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Extracting the effective bandgap of heterojunctions using Esaki diode I-V measurements

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The effective bandgap is a crucial design parameter of heterojunction tunneling field-effect transistors. In this letter, we demonstrate a method to measure the effective bandgap directly from the band-to-band tunneling current of a heterojunction Esaki diode, of which we only require knowledge of the electrostatic potential profile. The method is based on a characteristic exponentially increasing current with forward bias, caused by sharp energy filtering at cryogenic temperature. We apply this method experimentally to a n+In_{0.53}Ga_{0.47}As/pGaAs_{0.5}Sb_{0.5} Esaki diode and define requirements to apply it to other heterojunctions. © 2015 AIP Publishing LLC.
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The effective bandgap ($E_{g,\text{eff}}$, inset of Fig. 1) of heterojunctions is a crucial design parameter for Resonant Interband Tunneling Diodes (RITD) for high speed analog applications¹ and Tunneling Field-Effect Transistors (TFET) for ultra low power logic.² $E_{g,\text{eff}}$ is usually determined from the electron affinities and bandgaps of the bulk materials,³ or using optical measurements.^{4,5} However, there is significant uncertainty on $E_{g,\text{eff}}$, especially for the heterostructure In_{0.53}Ga_{0.47}As/GaAs_{0.5}Sb_{0.5} (InGaAs/GaAsSb, Fig. 1), which makes the prediction of TFET performance difficult.⁶ The lattice-matched In_xGa_{1-x}As/GaAs_{1-y}Sb_y heterojunction system is promising for TFET^{3,7-13} due to its tunable $E_{g,\text{eff}}$ (Fig. 1). In this letter, we present and experimentally demonstrate a method to measure $E_{g,\text{eff}}$ directly from the Band-To-Band Tunneling current density (J_{BTBT}) of a InGaAs/GaAsSb Esaki diode.

The method requires a p+/n or p/n+ Esaki diode (Figs. 2(a) and 2(c)) with a staggered (type II) or straddled (type I) band alignment, of which the highly doped region is highly degenerate and the lowly doped region is lowly degenerate or non-degenerate. Semiclassical¹⁴ (Figs. 2(b) and 2(d)) and Quantum Mechanical¹⁵ (QM) simulations at cryogenic temperature show a nearly exponentially increasing BTBT current with more negative reverse bias $0 > V_{\text{np}} > V_c$, which is unusual for p+/n+ Esaki diodes. V_c is the voltage where BTBT no longer increases exponentially and can easily be recognized visually. It will be theoretically shown that $E_{g,\text{eff}}$ can be extracted from V_c without requiring knowledge of the bandgaps or tunneling rates.

In order to intuitively understand the origin of the exponentially increasing current, we theoretically derive the approximate I-V relation for p/n+ diodes (Fig. 2(a)). A similar derivation can be made for p+/n diodes (Fig. 2(c)). The exponential current originates from a sharp energy filtering mechanism. Tunneling occurs dominantly at $E = E_{\text{fp}}$, along a path which starts at the hetero-interface and ends in the lowly p-type doped material (Fig. 2(a)). Tunneling at the highest energy levels ($E > E_{\text{fp}}$) is suppressed because these

tunnel paths are longer (Fig. 3(a)). At cryogenic temperature, tunneling at $E < E_{\text{fp}}$ is also suppressed due to a reduced amount of empty states $1 - f_{\text{FDp}}(E)$, with $f_{\text{FDp}}(E)$ the Fermi-Dirac occupation in the p-type region. This causes a peak in tunneling near E_{fp} . The BTBT current can therefore be described by considering tunneling only at this energy and using the Wentzel-Kramer-Brillouin (WKB) approximation

$$J_{\text{BTBT}} \propto \exp \left(-2 \int_0^L \kappa dx \right), \quad (1)$$

where κ is the magnitude of the imaginary wavevector k along the tunnel path in the forbidden gap¹⁶ and L is the length of the tunnel path. Due to the quadratic band bending in GaAsSb (Fig. 4(a)), the shape of $\kappa(x)$ in GaAsSb remains unchanged with more negative V_{np} , and only the limits of the integration change. For $0 > V_{\text{np}} > V_c$, the value of $\kappa(x=0)$ is nearly constant because the tunnel path starts close to midgap. We can locally approximate that L decreases linearly with $-V_{\text{np}}$ down to V_c (Fig. 4(c)). This causes J_{BTBT} to increase nearly exponentially (Fig. 4(b)). When $V_{\text{np}} < V_c$, the tunnel path extends into InGaAs and the current no longer increases exponentially, which allows the visual extraction of V_c from the I-V curve. More rigorous simulations with a fully QM 15-band k-p solver¹⁵ (not shown) confirm the same trends in the I-V curve. Contrary to the WKB approximation, the QM simulations do not neglect wavefunction reflections due to the discontinuity in $\kappa(x)$ at the heterointerface.^{17,18}

