Band offset determination of mixed As/Sb type-II staggered gap heterostructure for n-channel tunnel field effect transistor application


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I. INTRODUCTION

The tunnel field-effect transistor (TFET) is one of the devices that can achieve subthreshold swing (SS) < 60 mV/dec at 300 K based on band-to-band tunneling (BTBT) injection mechanism. Currently, it is under intensive study due to the promising applications for sub-0.5 V operation and low standby power. Heterostructures with type-II band alignment at source/channel heterointerface represent a steep p-n junction and have been investigated as TFET performance boosters, such as higher ON current (I_{ON}), lower OFF state leakage (I_{OFF}), and step sub-threshold swing. Among these heterostructures, mixed As/Sb based heterojunction enables a wide range of staggered band alignments depending on the alloy compositions in the source and channel materials. The band offset of the staggered gap heterojunction at the source/channel heterointerface also defines the effective tunneling barrier height (E_{b,eff}), which not only determines the ON-state tunneling current, but also sets the blocking barrier of OFF-state leakage. Therefore, efforts have been devoted to optimize the band offset to boost I_{ON} and suppress I_{OFF}; however, to our knowledge, there is no prior report of experimental demonstration of band offset on mixed As/Sb type-II staggered gap heterojunction n-channel tunnel FET structures. Very recently, we have demonstrated the valence band (VB) offset of the p-channel TFET structure. In this report, we work the experimental study of the valence band offset of a mixed As/Sb type-II staggered gap GaAs_{0.35}Sb_{0.65}/In_{0.7}Ga_{0.3}As n-channel tunnel FET structure that shows a great promise for low-power applications.

II. EXPERIMENTAL

In this study, n-channel TFET structures were grown by solid source molecular beam epitaxy (MBE) and Figure 1 shows the schematic of the layer structure used for this work. The details of the growth process can be found elsewhere. The crystalline quality of the structure was characterized by cross-sectional transmission electron microscopy (TEM). TEM samples were prepared using conventional mechanical thinning procedure followed by Ar+ ion milling. Reciprocal space maps (RSMs) were obtained using Panalytical X’pert Pro system with Cu Kα-1 line focused x-ray source to determine the layer compositions of the TFET structure. The detailed x-ray studies on this structure can be found elsewhere. The valence band offset (ΔE_v) of the internally lattice-matched GaAs_{0.35}Sb_{0.65}/In_{0.7}Ga_{0.3}As heterojunction at the source/channel interface was measured by x-ray photoelectron spectroscopy (XPS). The 5 nm In_{0.7}Ga_{0.3}As/310 nm GaAs_{0.35}Sb_{0.65} structure was used for the measurement of binding energy information at the heterointerface. To measure the binding energy value of bulk In_{0.7}Ga_{0.3}As and GaAs_{0.35}Sb_{0.65} layers, (i) 150 nm In_{0.7}Ga_{0.3}As/310 nm GaAs_{0.35}Sb_{0.65} heterostructure and (ii) 310 nm GaAs_{0.35}Sb_{0.65} without the top In_{0.7}Ga_{0.3}As layer were used. The 10 nm p++ GaAs_{0.35}Sb_{0.65} layer with heavily carbon (C) doping of 1×10^{20}/cm^3 in the source region was used to create abruptly doped junction and thus increasing the tunneling probability from source to channel. XPS measurements were performed using a Phi Quantera Scanning XPS Microprobe instrument with a monochromated Al-Kα (energy of 1486.6 eV) x-ray source. Oxide layer at sample surfaces was removed by wet chemical etching with citric acid/hydrogen peroxide (C_6H_8O_7:H_2O_2) at volume ratio of 50:1 for 10 s on In_{0.7}Ga_{0.3}As surface and 1 min on GaAs_{0.35}Sb_{0.65} surface.
respectively, prior to loading into the XPS chamber. Approximately, 2-3 nm was etched from each sample surface based on the premeasured etching rate. The Sb and In core level (CL) binding energy spectra as well as GaAs0.35Sb0.65 and In0.7Ga0.3As valence band binding energy spectra were collected with pass energy of 26 eV. An exit angle of 45° was used for all measurements. Curve fitting was performed by the CasaXPS 2.3.14 program using a Lorentzian convolution with a Shirley-type background.

