Determination of MgO/AlN heterojunction band offsets by x-ray photoelectron spectroscopy


Key Laboratory of Semiconductor Materials Science, Institute of Semiconductors, Chinese Academy of Sciences, P.O. Box 912, Beijing 100083, People’s Republic of China

(Received 9 December 2008; accepted 6 January 2009; published online 2 February 2009)

MgO is a promising gate dielectric and surface passivation film for GaN/AlGaN transistors, but little is known of the band offsets in the MgO/AlN system. X-ray photoelectron spectroscopy was used to measure the energy discontinuity in the valence band ($\Delta E_{\text{v}}$) of MgO/AlN heterostructures. A value of $\Delta E_{\text{v}}=0.22 \pm 0.08$ eV was obtained. Given the experimental band gap of 7.83 eV for MgO, a type-I heterojunction with a conduction band offset of $\sim 1.45$ eV is found. The accurate determination of the valence and conduction band offsets is important for use of III-N alloys based electronic devices. © 2009 American Institute of Physics. [DOI: 10.1063/1.3075060]

Wide-band gap semiconductors are very promising for their potential use in high temperature and high power electronics due to their low thermal carrier generation and high breakdown fields. The fundamental band gaps of the AlGaN material system span from $\sim 3.4$ to $\sim 6.2$ eV.1 This introduces the possibility for III-N alloys and heterostructures to be used in a wide variety of optoelectronic devices. AlGaN/GaN high electron mobility transistors (HEMTs) attracted considerable research interest.2–3 However, one of the continuing issues with microwave power AlGaN/GaN HEMTs is surface and bulk carrier trapping phenomena causing the continuing issues with microwave power AlGaN/GaN HEMTs.1 In particular, MgO is a 650-nm-thick AlN layer grown on Si (111), and 5 nm MgO/650 nm AlN grown on Si (111). All films in this study were grown by low-pressure metal-organic chemical vapor deposition. The growth conditions of the MgO and AlN films were the same as that in our previous study.14 The crystal structure of MgO is rocksalt, which is a fcc structure and grew epitaxial along the c-axis. The crystal structure of MgO is rocksalt, which is a fcc array of oxygen atoms with an interpenetrating fcc array of magnesium atoms. The (111) MgO film grown on Si (111) has a smooth surface with a root-mean-square roughness of 1.33 nm over a 1 $\mu$m$^2$ using a SH SPI-3800 atomic force microscope.

The XPS measurements were performed on a PHI Quantera SXM instrument with Al Kα (energy of 1486.6 eV) as the x-ray radiation source, which had been carefully calibrated utilizing work function and Fermi energy level ($E_F$). During the testing, because a large number of electrons are excited and emitted from the sample, the sample is always positively charged and the electric field caused by the charge can affect the measured kinetic energy of the photoelectron. Charge neutralization was performed with an electron flood gun and all XPS spectra were calibrated by the C 1s peak at 284.8 eV from contamination to compensate the charge effect. The surfaces of the specimens were examined initially by low-resolution survey scans to determine which elements were present. Very-high-resolution spectra were acquired to determine the binding energy (i.e., chemical state) in the survey spectra. Since only the relative energy position in each sample is needed to determine the VBO, the absolute energy calibration for a sample has no effect on the universal energy reference.

The VBO ($\Delta E_{\text{v}}$) can be calculated from the formula

$$\Delta E_{\text{v}} = \Delta E_{\text{CL}} + (E_{\text{Al}}^{\text{AIN}} - E_{\text{Mg}}^{\text{AIN}}) - (E_{\text{Mg}}^{\text{MgO}} - E_{\text{Mg}}^{\text{MgO}}),$$

where $\Delta E_{\text{CL}}=(E_{\text{Mg}}^{\text{MgO}} - E_{\text{Al}}^{\text{AlN}})$ is the energy difference between Mg 2p and Al 2p core levels (CLs), which are measured in the heterojunction sample, and $(E_{\text{Cl}}^{\text{AIN}} - E_{\text{Mg}}^{\text{AIN}})$ and $(E_{\text{Mg}}^{\text{MgO}} - E_{\text{Mg}}^{\text{MgO}})$ are the AlN and MgO bulk constants, which are obtained by XPS measurement on the respective thick films. Mg 2p and Al 2p XPS spectra are shown in Figs. 1(a)–1(d) fitted using Shirley backgrounds and Voigt (mixed Lorentzian–Gaussian) functions, the parameters for which are shown in Table I. Since considerable accordance of the fitted line to the original measured data has been obtained, the uncertainty of the CL position should be lower than 0.03 eV, as evaluated by numerous fittings with different parameters. The Mg 2p spectrum of both the MgO and the MgO/
AlN samples were fitted by a single contribution, attributed to the bonding configurations Mg–O. However, for the Al 2p spectrum of both the AlN and the MgO/AlN samples [Figs. 1(b) and 1(d)], an additional low-intensity higher-binding-energy component was also required. In Fig. 1(b) this extra component is attributed to Al–O bonding due to oxide contamination when AlN is present at the surface, and in Fig. 1(d), it is attributed to Al–O bonding at the MgO/AlN interface.

