Theoretical analysis of band-to-band tunneling in highly-mismatched semiconductor alloys

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***Abstract*—The requirement for improved mid-infrared sensing technologies motivates the development of photodiodes displaying high signal-to-noise ratio. Key to achieving this goal is minimisation of the dark current, to which band-to-band tunneling (BTBT) contributes significantly in narrow-gap materials. We present a theoretical analysis of BTBT in narrow-gap dilute nitride semiconductor alloys, and evaluate the impact of nitrogen (N) incorporation on the BTBT current density. For low field strengths our calculations suggest the potential to reduce BTBT by exploiting the impact of N-related band-anticrossing on the complex band structure (CBS). At high fields our analysis suggests that BTBT is governed by an interplay between the impact of N incorporation on the CBS and on the conduction band edge density of states, and is approximately equal to that in a conventional narrow-gap material.**

I. Introduction

The past two decades have seen significant interest in exploiting the unusual properties of highly-mismatched alloys (HMAs) to develop novel devices for applications in electronic, photonic and photovoltaic devices [1], [2]. Meanwhile, growing interest in mid-infrared sensing applications has motivated the exploration of new approaches to facilitate the development of high-performance long-wavelength photodiodes. To this end, the key challenges consist of exploring novel material systems and architectures to (i) access difficult spectral ranges, and (ii) enhance detector signal-to-noise ratio by suppressing the intrinsic loss mechanisms which contribute to photodiode dark current [3]. In narrow-gap (mid-infrared) photodiodes BTBT represents an important contribution to the dark current: here we explore the potential to exploit the unusual band structure of HMAs to suppress BTBT at mid-infrared wavelengths.

When substituted in dilute concentrations in conventional III-V compounds such as InAs, N acts as an isovalent impurity, strongly perturbing the conduction band (CB) structure. The unusual band structure evolution in InN_xAs_{1-x} and related alloys can be described in terms of a band-anticrossing (BAC) interaction between the extended states of the InAs CB edge, and highly localised N-related impurity states [1], [4]. This BAC interaction leads to a strong reduction in band gap with increasing N composition x which, unusually, is accompanied by an increase in the CB edge effective mass, and hence the CB edge density of states (DOS).

This increase in CB edge effective mass also modifies the CBS, suggesting the possibility to exploit N incorporation to engineer and suppress the BTBT current. We explore this possibility theoretically, via a comparative analysis of the dependence of the BTBT current on band gap and applied electric field in (001)-oriented highly-mismatched InN_xAs_{1-x} and conventional $InAs_{1-y}Sb_y$ alloys. Our calculations indicate that the impact of N incorporation on BTBT is determined by an interplay between the impact of N incorporation on the CBS (which acts to reduce the current) and CB edge DOS (which acts to increase the current), with the balance between these two effects depending strongly on the applied field.

II. Theoretical model

We calculate the CBS of dilute nitride InN_xAs_{1-x} using a 3-band $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian, describing the coupling of the lowest energy CB to the light-hole (LH) VB, and the coupling of the CB to a resonant N-related impurity state via a composition dependent band-anticrossing (BAC) interaction [1], [4].

Our calculation of the BTBT transmission coefficient is carried out using the Wentzel-Kramers-Brillouin (WKB) approximation, whereby the transmission at wave vector $\mathbf{k}_\perp$ in the plane perpendicular to the (001) direction is computed, for an applied electric field having strength F along (001), as [5]

$$T(\mathbf{k}_\perp) = \exp\left(-\frac{2}{eF}\int_{E_{\rm LH}(\mathbf{k}_\perp)}^{E_{\rm CB}(\mathbf{k}_\perp)} \kappa(E,\mathbf{k}_\perp)\,{\rm d}E\right), \quad (1)$$

where $E_{\rm LH}(\mathbf{k}_\perp)$ and $E_{\rm CB}(\mathbf{k}_\perp)$ describe the VB and CB edge dispersion, and $\kappa(E,\mathbf{k}_\perp)$ is the complex band linking the CB and VB. The calculation of the BTBT current density J for an applied voltage V proceeds by integrating Eq. (1) with respect to $\mathbf{k}_\perp$ and energy E (the upper limit on the energy integral being $eV - E_g(\mathbf{k}_\perp)$, where $E_g(\mathbf{k}_\perp) = E_{\rm CB}(\mathbf{k}_\perp) - E_{\rm LH}(\mathbf{k}_\perp)$ is the band gap at in-plane wave vector $\mathbf{k}_\perp$). We numerically evaluate Eq. (1) without commonly-employed approximations that neglect aspects of the impact of the CB and VB edge DOS [5]–[7]. For the calculations described below we consider a junction width of 90 nm and applied fields $F = 50$ kV cm^{-1} and 1 MV cm^{-1} – i.e. voltage drops $V = 0.45$ and 9 V.