III. RESULTS AND DISCUSSION

As fixed charges caused by defects at the source/channel heterointerface would influence the band lineup of the heterojunction,10 cross-sectional TEM was used to characterize the crystalline quality of the entire TFET structure. Figure 2 shows a cross-sectional TEM micrograph of such TFET structure with 150 nm intrinsic In0.7Ga0.3As channel and 200 nm n1 In0.7Ga0.3As drain layer. All layers were labeled in this figure and the GaAs0.35Sb0.65/In0.7Ga0.3As heterointerface was denoted by an arrow in the micrograph. It can be seen from this figure that the linearly graded InxAl1-xAs buffer layer effectively accommodates the lattice mismatch induced defects between the active layer and the InP substrate. Cross-sectional TEM micrograph shows high contrast at the source/channel heterointerface and no threading dislocations were observed in both the GaAs0.35Sb0.65 and In0.7Ga0.3As layers and their interface at this magnification, indicating a threading dislocation density in the lattice-matched source/channel layers on the order of or below 107 cm-2.

XPS measurement can provide binding energy information about the core level and the valence electrons emitted from each layer structure. This allows to determine AE of In0.7Ga0.3As channel relative to GaAs0.35Sb0.65 source by the method as described by Kraut et al.13 Using this approach, XPS spectra were collected from the following three samples: (i) 150 nm In0.7Ga0.3As/310 nm GaAs0.35Sb0.65, (ii) 5 nm In0.7Ga0.3As/310 nm GaAs0.35Sb0.65, and (iii) 310 nm GaAs0.35Sb0.65 without the top In0.7Ga0.3As layer. The AE can be determined using the following equation:

\[
\Delta E_v = \left( E_{GaAs}^{GaAsSb} - E_{VBM}^{GaAsSb} \right) - \left( E_{InGa}^{InGaAs} - E_{VBM}^{InGaAs} \right) - \Delta E_{CL}(i),
\]

where \( E_{GaAs}^{GaAsSb} \) and \( E_{InGa}^{InGaAs} \) are CL binding energy of Sb3d5/2 and In3d5/2 from thick GaAs0.35Sb0.65 and thick In0.7Ga0.3As film surfaces, respectively; \( E_{VBM}^{InGaAs} \) is the valence band maxima (VBM) of the corresponding samples and it can be determined by linear extrapolation of the leading edge of VB spectra to the base line.14 \( \Delta E_{CL}(i) = E_{InGaAs/GaAsSb}^{InGaAs} - E_{InGaAs/GaAsSb}^{Sb3d5/2} \) is the energy difference between Sb3d5/2 and In3d5/2 CLs which are measured at the In0.7Ga0.3As/GaAs0.35Sb0.65 heterointerface. Figures 3(a)–3(f) show the CL and VB spectra from each sample. High resolution XPS measurements with a step-size of 0.025 eV were performed to resolve the spin-orbit splitting of In3d and Sb3d peaks. XPS survey scan in the range of 0-600 eV and high resolution scan around the O1s peak (~530 eV) was taken before each measurement to confirm that no oxygen component was left on each film surface. Figure 3(g) shows the high resolution scan from 526 eV to 540 eV on GaAs0.35Sb0.65 surface. No oxygen 1s peak and Sb-O bond (~530 eV)15 was detected at an exit angle of 45°. Similar scans on other sample surfaces (not shown in Figure 3) also show that no oxygen component was detected at this exit angle. Furthermore, the symmetric CL peaks of In3d5/2 and Sb3d5/2 also indicate that only single bond, either In-As or Sb-Ga, presents within the sample surfaces studied in this work, suggesting that no In-O or Sb-O bonds formed on the sample surface. All measured binding energy values are summarized in Table I. From the XPS measurements, the values of \( \left( E_{GaAs}^{GaAsSb} - E_{VBM}^{GaAsSb} \right), \left( E_{InGa}^{InGaAs} - E_{VBM}^{InGaAs} \right), \) and \( \Delta E_{CL}(i) \) were determined to be 527.70 eV, 443.79 eV, and 83.52 eV, respectively. The valence band offset of In0.7Ga0.3As channel relative to GaAs0.35Sb0.65 source is determined to be 0.39 ± 0.05 eV using Eq. (1). The uncertainty value of 0.05 eV is from the
scatter of VB data with respect to the fitting in VBM position.