We can easily extract $E_{g,\text{eff}}$ from V_c , because at this bias condition, E_c of InGaAs at the hetero-interface is equal to E_{fp} (Fig. 4(a)). Therefore, we obtain the relation

$$E_{g,\text{eff}} = q(\Delta\Psi_n + \Delta\Psi_p - V_c) - \xi_n - \xi_p, \quad (2)$$

where q is the elementary charge, $\Delta\Psi_n$, $\Delta\Psi_p$ are the band bending of the n and p regions at $V_{\text{np}} = V_c$ (Fig. 4(a)), and the degeneracies are $\xi_n = E_{\text{fn}} - E_{c,n,\text{bulk}}$ and $\xi_p = E_{v,p,\text{bulk}} - E_{\text{fp}}$ or zero if non-degenerate. In order to be valid for staggered and straddled heterojunctions, we define the effective

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FIG. 1. Many lattice matched $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}_{1-y}\text{Sb}_y$ heterojunction TFETs have been demonstrated in literature, but there is significant uncertainty on the reported $E_{g,\text{eff}}$. The full line is calculated from electron affinities and bandgaps of the bulk materials.^{3,9}

bandgap at the hetero-interface as $E_{g,\text{eff}} = E_{c,n} - E_{v,p}$ with $E_{c,n}$ the n-type region conduction band edge and $E_{v,p}$ the p-type region valence band edge, both taken at the hetero-interface (Figs. 2(a) and 2(c)).

Four requirements are identified to obtain nearly exponentially increasing current in p/n+ Esaki diodes. First, the temperature must be sufficiently low (Fig. 3(b)). Simulations show the required temperature decreases with higher p-type dopant concentration, lower $E_{g,\text{eff}}$, and higher degeneracy ξ_p . Experimentally this required temperature can be found easily

FIG. 2. (a) The band diagram of a forward biased p/n+ Esaki diode with staggered alignment shows tunneling from the heterointerface to the lowly doped region. E_c , E_v are conduction and valence band edges and E_{fn} , E_{fp} are the quasi Fermi energy levels. (b) The corresponding simulation¹⁴ shows J_{BTBT} increases exponentially with forward bias at sufficiently low temperature. (c) and (d) Similar behavior for a p+/n heterojunction with straddled alignment.

FIG. 3. (a) The dashed arrows in the GaAsSb band diagram show suppressed tunneling at $E > E_{fp}$ and $E < E_{fp}$. The Transmission Probability (TP) weighted with Fermi-Dirac shows a peak in tunneling near E_{fp} at $T = 50$ K. The TP is calculated with a 15-band k-p solver¹⁵ and $k_{\perp}$ is the wavevector perpendicular to the tunneling direction. (b) Simulations¹⁴ show that at small forward bias, J_{BTBT} is temperature dependent for $T > 100$ K and exponential for $T < 100$ K.

by performing I-V measurements and lowering the temperature until the I-V no longer changes. Second, intermixing of both semiconductors near the heterointerface must be sufficiently low. Simulations show that the current is no longer exponential if the intermixing region is larger than 1 nm. Third, the degeneracy ξ_n must be larger than the band bending of the n+ region ($\Delta\Psi_n$ in Fig. 4(a)) at $V_{np} = 0$. This is easily achieved in n+InGaAs due to its low conduction band density of states, but not in n+ silicon. Finally, the conduction band offset at the hetero-interface (ΔE_c in Fig. 2(a)) must be positive and sufficiently large ($q\Delta E_c > \xi_n - q\Delta\Psi_n$) such that the tunnel path starts at the heterointerface at $V_{np} = 0$. This is the case for n+InGaAs/pGaAsSb but not for n+InGaAs/pInP. Furthermore, simulations show that the method remains valid in the limit of a near-broken bandgap heterojunction with $E_{g,\text{eff}} = 0$ eV.

We experimentally verify our prediction of exponential BTBT current in a forward biased diode.⁶ An InGaAs/GaAsSb heterojunction is grown on a lattice matched InP substrate with Molecular Beam Epitaxy (MBE) as described in Ref. 20. The active dopant concentrations $n = 3.3 \times 10^{19} \text{ cm}^{-3}$ and $p = 1.1 \times 10^{19} \text{ cm}^{-3}$ are obtained with Hall measurements and satisfy the previously mentioned requirements for exponential BTBT current. Transmission Electron Microscopy (HR-HAADF-STEM, Fig. 5) analysis confirms a sharp hetero-interface with less than 1 nm of intermixing. Diodes with junction areas $A_j = 0.01\text{--}2 \mu\text{m}^2$ are fabricated according to the process flow in Ref. 21. We measure the diode I-V characteristics with an Agilent 4156C parameter analyzer. Perimeter effects are negligible, since I_{BTBT} scales with A_j in reverse (inset of Fig. 6) and forward bias, but only after correction for series resistance R_s according to the

FIG. 4. (a) and (c) The tunnel path at $E = E_{Fp}$ is located entirely in GaAsSb for $0 > V_{np} > V_c$, and extends to InGaAs for $V_{np} < V_c$. κ is calculated using the Kane 2-band dispersion relation.¹⁹ (b) The current no longer increases exponentially when $V_{np} < V_c$.

procedure described in Ref. 20. The measured V_c can be severely impacted by a high R_s if the I-V curves are not corrected.⁶ While the peak voltage of diodes with $A_j = 0.04 \mu\text{m}^2$ shifts by only 0.02 V, diodes with $A_j = 2 \mu\text{m}^2$ carry more current and the peak voltage is shifted by 0.1 V when correcting for $R_s = 350 \Omega$. When the temperature is lowered, we observe a decrease of BTBT in forward bias, and the I-V becomes more exponential (Fig. 6) as predicted by simulations (Fig. 3(b)). The exponential current also confirms that the intermixing region at the heterojunction is smaller than 1 nm. At $T = 78$ K, we extract $V_c = -0.27$ V from 4 diodes with different areas.

