Structural properties and band offset determination of p-channel mixed As/Sb type-II staggered gap tunnel field-effect transistor structure


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The structural properties and band offset determination of p-channel staggered gap In$_{0.7}$Ga$_{0.3}$As/GaAs$_{0.35}$Sb$_{0.65}$ heterostructure tunnel field-effect transistor (TFET) grown by molecular beam epitaxy (MBE) were investigated. High resolution x-ray diffraction revealed that the active layers are strained with respect to “virtual substrate.” Dynamic secondary ion mass spectrometry confirmed an abrupt junction profile at the In$_{0.7}$Ga$_{0.3}$As/GaAs$_{0.35}$Sb$_{0.65}$ heterointerface and minimal level of intermixing between As and Sb atoms. The valence band offset of $0.37 \pm 0.05$ eV was extracted from x-ray photoelectron spectroscopy. A staggered band lineup was confirmed at the heterointerface with an effective tunneling barrier height of 0.13 eV. Thus, MBE-grown staggered gap In$_{0.7}$Ga$_{0.3}$As/GaAs$_{0.35}$Sb$_{0.65}$ TFET structures are a promising p-channel option to provide critical guidance for the future design of mixed As/Sb type-II based complementary logic and low power devices.
was used for the measurement of binding energy information at the heterointerface, while 200 nm In0.7Ga0.3As/450 nm GaAs0.35Sb0.65 and 450 nm GaAs0.35Sb0.65 without the top In0.7Ga0.3As layer were used to measure the binding energy information of bulk In0.7Ga0.3As and GaAs0.35Sb0.65, respectively. XPS measurements were performed on a Phi Quantera Scanning XPS Microprobe instrument using a monochromatic Al Kα (1486.6 eV) x-ray source. A take-off angle of 45° and pass energy of 26 eV was used in all measurements. The binding energy was corrected by adjusting the carbon (C) 1s core level (CL) peak position to 285 eV for each sample surface. Curve fitting was done by the CasaXPS 2.3.14 using a Lorentzian convolution with a Shirley-type background.

As shown in Fig. 1, due to the lattice constant difference between active layers (In0.7Ga0.3As and GaAs0.35Sb0.65) and the InP substrate, a linearly graded InxAl1–xAs buffer was used to accommodate the lattice mismatch induced defects. Reciprocal space maps (RSMs) were obtained using Panalytical X’pert Pro system with Cu Kα1 line focused x-ray source to determine the amount of strain relaxation and the layer compositions of the p-channel TFET structure. Figures 2(a) and 2(b) show RSMs for (004) and (115) reflections corresponding reciprocal space points (RLPs) in these layers with measured compositions were labeled to with the projection of incident x-ray beam along [110] direction with respect to the In0.7Al0.3As “virtual substrate” was used for the measurement of binding energy information of bulk In0.7Ga0.3As and GaAs0.35Sb0.65 heterointerface. The transition between In0.7Ga0.3As/GaAs0.35Sb0.65 is less than 10 nm, within the sputter-induced broadening of the ion beam, thereby improves the Ion and SS. Figure 3(b) shows the Si and C doping profiles in the same p-channel TFET structure. It depicts an abrupt junction profile at the In0.7Ga0.3As/GaAs0.35Sb0.65 interface, suggesting a steep junction is formed at the heterointerface.

The valence band offset at the In0.7Ga0.3As/GaAs0.35Sb0.65 interface was determined with the method by Kraut et al.,

\[ \Delta E_V = \left( E_{GaAs}^{CL} - E_{VBM} \right) - \left( E_{InGaAs}^{CL} - E_{VBM} \right) - \Delta E_{CL}^{(i)} \]

where \( E_{GaAs}^{CL} \) and \( E_{InGaAs}^{CL} \) are CL binding energies of Sb3d5/2 and In3d5/2; \( E_{VBM} \) is the valence band maxima (VBM) of the corresponding samples. \( E_{VBM} \) was determined by linearly fitting the leading edge of the valence band (VB) spectrum to the base line. \( D \) and \( E_{InGaAs}^{CL} - E_{GaAs}^{CL} \) were measured from 200 nm In0.7Ga0.3 As/450 nm GaAs0.35Sb0.65 and 450 nm GaAs0.35Sb0.65 without the In0.7Ga0.3As overlayer, respectively. \( \Delta E_{CL}^{(i)} = E_{GaAs}^{CL} - E_{InGaAs}^{CL} \) is the binding energy difference between Sb3d5/2 and In3d5/2 CLs measured at the