III. Results

Figure 1(a) shows the CBS of InN_xAs_{1-x} (solid lines) and $InAs_{1-y}Sb_y$ (dashed lines) alloys having $E_g = 0.257$ eV (≈ 4.8 μm). From Eq. (1), $T(\mathbf{k}_\perp) = \exp\left(-\frac{2A(\mathbf{k}_\perp)}{eF}\right)$, where $A(\mathbf{k}_\perp)$ is the area bounded in the complex plane by $\kappa(E,\mathbf{k}_\perp)$. Comparing the two CBSs we note (i) that $\kappa(E,0)$ bounds a greater area in the complex plane in InN_xAs_{1-x}, a result of (ii) an increase in the band edge effective masses in InN_xAs_{1-x} due to the BAC interaction. The N-induced changes (i) and (ii) to the CBS have competing impact on BTBT. (i) increases $A(\mathbf{k}_\perp)$ at small $k_\perp$, acting to decrease T (and hence J). (ii) decreases $E_g(\mathbf{k}_\perp)$ at fixed $k_\perp$, which is equal to the difference in energy between the limits of integration in Eq. (1). This limits the growth of $A(\mathbf{k}_\perp)$ with increasing $k_\perp$, acting to

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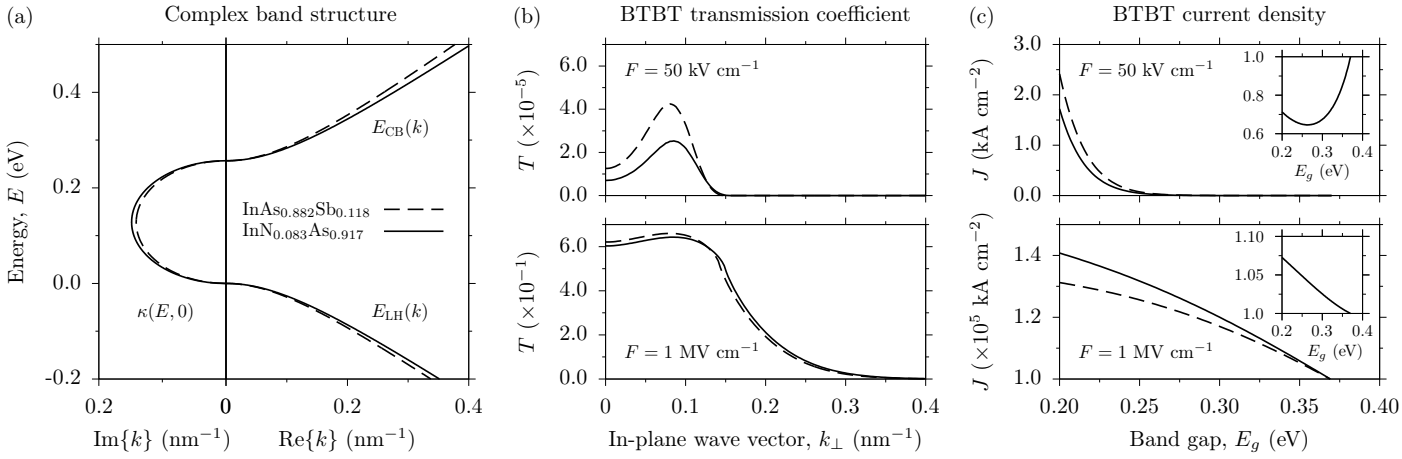

