Band Alignment Parameters of $\text{Al}_2\text{O}_3$/InSb Metal–Oxide–Semiconductor Structure and Their Modification with Oxide Deposition Temperatures

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II–V compounds have been widely studied for future scaling down of low power, high speed field-effect transistors (FETs) due to their high electron mobility and saturation velocity. Among them, InSb has the highest electron mobility (7.7 × 10^5 cm^2 V−1 s−1) and high hole mobility (840 cm^2 V−1 s−1) that has potential for both high speed n- and p-FETs. Due to its narrow bandgap, InSb has been suggested to be applicable to quantum-well heterostructure including conduction and valence band offsets by Fowler–Nordheim (F–N) current–voltage (I–V) characteristics is consistent with that determined by the IPE measurements were performed in a commercial Microlab 350 XPS system equipped with an Al Kα source in an ultrahigh-vacuum chamber (5 × 10^−9 Torr) with a 60° take-off angle. The In 4d, Al 2p core levels and VBM spectra of the InSb, Al2O3/InSb interface was determined to be 2.9 ± 0.1 eV. In the present work, we further investigate the band alignment of ALD Al2O3/100nmInSb structure including conduction and valence band offsets by using Fowler–Nordheim (FN) current–voltage (I–V) characteristic and X-ray photoelectron spectroscopy (XPS) analysis. The ΔEc value determined from the FN characteristic is consistent with that determined by the IPE method. Since the characteristics of high-k/InSb structure are very sensitive to the thermal process due to the low thermal budget in InSb, the effect of oxide deposition temperatures on the band alignment modification of Al2O3/InSb is also investigated. The wafers used in this work were n-type (100)InSb substrates with a donor concentration of 2.2 × 10^{16} cm^{-3} at room temperature (determined by Hall measurement). After increasing in acetone and iso-propanol, the samples were dipped in diluted HCl (4%) solution for removing native oxides. The samples were then loaded into the ALD chamber (Cambridge NanoTech Fiji 202 DSC) for Al2O3 deposition using trimethylaluminium (TMA) and water as precursors. In the ALD chamber, 10 pulses of TMA/Ar were used to further removing native oxides before the deposition of 100 CYC (~9.2 nm) Al2O3. The use of in-situ TMA pre-cleaning before oxide deposition was proved to improve the Al2O3/InGaAs, Al2O3/InAs, Al2O3/InSb interfaces by self-cleaning effect. Beside the effect on the reduction of III–V native oxides, the reduction of dangling bonds at Al2O3/InSb interface after using some pulses of TMA/Ar is also expected. For the fabrication of metal–oxide–semiconductor capacitors (MOSCAPs), Ni/Au gate metal was formed via photolithography/e-beam evaporation/lift-off process. Finally, the Au/Ge/Ni/Au was deposited for back side ohmic contact followed by post metal annealing at 200 °C in N2 for 30 s.

The valence band offset (ΔEv) of Al2O3/InSb was determined for the sample deposited at 200 °C by using XPS measurement via the following formula:20)

\[ ΔE_v = E_{cl} + \left( E^{InSb}_{In4d} - E^{VBM}_{InSb} \right) - \left( E^{Al2O3}_{Al2p} - E^{VBM}_{Al2O3} \right). \]  

where \( E_{cl} = E^{Al2O3}_{Al2p} - E^{NOx}_{InSb} \) is the energy difference between Al 2p and In 4d core levels measured in 2 nm Al2O3/InSb interface, while \( E^{InSb}_{In4d} - E^{InSb}_{VBM} \) and \( E^{Al2O3}_{Al2p} - E^{VBM}_{Al2O3} \) are the differences between valence band maximum (VBM) energies and corresponding In 4d core level in InSb and Al 2p core level in 9.2-nm-thick Al2O3. XPS measurements were performed in a commercial Microlab 350 XPS system equipped with an Al Kα source in an ultrahigh-vacuum chamber (5 × 10^{-9} Torr) with a 60° take-off angle. The In 4d, Al 2p core levels and VBM spectra of the InSb, Al2O3/InSb interface and Al2O3 are shown in Fig. 1. The core levels were determined by using XPSPEAK software package (version 4.1) with Gaussian–Lorentz line shape and a Shirley background. The uncertainty of the core positions is 0.05 eV. The VBM positions were determined by the linear extrapolation of the leading valence band edge on the semiconductor and oxide. The uncertainty of determining VBM positions was also 0.05 eV. From the measurement values shown in Fig. 1 and Eq. (1), the value of \( ΔE_v ~ 3.76 ± 0.1 \) eV is extracted.

Figure 2(a) shows the current density–voltage (J–V) characteristics of the MOSCAP samples that were deposited at 150, 200, and 250 °C. J–V measurement was performed using a Keithley 4200 analyzer. All the samples exhibit a low leakage current with a breakdown field of above 7.2 MV/cm. In the FN regime, the current density can be expressed as:

\[ J_{FN} = \frac{m}{m^*} \frac{q}{16\pi^2\hbar^2\phi_h} E^2 \exp \left( -\frac{4\sqrt{2}m^*}{3\hbar q}\phi_h^{1/2}\frac{E}{E_0} \right), \]

(2)

where \( m, m^*, q, h, E, \) and \( \phi_h \) are the electron mass, electron effective mass in Al2O3 oxide, elementary charge, Plank’s...
constant, oxide electrical field \((E = V_g/l_{ox}, V_g: \text{gate bias and } l_{ox}: \text{oxide thickness})\), and tunneling barrier height, respectively. According to Eq. (2), the plot of \(\ln J_{FN}/E^2\) versus \(1/E\) (so-called FN plot) should be linear with slope \(S\) given by

\[
S = \frac{d[\ln(J_{FN}/E^2)]}{d(1/E)} = -\frac{4\sqrt{2m^*/q}}{3\hbar^2/2}\phi_B^{3/2}.
\]

