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Dilute bismide alloys grown on GaAs and InP substrates for improved near- and mid-infrared semiconductor lasers

Christopher A. Broderick[1,*], Wanshu Xiong[1], Stephen J. Sweeney[2], Eoin P. O'Reilly[3,4], and Judy M. Rorison[1,†]

[1]*Department of Electrical and Electronic Engineering, University of Bristol, Bristol BS8 1UB, U.K.*

[2]*Advanced Technology Institute and Department of Physics, University of Surrey, Guildford GU2 7XH, U.K.*

[3]*Tyndall National Institute, Lee Maltings, Dyke Parade, Cork, Ireland*

[4]*Department of Physics, University College Cork, Cork, Ireland*

e-mail: [*]`christopher.broderick@bristol.ac.uk`, [†]`judy.rorison@bristol.ac.uk`

ABSTRACT

We present an analysis of dilute bismide quantum well (QW) lasers grown on GaAs and InP substrates. Our theoretical analysis is based upon a 12-band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian which directly incorporates the strong impact of Bi incorporation on the band structure using a band-anticrossing approach. For GaBiAs QWs grown on GaAs we analyse the device performance as a function of Bi composition, and quantify the potential to use GaBiAs alloys to realise highly efficient, temperature stable 1.55 μm lasers. We compare our calculations to measured spontaneous emission (SE) and gain spectra for first-generation GaBiAs lasers and demonstrate quantitative agreement between theory and experiment. We also present a theoretical analysis of InGaBiAs alloys grown on InP substrates. We show that this material system is well suited to the development of mid-infrared lasers, and offers the potential to realise highly efficient InP-based diode lasers incorporating type-I QWs and emitting at > 3 μm. We quantify the theoretical performance of this new class of mid-infrared lasers, and identify optimised structures for emission across the application-rich $3 - 5$ μm wavelength range. Our results highlight and quantify the potential of dilute bismide alloys to overcome several limitations associated with existing GaAs- and InP-based near- and mid-infrared laser technologies.

Keywords: *Highly-mismatched semiconductors, dilute bismide alloys, long-wavelength semiconductor lasers*

1. INTRODUCTION

Interest in dilute bismide alloys – in which a small fraction of the group-V atoms in a conventional III-V semiconductor are replaced by bismuth (Bi) – has been steadily increasing in recent years. The growing interest in these "highly-mismatched" materials is due to fundamental interest in the unusual properties of dilute bismide alloys, as well as their potential for specific device applications. Of particular interest is the exploitation of the effects of Bi incorporation to facilitate band structure engineering in semiconductor lasers [1]–[4].

The replacement of As by Bi to form the GaBiAs alloy causes a rapid reduction of the band gap (E_g) and increase of the spin-orbit-splitting energy (Δ_{SO}), both of which are characterised by strong, composition-dependent bowing arising from the impurity-like behaviour of substitutional Bi atoms, as shown in Fig. 1 (left). Incorporation of $> 10\%$ Bi in GaBiAs produces a band structure in which $\Delta_{\mathrm{SO}} > E_g$. This offers the possibility to suppress the non-radiative (Auger) recombination and inter-valence band absorption (IVBA) loss mechanisms involving the spin-split-off band, which dominate the threshold current and degrade the temperature stability of conventional InP-based QW lasers operating at telecommunication wavelengths [2], [3]. The suppression of the "CHSH" Auger recombination process in this manner is depicted schematically in Fig. 1 (right).

Despite challenges associated with the growth of Bi-containing alloys, significant progress has been made towards developing dilute bismide materials and devices. Refinement of growth techniques has led to the development of electrically pumped GaAs-based dilute bismide QW lasers [7] which, from a theoretical perspective, has mandated the development of models of the electronic and optical properties of Bi-containing nanostructures. Here, we (i) provide an overview of the theoretical approach we have developed to study dilute bismide materials and semiconductor lasers [5], [6], (ii) identify key trends relating to the impact of Bi incorporation on the properties of GaAs- and InP-based dilute bismide QW lasers [6], (iii) identify optimised laser structures for emission across a wide range of wavelengths in the near- and mid-infrared [6], [8], and (iv) demonstrate how Bi incorporation can be exploited to deliver highly efficient near- and mid-infrared semiconductor lasers grown respectively on GaAs and InP substrates. We compare the results of our theoretical calculations directly to measurements of the SE and gain spectra performed on first-generation GaAs-based dilute bismide QW lasers and demonstrate quantitative agreement between theory and experiment, thereby verifying the accuracy of our theoretical model of the optical properties and highlighting its potential for use in the design and optimisation of dilute bismide materials and devices for a range of applications [9].