Fig. 1. (a) CBS of $\rm InN_{0.083}As_{0.917}$ (solid lines) and $\rm InAs_{0.882}Sb_{0.118}$ (dashed lines) alloys having band gap $E_g = 0.257$ eV at $k_\perp = 0$. In both cases the zero of energy is taken at the VB edge. (b) BTBT transmission coefficient T as a function of in-plane wave vector $k_\perp$ for $\rm InN_{0.083}As_{0.917}$ (solid lines) and $\rm InAs_{0.882}Sb_{0.118}$ (dashed lines) alloys, for applied electric fields $F = 50$ kV $\rm cm^{-1}$ (upper panel) and 1 MV $\rm cm^{-1}$ (lower panel). (c) BTBT current density J as a function of the $k_\perp = 0$ band gap E_g for $\rm InN_xAs_{1-x}$ (solid lines) and $\rm InAs_{1-y}Sb_y$ (dashed lines), for applied electric fields $F = 50$ kV $\rm cm^{-1}$ (upper panel) and 1 MV $\rm cm^{-1}$ (lower panel). The inset in each panel shows the ratio of the $\rm InN_xAs_{1-x}$ current density to that of $\rm InAs_{1-y}Sb_y$.

increase T (and hence J), and describing that the N-induced increase in the CB and VB edge DOS in $\rm InN_xAs_{1-x}$ makes more carriers available to contribute to BTBT.

The impact of the N-induced modifications of the CBS on T are shown in Fig. 1(b) where we compare the cases of low ($F = 50$ kV $\rm cm^{-1}$; upper panel) and high ($F = 1$ MV $\rm cm^{-1}$; lower panel) applied fields. At low F (i) dominates over (ii), leading to a significantly reduced transmission coefficient in $\rm InN_xAs_{1-x}$. Conversely, at higher F (ii) acts to produce higher T at large $k_\perp$ in $\rm InN_xAs_{1-x}$, leading to little difference in T between the two alloys. The implications of this field-dependent interplay of N-related band structure effects on the BTBT current density J are shown in Fig. 1(c). Here, J is calculated as a function of band gap E_g for $\rm InN_xAs_{1-x}$ (solid lines) and $\rm InAs_{1-y}Sb_y$ (dashed lines), with E_g reducing via N or Sb incorporation. At low F, J tends to remain low as E_g is reduced to 0.25 eV, beyond which point it increases exponentially. In this low-field regime N incorporation significantly reduces J at fixed E_g, with the ratio of J in $\rm InN_xAs_{1-x}$ to that in $\rm InAs_{1-y}Sb_y$ (cf. upper panel inset) reaching a minimum value of 0.65 at $E_g = 0.264$ eV. At high F, J in $\rm InN_xAs_{1-x}$ is comparable to, but slightly exceeds, that in $\rm InAs_{1-y}Sb_y$ at fixed E_g, a consequence of the small difference in T between the two alloys, and the N-induced increase of the CB and VB edge DOS making more carriers available to contribute to BTBT at the larger range of $k_\perp$ from which carriers originate at high F.

IV. Conclusion

We have undertaken a theoretical analysis of BTBT in narrow-gap dilute nitride HMAs. We find that BTBT in $\rm InN_xAs_{1-x}$ and related HMAs is governed by a field-dependent interplay between the impact of N incorporation on the CBS and on the CB edge DOS. Comparative analysis for highly-mismatched $\rm InN_xAs_{1-x}$ and conventional $\rm InAs_{1-y}Sb_y$ alloys identified two distinct regimes. For low applied fields the N-induced modification of the CBS in $\rm InN_xAs_{1-x}$ decreases the inter-band transmission coefficient, leading to reduced BTBT current density at fixed band gap. For high applied fields the N-induced increase in the CB edge DOS makes more states available to contribute to BTBT in $\rm InN_xAs_{1-x}$, counteracting the N-induced modification of the CBS and leading to approximately equal BTBT current density at fixed band gap as in $\rm InAs_{1-y}Sb_y$.

Overall, our analysis suggests that the development of mid-infared photodiodes based on $\rm InN_xAs_{1-x}$ and related HMAs is unlikely to lead to devices displaying significantly reduced dark currents. However, given that HMAs can in general provide access to longer wavelengths at fixed lattice mismatch compared to conventional alloys, it is possible that HMAs can nonetheless play an important role in enabling the development of mid-infrared photodetectors at wavelengths which are challenging to access using conventional semiconductor materials.

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