The barrier heights can be expressed as \(\phi_B^+ = \chi_S - \chi\) under forward gate bias and \(\phi_B^- = \phi_m - \chi\) under reverse gate bias, where \(\chi_S, \phi_m,\) and \(\chi\) are semiconductor electron affinity, metal work function and oxide electron affinity, respectively. The FN plots of the three samples are shown in Figs. 2(b)–2(d). It can be seen that the curves exhibit a linear relationship at high electrical field, indicating the dominance of the FN mechanism. The slopes under forward and reverse bias \((S_+ \text{ and } S_-\text{, respectively})\) can be extracted from these data and the values of \(m^*\), \(\phi_B^+\), and \(\chi\) can be determined using the following formulas:

\[
m^* = \frac{9q^2h^4}{32m^*\left(\phi_m - \chi_S^3\right)^3},
\]

\[
\phi_B^+ = \left(\frac{-3qh\chi_S}{4\sqrt{2m^*}}\right)^{2/3},
\]

\[
\chi = (\chi_S - \phi_B^+).
\]

By taking the values of Ni work function \(\phi_m = 5.05 \text{ eV}\) and InSb electron affinity \(\chi_S = 4.6 \text{ eV}\), the extracted parameters of the MOS structures are listed Table I. As shown in the table, the extracted values of the two samples deposited at 150 and 200°C are very similar. The conduction band offset \(\Delta E_C\) values are found to be 2.71 and 2.77 eV, respectively. These values are in agreement and very close to that reported by Chou et al. by using the IPE method.\(^8\) The values of \(m^*\) and \(\chi\) are about 0.2–0.22\(m_0\) and 1.8–1.9 eV, respectively. For the sample deposited at 250°C, \(\Delta E_C, m^*\), and \(\chi\) are 3.84 eV, 0.092\(m_0\), and 1.21 eV, respectively, which are very different from those of the other samples.

To find out the reason for this difference, the capacitance–voltage \((C–V)\) measurement was performed using an HP4284A meter for further study. Figure 3(a) shows the \(C–V\) curves at 1 kHz of the three samples. While the \(C–V\) curves of the two samples deposited at 150 and 200°C are very similar, that of the sample deposited at 250°C shifts positively to \(\Delta V = 0.09 \text{ V}\). In the previous work, we found that there was an In, Sb out diffusion layer with a thickness of 1.5 nm at the \(\text{Al}_2\text{O}_3/\text{InSb}\) interface when the sample was deposited at 250°C [see the transmission electron microscopy (TEM) image of the sample with 7.5 nm ALD \(\text{Al}_2\text{O}_3/\text{InSb} \) at 250°C in Fig. 3(b)].\(^9\) This out diffusion layer might cause a negative fixed charge which results in lowering the Fermi level in InSb side to \(\Delta \phi = 0.09 \text{ eV}\) below that in the metal side [Fig. 3(b)]. The root cause of negative charge layer needs further investigating but it may attribute to the dominant diffusion of Sb at low thermal temperature.

![Fig. 1. XPS spectra of (a) In 4d core level and valence band of InSb surface (after HCl cleaning), (b) Al 2p and In 4d core levels at the 2 nm \(\text{Al}_2\text{O}_3/\text{InSb}\) interface, and (c) Al 2p and valence band of \(\text{Al}_2\text{O}_3\) film.](image1)

![Fig. 2. (a) \(I–V\) characteristics of samples; (b) and (c) FN plots of samples deposited at 150 and 200°C; (d) FN plots after revision of samples deposited at 250°C.](image2)

![Table 1. Band parameters of the samples extracted by FN characteristics.](table1)
In conclusion, the band alignment parameters of Al₂O₃/InSb structures have been evaluated by using XPS analysis and FN characteristics. The conduction band offset $\Delta E_C \approx 2.73 \pm 0.1\,\text{eV}$, and valence band offset $\Delta E_V \approx 3.76 \pm 0.1\,\text{eV}$ are extracted. For the ALD Al₂O₃ film parameters, an energy band gap of $6.66 \pm 0.1\,\text{eV}$, an electron affinity of $1.8-1.9\,\text{eV}$, and an electron effective mass of 0.2-0.22$m_0$ were deduced. The $I-V$ and $C-V$ analyses also indicated the band modification of the sample deposited at 250°C caused by the In, Sb out diffusion layer at the Al₂O₃/InSb interface. These results would be useful for the future study of high-$k$/InSb MOS devices.

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Fig. 3. (a) $C-V$ curves of samples, and (b) the band modification diagram of the sample deposited at 250°C caused by In, Sb out diffusion layer as indicated by TEM image.

The FN plot after revision is also linear as indicated in Fig. 2(d). The band alignment parameters were extracted again and interestingly, all the parameters became very similar to those of others samples (see Table I). By this revision, one can conclude that the conduction band offset of Al₂O₃/InSb is $\Delta E_C \approx 2.73 \pm 0.1\,\text{eV}$. Combining this value of conduction band offset with the valence band offset $\Delta E_V$ extracted above and the InSb band gap of 0.17 eV at room temperature, the band gap of the Al₂O₃ film can be deduced to be $E_g \approx 6.66 \pm 0.1\,\text{eV}$. This value is consistent with that reported by Huang et al. (6.8 ± 0.1 eV) by using energy loss spectra analysis.