![FIG. 2. Symmetric (004) and asymmetric (115) RSMs of the p-channel TFET structure with the projection of incident x-ray beam along [110] direction. Only 10% strain relaxation values in In0.7Ga0.3As and GaAs0.35Sb0.65 layers were extracted from RSMs, indicating low defect density in this region.](Image 57x96 to 291x233)

![FIG. 3. (a) Dynamic SIMS depth profiles of Ga, In, As, and Sb of the TFET structure. An abrupt In0.7Ga0.3As/GaAs0.35Sb0.65 interface with a transition between In0.7Ga0.3As/GaAs0.35Sb0.65 of less than 10 nm was confirmed, indicating low level of As and Sb intermixing at the interface; (b) doping concentration profiles of Si in the n` source and C in the p` drain region. An abrupt junction profile at the In0.7Ga0.3As/GaAs0.35Sb0.65 interface suggests a formation of steep junction.](Image 336x115 to 540x325)
heterointerface from 5 nm In0.7Ga0.3As/450 nm GaAs0.35Sb0.65 sample. The CL and VB spectra from each sample were shown in Figs. 4(a)–4(f). In order to improve accuracy of the measured binding energy information, high resolution measurements with a step-size of 0.025 eV was performed to resolve the spin-orbit splitting of In and Sb 3d peaks. Curve fitting was done on each CL spectra to separate In-As and Sb-Ga bonds from the In-O and Sb-O bonds. The measured binding energy of In-O and Sb-O bonds was about 444.90 eV and 530 eV, respectively, which were in agreement with the reported values.12,13 The binding energy difference between Sb-O and Sb-Ga bonds from the In-O and Sb-O bonds. The measured fitting was done on each CL spectra to separate In-As and Sb-Ga bonds large enough to resolve the Sb-O bond as a separated peak (not shown in Fig. 4) from Sb-Ga spectrum. As a result, unlike In3d5/2 CL spectrum, which was a combination of In-As and Sb-Ga bonds, the measured Sb3d5/2 CL peak was Lorentzian shape without curve fitting.

All measured binding energy values are summarized in Table. I. The values of \( E_{\text{InGaAs}} - E_{\text{VBM}} \) and \( E_{\text{GaAsSb}} - E_{\text{VBM}} \) were found to be 443.79 eV and 527.66 eV, respectively. The VBO of In0.7Ga0.3As source relative to GaAs0.35Sb0.65 channel from the Eq. (1) is \( \Delta E_v = 0.37 \pm 0.05 \) eV. The uncertainty value 0.05 eV is due to the scatter of VB with respect to the fitting in VBM position.

The conduction band offset (CBO) can be calculated from the following equation:11

\[
\Delta E_C = E_{\text{GaAsSb}}^g + \Delta E_V - E_{\text{InGaAs}}^g,
\]

where, \( E_{\text{GaAsSb}}^g \) and \( E_{\text{InGaAs}}^g \) are the band gaps of GaAs0.35Sb0.65 and In0.7Ga0.3As, respectively. The bandgap of intrinsic GaAs0.35Sb0.65 at 300 K was found to be 0.70 eV by the commonly used empirical law.14 The bandgap of heavily doped In0.7Ga0.3As was determined to be 0.50 eV using the experimental measured bandgap of intrinsic In0.7Ga0.3As15 and by considering the band gap narrowing (BGN) effect caused by heavily Si doping.16,17 Using these results, the CBO of In0.7Ga0.3As with respect to GaAs0.35Sb0.65 was calculated to be \( \Delta E_C \sim 0.57 \) eV.

The strain relaxation of the active layers (In0.7Ga0.3As/GaAs0.35Sb0.65) of the p-channel heterojunction TFET structures is only limited to 10% with respect to the uppermost layer (In0.7Al0.3As) of the linearly graded InAs graded buffer. These active layers are considered to be strained or near lattice matched with respect to the “virtual substrate.” However, the active layers are about 1.1% lattice mismatched to InP substrate and the measured strain relaxation was \(~80%\) relative to InP substrate. The 1.1% lattice mismatch was mitigated by the linearly graded InxAl1-xAs (x = 0.52 to 0.7) buffer starting with the lattice matched composition of In0.52Al0.48As to InP and ending with In0.7Al0.3As, which is closely internal lattice matched to In0.7Ga0.3As/GaAs0.35Sb0.65 active layers. Growing of such In0.7Ga0.3As/GaAs0.35Sb0.65 p-channel TFET structure on Si will be lattice mismatched with respect to Si substrate, however, the active layers (In0.7Ga0.3As/GaAs0.35Sb0.65) and the uppermost layer (In0.7Al0.3As) of InAs graded buffer will also be closely internal lattice matched. Thus, the entire p-channel TFET on Si will be considered as a “metamorphic” (fully or partially relaxed) structure and the active layers will be either pseudomorphic (strained) or lattice matched. In the past, the In0.7Ga0.3As quantum well FET has been demonstrated on Si where the entire structure was metamorphic while the active layers were pseudomorphic.18 Thus, the value of valence band offset will not change, once the In0.7Ga0.3As/GaAs0.35Sb0.65 p-channel tunnel FET structures are grown on Si.

