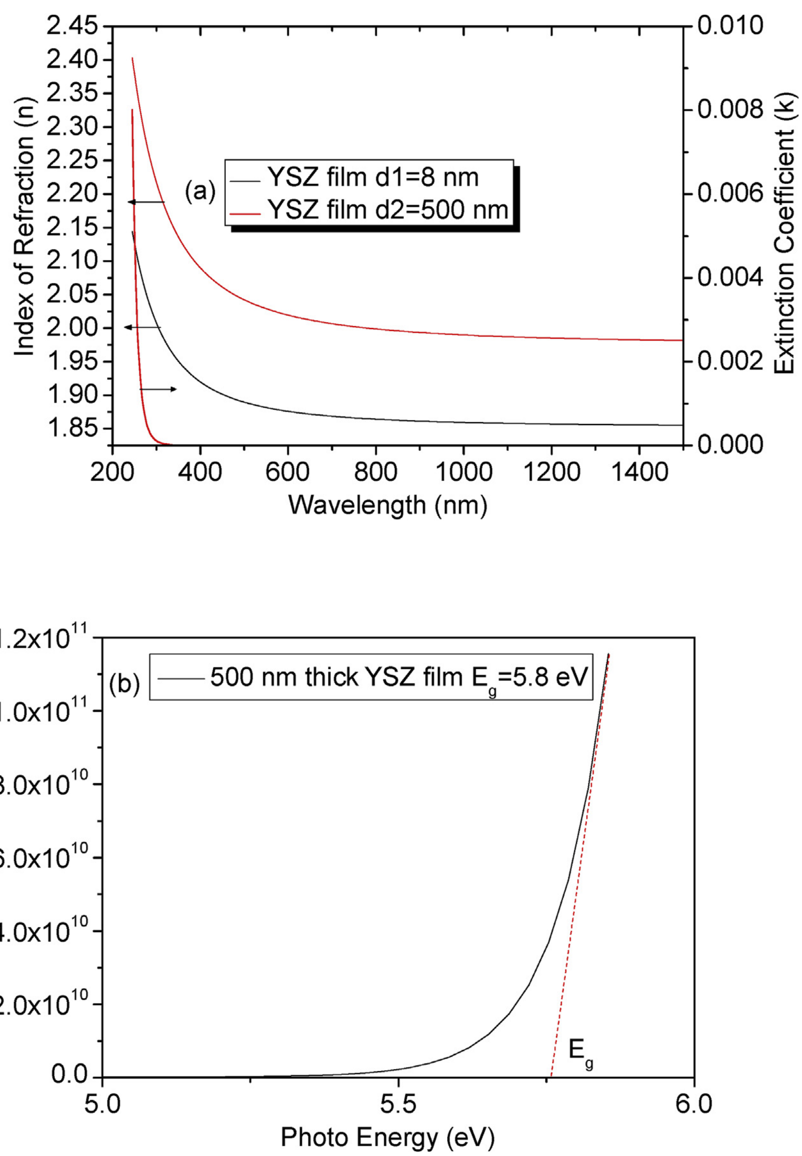

Fig. 1. (a) n, k, d and (b) E_g for YSZ films.