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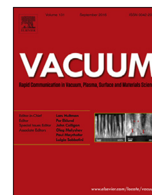

# Determination of band offset in MgO/InP heterostructure by X-ray photoelectron spectroscopy

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A B S T R A C T

X-ray photoelectron spectroscopy was used to measure the valence-band offset ($\Delta E_V$) of MgO/InP heterostructure. Two sets of core level pairs in the MgO/InP system were used to demonstrate the accuracy of the calculation, the $\Delta E_V$ value was the same (5.33 ± 0.15 eV) when using the In $3d_{3/2}$, Mg 2p pair and In $3d_{5/2}$, Mg 2p pair, indicating our calculations are accuracy and reasonable. Taking the band gaps of 7.83 eV for MgO and 1.34 eV for InP into consideration, a type-I band alignment of MgO/InP heterostructure was obtained with conduction band offset (CBO) of 1.16 ± 0.15 eV for two sets of core level pairs, indicating a nested interface band alignment heterostructure was prepared. The accurate determination of the band alignment of MgO/InP has a significant impact on the performance of InP-based devices.

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## 1. Introduction

With the continued scaling of the gate dielectric in transistors, silicon dioxide is reaching its fundamental limit to satisfy device performance, so thinner layers with low leakage current are needed. Therefore, it is necessary to investigate other materials to replace silicon dioxide in the future for device applications and a large research efforts had been devoted [1]. Researchers had investigate materials as the dielectric layer to passivate the transistors structure such as $SiN_X$ [2,3], $Sc_2O_3$ [4,5], or MgO [6,7]. In particular, MgO with a wide bandgap (7.83 eV) is a candidate for the buffer layer in transistors to inhibit chemical reactions and mitigate tunneling current, and it has the potential to ensure band offsets of sufficient magnitude to minimize leakage currents. The dielectric properties of MgO layers, which deposited on GaAs [8,9], GaN [10], InN [11], and ZnO [12–14], have also been reported. Yan et al. [15] have reported MgO is better than other oxides due to its high secondary electron emission coefficient and it can be further enhanced by adding low concentrations of other compounds. These findings indicate that MgO is a promising gate dielectric and this property can be used to passivate the surface of III-V group semiconductors such as transistors and other devices. Therefore the band offset at MgO/III-V heterojunction interface is a very important parameter for developing III-V group transistor devices. Like other III-V group semiconductors, InP attracts considerable attention as possible high-mobility channel material for next generation transistor devices. Meanwhile $Al_2O_3$ deposited on InP by atomic-layer-deposition (ALD) have been demonstrated [16]. However, $Al_2O_3$/InP devices suffer from the threshold voltage instability caused by charge injection and trapping in the insulator [17], the MgO film grow on InP substrate don't suffer this problem. Kim et al. have prepared MgO thin films on InP substrates by using electron-beam-deposition [18]. The I–V and C–V results showed that the dielectric constant of the MgO thin films was very low (9.67) and the MgO/InP heterointerface has no significant interdiffusion problem. These results indicating MgO/InP heterostructure hold promise for potential electronic devices based on InP substrates. However, there is lacking of systematically study for the interface band alignment parameters of MgO/InP heterostructure. In

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addition, accurate determination and reliable knowledge of band alignment is needed for proper engineering of InP-based transistor devices. Therefore, determining the band offset of MgO/InP heterojunction is very important.

In present, X-ray photoelectron spectroscopy (XPS) has been proven to be a powerful tool for direct and precise measurement of the band offsets at heterojunction interfaces [19]. However, the sample is always positively charged and the electric field caused by the charge can affect the measured kinetic energy of the photoelectron because a large number of electrons are excited and emitted from the sample during the XPS measurement. Researchers had pointed out that due to the charging effect, it is not straightforward to determine VBO in dielectric/semiconductor heterojunction when the XPS method is used. Fortunately, the C 1s peak position was found also changed [20]. So the core levels and VBM for the samples were calibrated by the respective C 1s peak (284.6 eV) from contamination to compensate the charge effect.

In this paper, MgO/InP heterojunction have been successfully prepared by atomic-layer-deposition (ALD). By using XPS, we determine the band offset at the MgO/InP interface. Our results suggest the MgO/InP heterojunction particularly promising for application in transistor devices.

## 2. Material and methods

### 2.1. Materials

Three samples were used in our XPS measurements, namely, a InP comparative sample, 5-nm-thick and 100-nm-thick MgO layer deposited on the InP substrate directly, respectively.

### 2.2. Preparation

The MgO films were grown by a LabNano TM 9100 atomic-layer-deposition system. In the deposition processes, $H_2O$ and $Mg(C_5H_5)_2$ were used as precursors. Water and $Mg(C_5H_5)_2$ were introduced into the growth chamber separately, the growth temperature was 250 °C. The detail growth process of MgO film by ALD is described in Ref. [21].