Figure 5 shows the schematic band alignment based on the band gap energy values determined above and the experimental result of \( \Delta E_V \) measured by XPS. One can find that a type-II band alignment was formed at the In0.7Ga0.3As/GaAs0.35Sb0.65 heterointerface. An effective tunneling barrier height \( E_{\text{eff}} = E_{\text{InGaAs}}^g - \Delta E_V \) of 0.13 eV was extracted from the present result. This effective tunneling barrier height plays a significant role on the performance of either n-channel or p-channel TFETs, which not only determines the ON-state BTBT rate but also sets the blocking barrier for...
OFF-state leakage.\cite{1,6,7} In order to increase $I_{\text{ON}}$ and improve the switching efficiency, a reduced energy barrier for tunneling is required.\cite{6,8,9} Large increase in BTBT current has been measured in type-II mixed As/Sb staggered gap TFETs by reducing $E_{\text{beff}}$.\cite{6,8} However, if $E_{\text{beff}}$ is reduced to a negative value, a broken band lineup will be formed at the heterointerface. Although a broken band alignment yields better ON-state performance,\cite{1} the increase in $I_{\text{OFF}}$ becomes another roadblock for boosting the performance of TFET devices. In that case, an additional gate bias is required to turn off this tunneling mechanism.\cite{19} As a result, the $E_{\text{beff}}$ value should be well optimized to guarantee high performance operation for both ON and OFF states in a p-channel or n-channel TFET structure. It has been reported that high $I_{\text{ON}}$ of 135 $\mu$A/$\mu$m with high $I_{\text{ON}}/I_{\text{OFF}}$ ratio of $2.7 \times 10^4$ ($V_{\text{DS}} = 0.5$ V, and $V_{\text{ON}} - V_{\text{OFF}} = 1.5$ V) was achieved using the similar device structure for n-channel TFET,\cite{9} indicating promising device performance is expected in the structure studied here for complementary p-channel TFET application.

In conclusion, the experimental determination of structural properties and valence band offset of a p-channel In$_{0.7}$Ga$_{0.3}$As/GaAs$_{0.35}$Sb$_{0.65}$ heterostructure tunnel FET grown by MBE was investigated. Symmetric (004) and asymmetric (115) reciprocal space maps demonstrated the strain relaxation of the In$_{0.7}$Ga$_{0.3}$As/GaAs$_{0.35}$Sb$_{0.65}$ active layers is limited to only 10% with respect to the uppermost layer (In$_{0.7}$Ga$_{0.3}$As) of the graded In$_{x}$Al$_{1-x}$As buffer. Dynamic SIMS measurement confirmed a low level intermixing between As and Sb atoms as well as an abrupt junction profile at the In$_{0.7}$Ga$_{0.3}$As/GaAs$_{0.35}$Sb$_{0.65}$ heterointerface. A valence band offset of $0.37 \pm 0.05$ eV at In$_{0.7}$Ga$_{0.3}$As/GaAs$_{0.35}$Sb$_{0.65}$ heterointerface was obtained from XPS measurements. The corresponding conduction band offset of $\sim 0.57$ eV was calculated using bandgaps of GaAs$_{0.35}$Sb$_{0.65}$ and In$_{0.7}$Ga$_{0.3}$As. A type-II band lineup was formed at the heterointerface with an effective tunneling barrier height of 0.13 eV. Knowledge of band alignment parameters, especially the valence band offset and effective tunneling barrier height of In$_{0.7}$Ga$_{0.3}$As/GaAs$_{0.35}$Sb$_{0.65}$ heterointerface, is believed to facilitate the design of mixed As/Sb staggered gap p-channel tunnel FETs for ultra-low power applications.

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