Shallow CL spectra of In4d and Sb4d were also recorded to confirm the results obtained from In3d and Sb3d spectra. Curve fittings were used to separate the spin-orbit splitting of In4d and Sb4d peaks as well as to resolve In4d from the combined Ga/In 3d peaks. Figures 4(a)–4(c) show the CL and VB spectra from 150 nm In0.7Ga0.3As/310 nm GaAs0.35Sb0.65, 310 nm GaAs0.35Sb0.65 without the top In0.7Ga0.3As layer

![Figure 3](image1.jpg)

**FIG. 3.** XPS spectra of (a) Sb3d5/2 CL and (b) VB spectra from 310 nm GaAs0.35Sb0.65 without the top In0.7Ga0.3As layer; (c) In3d5/2 CL and (d) VB spectra from 150 nm In0.7Ga0.3As/310 nm GaAs0.35Sb0.65 sample; (e) Sb3d5/2 CL and (f) In3d5/2 CL spectra from 5 nm In0.7Ga0.3As/310 nm GaAs0.35Sb0.65 sample measured at the interface; (g) high resolution scan in the range of 526-540 eV and no O1s peak or Sb-O bond was detected. CL spectra curves were fitted using a Lorentzian convolution with a Shirley-type background.

![Figure 4](image2.jpg)

**FIG. 4.** XPS spectra of (a) Sb4d CL and VB spectra from 310 nm GaAs0.35Sb0.65 without the top In0.7Ga0.3As layer; (b) In4d CL and VB spectra from 150 nm In0.7Ga0.3As/310 nm GaAs0.35Sb0.65 sample; (c) Sb4d CL and In4d CL spectra from 5 nm In0.7Ga0.3As/310 nm GaAs0.35Sb0.65 sample measured at the interface. The insets of (a) and (b) show the magnified VB spectrum of the corresponding sample.

TABLE I. Measurement results of XPS CL spectra and VBM positions obtained by linear extrapolation of the leading edge to the extended base line of the valence band spectra.

<table>
<thead>
<tr>
<th>Sample</th>
<th>States</th>
<th>Binding energy (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>310 nm GaAs0.35Sb0.65</td>
<td>Sb CL</td>
<td>527.95</td>
</tr>
<tr>
<td></td>
<td>VBM</td>
<td>0.25</td>
</tr>
<tr>
<td>150 nm In0.7Ga0.3As/310 nm GaAs0.35Sb0.65</td>
<td>In CL</td>
<td>444.25</td>
</tr>
<tr>
<td></td>
<td>VBM</td>
<td>0.46</td>
</tr>
<tr>
<td>5 nm In0.7Ga0.3As/310 nm GaAs0.35Sb0.65</td>
<td>Sb CL</td>
<td>528.17</td>
</tr>
<tr>
<td></td>
<td>In CL</td>
<td>444.65</td>
</tr>
</tbody>
</table>

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and 5 nm In$_{0.7}$Ga$_{0.3}$As/310 nm GaAs$_{0.35}$Sb$_{0.65}$ samples, respectively. An accurate determination of valence band maximum value of each material is the key point of the measurement of valence band offset. According to Kraut’s method, the VBM was determined by fitting a instrumentally broadened valence band density of states (DOS), for which the VBM is uniquely identified as the energy at which the DOS goes to zero, to the leading edge of the experimental valence band spectrum. Based on this method, the insets of Figs. 4(a) and 4(b) show the corresponding magnified VB spectra of In$_{0.7}$Ga$_{0.3}$As and GaAs$_{0.35}$Sb$_{0.65}$, respectively. The intersection of two straight lines, one fits to the linear portion of the valence band leading edge and one fits to the base line of valence band spectrum, determines the VBM value of the corresponding material. All measured binding energy information was also summarized in Table I. The $\Delta E_c$ of In$_{0.7}$Ga$_{0.3}$As channel relative to GaAs$_{0.35}$Sb$_{0.65}$ source measured from shallow CL spectra was determined to be 0.36 ± 0.05 eV using Eq. (1). It should be noted that the difference between measured $\Delta E_c$ values from 4d CL peaks (0.36 ± 0.05 eV) and 3d CL peaks (0.39 eV ± 0.05 eV) could be caused by the uncertainty during the curve fitting process. However, the $\Delta E_c$ value difference within these two measurements (0.03 eV) is in the range of experimental error (0.05 eV) labeled in the paper, indicating good consistency between the results from 4d CL and 3d CL measurements.