### 2.3. Characterization

XPS was used to determine the band offset at the MgO/InP interface. In this XPS measurements, the experiments were performed on a PHI Quantera SXM instrument with the Al $K\alpha$ ($h\nu = 1468.60$ eV) as the X-ray radiation source. The sample, which used for XPS experiment, was seting in an ultra-high vacuum system operating at $10^{-8}$-$10^{-11}$ Torr, and the XPS data acquired.

## 3. Calculations

The VBO ($\Delta E_V$) of MgO/InP heterostructure can be calculated from the Kraut's equation [22,23]:

$$\Delta E_V = \Delta E_{CL} + \left(E^{InP}_{In3d} - E^{InP}_{VBM}\right) - \left(E^{MgO}_{Mg2p} - E^{MgO}_{VBM}\right) \text{ QUOTE} \quad (1)$$

where$\Delta E_{CL} = E^{\frac{MgO}{InP}}_{Mg2p} - E^{\frac{MgO}{InP}}_{In3d}$ is the energy difference between Mg 2p and In 3d core levels (CLs) measured in MgO/InP interface, $E^{InP}_{In3d} - E^{InP}_{VBM}$ and $E^{MgO}_{Mg2p} - E^{MgO}_{VBM}$ are the differences between valence band maximum and In 3d core level in InP and Mg 2p core level in MgO, respectively.

Conduction band offset (CBO) was calculated by using the following equation:

$$\Delta E_C = E^{MgO}_g - E^{InP}_g - \Delta E_V \quad (2)$$

where $E^{MgO}_g$ and $E^{InP}_g$ are the energy band gap of MgO and InP, respectively.

## 4. Results and discussion

The C core level spectra for the InP sample is shown in Fig. 1. The C 1s core level spectra contain only one peak which located in 284.59 eV. Compared with the value of 284.60 eV, it has a peak offset about 0.01 eV and this value should be added when calculating the core level for InP sample. MgO sample and MgO/InP heterostructure also calibrated by the C 1s peak at 284.6 eV like this.

In order to obtain reliable results from the heterojunction, the strain must be considered, for it may affect the results of experiment. This strain has the potential to induce a large piezoelectric field [24]. Since the InP substrate is thick enough and the strain is completely relaxed, so it is unnecessary to consider the strain for InP sample. The critical thickness ($t_c$) of the MgO film deposited on InP substrate determined by the following empirical formula [24]:

$$t_c = a_e^2 \Big/ 2|a_e - a_s| \quad (3)$$

where $a_e$, $a_s$ denote the crystal lattice constants of MgO and InP.

The lattice constant of MgO is 0.42 nm, and InP is 0.59 nm. Using these values, $t_c$ is calculated as 0.53 nm, which is far below the thickness of the MgO films, therefore, 5-nm-thick and 100-nm-thick MgO films are thick enough to consider strain-relaxed. Although 5-nm-thick MgO film is thick enough to eliminate the effect of strain, the X-ray can pass through 6.48 nm in the XPS experiment, so 5-nm-thick MgO film is thin enough to detect the core levels of InP in MgO/InP heterostructure. To confirm the In signal in MgO/InP heterostructure can be detected, the core level survey spectra of InP, 100-nm-thick MgO on InP and MgO/InP heterostructure were tested, as shown in Fig. 2. We can easily find In 3d covel level in MgO/InP sample, indicating the X-ray can pass through 5-nm-thick MgO film and reach the InP substrate. Therefore, 5-nm-thick MgO film on InP substrate can be used for the band offset of MgO/InP heterostructure.

The XPS spectra of CL and VB region for InP, MgO and MgO/InP samples are shown in Fig. 3. The software of XPSPEAK 4.1 was used to fit all the XPS spectra. The spin-orbit doublet with a splitting energy of 7.75 eV of In 3d spectrum in the InP sample is shown in

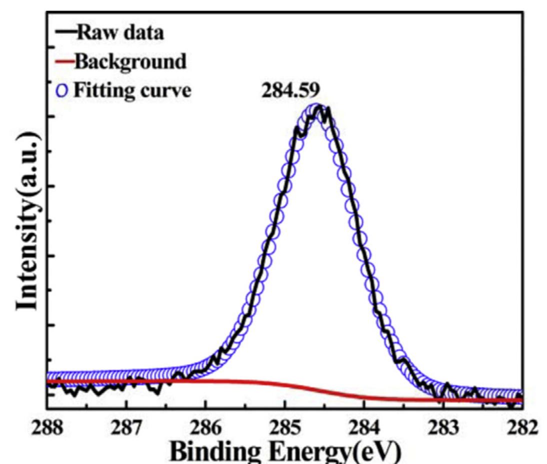


**Fig. 1.** Optimized peak fit of C 1s spectra for the InP sample.

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