In order to extract $E_{g,eff}$ from V_c using Eq. (2), we calculate the degeneracies $\xi_{n,p}$ and band bending $\Delta\Psi_{n,p}$ at V_c using the measured active dopant concentrations and Sentaurus Device.¹⁴ We use Fermi-Dirac statistics and the effective mass approximation for the light hole, heavy hole, and conduction bands with a nonparabolicity correction in the Γ , L , and X valleys.^{3,9,22} We assume dopant-dependent bandgap narrowing (dopant-BGN) does not increase the degeneracy, and we obtain $\xi_n = 0.47$ eV and $\xi_p = 0.04$ eV at $T = 78$ K. We obtain a match between simulated and measured $V_c = -0.27$ V at $T = 78$ K with $E_{g,eff} = 0.27$ eV. We then extrapolate this result to $T = 300$ K using literature data

FIG. 5. (a) HR-HAADF-STEM analysis and (b) the intensity traces along A-A', B-B', and C-C' show a locally smooth and sharply defined heterointerface with an intermixing region smaller than 1 nm and no visible defects.

on temperature dependent bandgap narrowing^{23,24} and obtain $E_{g,eff} = 0.21$ eV. Currently, we cannot quantitatively compare the full measured and simulated I-V, since this requires a profound understanding of dopant-BGN on BTBT rates.

We assess the sensitivity of $E_{g,eff}$ to the different input parameters in Eq. (2) using semiclassical simulations. If an error $\Delta V_c = \pm 20$ mV is made during the experimental extraction in Fig. 6, this results in an error $\Delta E_{g,eff} = \pm 45$ meV. If an error is made on ξ_n , ξ_p due to a possibly inaccurate density of states model, $\Delta \xi_p = \pm 20$ meV results in an error $\Delta E_{g,eff} = \mp 20$ meV, and $\Delta \xi_n = \pm 20$ meV results in $\Delta E_{g,eff} = \pm 11$ meV.

Even when considering these possible error bars, our obtained $E_{g,eff}$ is lower than other literature values for the undoped $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{GaAs}_{0.5}\text{Sb}_{0.5}$ heterojunction⁷⁻¹⁰ ($E_{g,eff} = 0.27$ – 0.5 eV, see Fig. 1). We identify three possible explanations for this discrepancy: First, dopant-BGN could

FIG. 6. The measured I-V curves become more exponential at $T = 78$ K. We extract $V_c = -0.27$ V from 2 diodes with different areas. The inset shows I_{BTBT} scales with the junction area, but only after correcting for series resistance.

increase ξ_n and ξ_p and therefore also $\Delta\Psi_{n,p}$. This would result in a underestimated $E_{g,\text{eff}}$ for the same measured $V_c = -0.27$ V. Our obtained value $E_{g,\text{eff}} = 0.21$ eV is therefore a lower limit.

Second, heavy doping could shift ΔE_c and ΔE_v and decrease $E_{g,\text{eff}}$.²⁵ Further extrapolation to an undoped heterojunction using literature values of Jain Roulston dopant-BGN^{25,26} results in $E_{g,\text{eff}} = 0.39$ eV, which brings our measured value in the range found in literature.

The third possibility is a fixed interface charge affecting the band bending, as reported in Ref. 5 for a $\text{In}_{0.7}\text{Ga}_{0.3}\text{As}/\text{GaAs}_{0.35}\text{Sb}_{0.65}$ heterojunction. It was reported that a fixed positive charge of $6 \times 10^{12} \text{ cm}^{-2}$ changed the band alignment from staggered to broken. However, HR-HAADF-STEM analysis shows no visible defects in our diodes (Fig. 5), thus we do not expect fixed charge to affect the measured $E_{g,\text{eff}}$.

In conclusion, simulations and experiments of heterojunction Esaki diodes at cryogenic temperature demonstrate a characteristic exponentially increasing BTBT current. It allows us to determine a lower limit $E_{g,\text{eff}} > 0.21$ eV for the $n + \text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{pGaAs}_{0.5}\text{Sb}_{0.5}$ heterojunction using a method that requires knowledge of the dopant concentrations and degeneracies $\xi_{n,p}$ but not the bandgaps and tunnel rates. The exponential current also allows us to determine that the intermixing region at the junction is < 1 nm, which is verified by HR-HAADF-STEM analysis. Other applications include the analysis of fixed charge at the heterojunction and further understanding of dopant-BGN and its impact on TFET.

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