The conduction band offset ($\Delta E_c$) can be estimated by the following equation:

$$\Delta E_c = E_g^{GaAs} + \Delta E_v - E_v^{InGaAs},$$

where $E_g^{GaAs}$ and $E_v^{InGaAs}$ are the band gaps of GaAs$_{0.35}$Sb$_{0.65}$ and In$_{0.7}$Ga$_{0.3}$As, respectively. The bandgap of intrinsic GaAs$_{0.35}$Sb$_{0.65}$ at 300 K was found to be ~0.7 eV by the commonly used empirical law and the experimental measured bandgap of intrinsic In$_{0.7}$Ga$_{0.3}$As material at 300 K is 0.6 eV. Using these data, the $\Delta E_c$ is calculated to be ~0.49 eV. It should be noted that, in reality, the value of $\Delta E_c$ could be smaller than the evaluated one due to the band gap narrowing effect caused by the heavy C doping in the GaAs$_{0.35}$Sb$_{0.65}$ layer.

Figure 5 shows the schematic band alignment diagram of the GaAs$_{0.35}$Sb$_{0.65}$/In$_{0.7}$Ga$_{0.3}$As heterojunction based on the present results above. A type-II staggered band lineup is formed at the source/channel interface of the n-channel TFET structure. The effective tunneling barrier height ($E_{eff}$) is determined to be 0.21 ± 0.05 eV. This effective tunneling barrier height plays a key role on the performance of TFET devices such as, $I_{ON}$ and $I_{OFF}$. It has been reported that reducing $E_{eff}$ from 0.5 eV to 0.25 eV results in at least 200% improvement of $I_{ON}$ in mixed As/Sb heterojunction TFETs due to the increase of tunneling transmission coefficient. On the other hand, the reduced $E_{eff}$ also improves the drain induced barrier thinning (DBT) due to the fact that the inter band generation process occurs closer to the source/channel junction, thus improving electrostatics of devices. Nevertheless, if $E_{eff}$ < 0, a broken bandgap lineup will occur at the source/channel heterointerface. Although, further improvement is expected on $I_{ON}$ and SS by decreasing $E_{eff}$, the $I_{OFF}$ will increase simultaneously and thus additional gate bias is required to turn off this tunneling mechanism. As a result, the $E_{eff}$ should be well modulated to guarantee both the ON-state and OFF-state performance of a TFET device. An $I_{ON}/I_{OFF}$ ratio of greater than 10$^4$ with high $I_{ON} > 100$ μA/μm has been reported experimentally using the same TFET structure as studied in this paper, indicating that a 0.21 eV effective barrier at GaAs$_{0.35}$Sb$_{0.65}$/In$_{0.7}$Ga$_{0.3}$As interface can provide promising performance for n-channel TFET device application.

**IV. CONCLUSION**

In summary, the experimental study of the valence band offset of an n-channel GaAs$_{0.35}$Sb$_{0.65}$/In$_{0.7}$Ga$_{0.3}$As heterostructure tunnel FET structure grown by MBE was investigated using XPS. Cross-sectional TEM micrograph indicated threading dislocation free interface at the source/channel region. XPS results showed the valence band offset of 0.39 ± 0.05 eV at the GaAs$_{0.35}$Sb$_{0.65}$/In$_{0.7}$Ga$_{0.3}$As source/channel heterointerface. The conduction band offset is calculated to be ~0.49 eV using bandgaps of GaAs$_{0.35}$Sb$_{0.65}$ and In$_{0.7}$Ga$_{0.3}$As, and the effective tunneling barrier height was found to be 0.21 eV. These results and the self-consistency among device, material, and growth properties indicate that mixed As/Sb material systems provide access to various combinations of band gaps and band offset energies while maintaining high material quality to design metamorphic staggered gap TFET devices for ultra-low power logic applications.

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