The VB XPS spectra for the thicker MgO and AlN samples are shown in Figs. 1(e) and 1(f). The VBM positions in the VB spectra were determined by linear extrapolation of the leading edges of VB spectra to the base lines in order to account for the finite instrument resolution. The parameters deduced from Fig. 1 are summarized in Table I for clarity. The VB spectra recorded on the MgO sample in Fig. 1(d) gives a VBM of 3.23 eV by the same method as AlN. The scatter of the data relative to the fit are estimated as an uncertainty in VBM positions of less than 0.08 eV, as also estimated from fitting with different parameters. The VBO value is calculated to be $0.22 \pm 0.08$ eV by substituting those values obtained in experiments into Eq. (1). As XPS measurements are spatially averaged due to the finite mean free path of elastic electrons (1.5–2 nm), band bending could induce a systematic error in our measurements. We estimate that this error is much smaller than the average standard deviation of 0.08 eV given above. Another factor that may affect the precision of the VBO value is the strain-induced piezoelectric field in the overlayer of the heterojunction, as described in the III-nitrides system. The (111)//(0001) is the lowest energy configuration for the interface of the two materials and the expected growth plane for the MgO, which produces the lattice mismatch between the MgO (111) and the AlN (0001) of $-4.2\%$. This value is comparable to the lattice mismatch between MgO/GaN interface, in which the strain-induced piezoelectric field is not considered. It has been previously noted that $\Delta E_v$ has transitive property. It means for heterojunctions formed between three semiconductors (A, B, and C), if $\Delta E_v$ (A-B) and $\Delta E_v$ (B-C) are known, $\Delta E_v$ (A-C) is also specified. From the reported experiment data, $\Delta E_v$ (InN–GaN) is $0.58 \pm 0.08$ eV, $\Delta E_v$ (InN–AlN) is $1.52 \pm 0.17$ eV, $\Delta E_v$ (MgO–GaN) is $1.06 \pm 0.15$ or $1.2 \pm 0.2$ eV, and we can deduce $\Delta E_v$ (MgO–AlN) is $0.26$ or $0.12$ eV, which is comparable to our calculated result within the experiment error, and thus, further confirm the reliability of the experimentally obtained VBO value. Lastly, using the room temperature band gaps for MgO and AlN [7.83 (Ref. 13) and 6.16 eV, respectively], the MgO/AlN heterojunction is found to have a type-I (staggered) band line-up, as shown in Fig. 2, with a corresponding conduction band offset of $1.45 \pm 0.1$ eV, the ratio of $\Delta E_v : \Delta E_c$ is close to 13:2.

In summary, the VBO of the MgO/AlN heterojunction has been measured by XPS. A type-I band alignment with a VBO of $\Delta E_v$ was $0.22 \pm 0.08$ eV and conduction band offset of $\Delta E_c \sim 1.42$ eV is obtained. The accurate determination of the band alignment of MgO/AlN indicates that the MgO (111) can provide an effective carrier confinement in III-N alloys based electronic devices.

![Energy band diagram of MgO/AlN heterojunction. A type-I heterojunction is formed in the staggered arrangement.](image)

**Table I.** XPS CL spectra fitting results and VBM positions obtained by linear extrapolation of the leading edge to the extended base line of the VB spectra. The errors in the peak positions and VBM are $\pm 0.03$ and $\pm 0.08$ eV, respectively.

<table>
<thead>
<tr>
<th>Sample</th>
<th>State</th>
<th>Binding</th>
<th>Energy (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MgO</td>
<td>Mg 2p</td>
<td>50.25</td>
<td>(Mg–O)</td>
</tr>
<tr>
<td></td>
<td>VBM</td>
<td>3.23</td>
<td></td>
</tr>
<tr>
<td>AlN</td>
<td>Al 2p</td>
<td>73.83</td>
<td>(Al–N)</td>
</tr>
<tr>
<td></td>
<td>VBM</td>
<td>74.86</td>
<td>(Al–O)</td>
</tr>
<tr>
<td>MgO/AlN</td>
<td>Mg 2p</td>
<td>50.38</td>
<td>(Mg–O)</td>
</tr>
<tr>
<td></td>
<td>Al 2p</td>
<td>73.94</td>
<td>(Al–N)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>75.44</td>
<td>(Al–O)</td>
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This work was supported by the 863 High Technology R&D Program of China (Grant Nos. 2007AA03Z402 and 2007AA03Z451), the Special Funds for Major State Basic Research Project (973 program) of China (Grant No. 2006CB604907), and the National Science Foundation of China (Grant Nos. 60506002 and 60776015).