2. THEORETICAL MODEL

Our theoretical description of the (In)GaBiAs band structure is based on a 12-band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian which we have derived directly using atomistic supercell calculations [5]. This extended basis set Hamiltonian directly
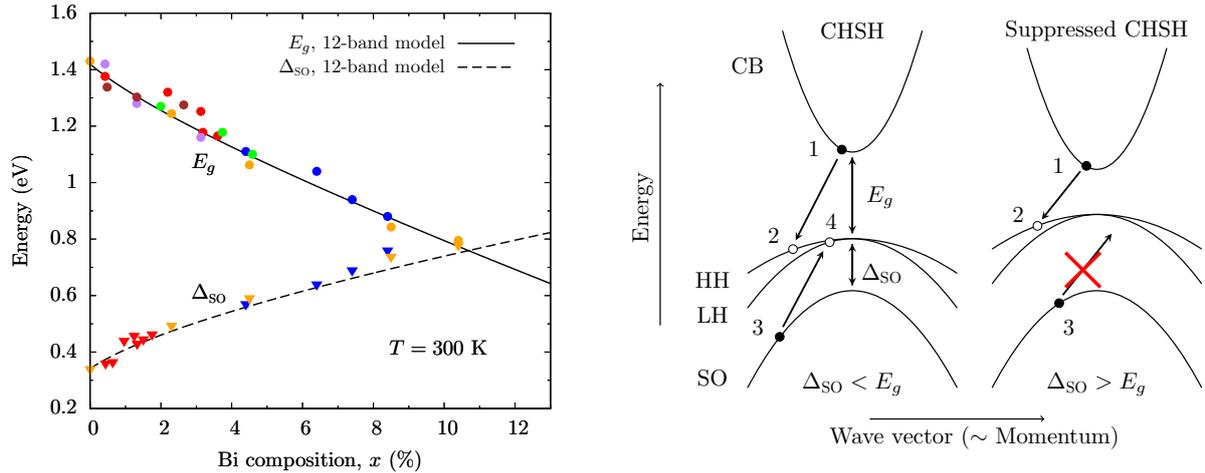
*Figure 1: Left – Measured variation of the band gap (E_g; closed circles) and spin-orbit-splitting energy (Δ_{SO}; closed triangles) as a function of Bi composition x in GaBi$_x$As$_{1-x}$. Solid and dashed black lines show, respectively, the variation of E_g and Δ_{SO} with x calculated using an extended basis set 12-band **k·p** Hamiltonian [5], [6]. Right – Schematic illustration of the suppression of the CHSH Auger recombination process described in the text [1]–[3]: when $\Delta_{SO} > E_g$, as in GaBi$_x$As$_{1-x}$ with $x > 10\%$, there is insufficient energy made available by a recombining electron-hole pair (1,2) to promote a valence electron from the spin-split-off (SO) band (3) to a light- or heavy-hole (LH or HH) valence band edge state (4).*

incorporates Bi composition-dependent band-anticrossing interactions between the valence band edge states of the (In)GaAs host matrix and localised Bi-related impurity states. Having been obtained directly on the basis of ordered alloy supercell calculations [5], the parameters describing the impact of Bi incorporation on the band structure have been constrained and refined by comparing the band offsets and transition energies calculated using the 12-band Hamiltonian to the results of polarisation-resolved photovoltage measurements performed on a series of GaBiAs/(Al)GaAs QW laser structures [10]. Key to our calculation of the performance of dilute bismide laser structures is the direct use of the eigenstates of the 12-band Hamiltonian in the computation of the optical properties, so that our theoretical model explicitly includes the impact of key band structure effects such as band mixing brought about by Bi-induced hybridisation of valence states and pseudomorphic strain [6]. For mid-infrared emitting materials and QW lasers grown on InP substrates we have extended our model for GaBiAs to treat pseudomorphically strained InGaBiAs alloys, by including parameterisation of the effects on the alloy band structure of co-alloying of In and Bi into an InGaAs host matrix [11]. Full details of the theoretical model we have developed for dilute bismide QW lasers can be found in Ref. [6].

3. RESULTS

A. GaAs-based dilute bismide alloys and near-infrared semiconductor lasers

We have used our theoretical model to identify and quantify trends in the performance of ideal GaBi$_x$As$_{1-x}$/(Al)-GaAs QW lasers as a function of Bi composition x. Our calculations indicate that Al incorporation in the barrier layers is required for Bi compositions $x < 6\%$ in order to mitigate the low GaBi$_x$As$_{1-x}$/GaAs conduction band offset and bring about appreciable material gain. This leads to a trade-off between the carrier and optical confinement, which can be engineered to minimise the threshold current density [6]. The results of this analysis at low Bi composition ($x \approx 2\%$) are summarised in Fig. 2 (left). As x is increased, the beneficial effects of compressive strain on the band structure dominate. We calculate that ideal GaBi$_x$As$_{1-x}$ QWs designed to emit at 1.55 μm ($x \approx 13\%$) have intrinsically superior gain characteristics than at lower x – leading to reduced threshold carrier densities and enhanced differential gain – as a result of (i) improved carrier confinement, and (ii) a strong reduction in the density of states at the valence band edge, brought about respectively by the increased conduction band offset and compressive strain in QWs with $x > 10\%$. The calculated improvement in the modal and differential gain in ideal GaBi$_x$As$_{1-x}$ QWs at $x > 10\%$ is shown in Fig. 2 (right) [6].

We have also performed a detailed comparison between theory and experiment for GaBi$_x$As$_{1-x}$/(Al)GaAs QW lasers at low x [9]. For the experimental analysis, multi-section devices were fabricated and measurements of the SE and optical gain spectra were undertaken using the segmented contact method. By comparing the measured and calculated SE spectra, we have determined that (i) the spectral broadening is well described using a hyperbolic secant lineshape, and (ii) the large spectral linewidth, $\delta = 25$ meV, is relatively independent of temperature, indicating strong inhomogeneous broadening associated with Bi-related alloy disorder [6], [10]. For this comparison the theoretical SE and gain spectra were computed directly for the laser structure [6], and the internal (cavity) losses were extracted from optical absorption measurements [9]. The SE and gain spectra calculated using our theoretical model are in quantitative agreement with experiment across a wide range of current densities, as well as for a range of multi-section and Fabry-Perot devices [9], confirming the predictive capability of the theoretical model we have developed for dilute bismide QW lasers.
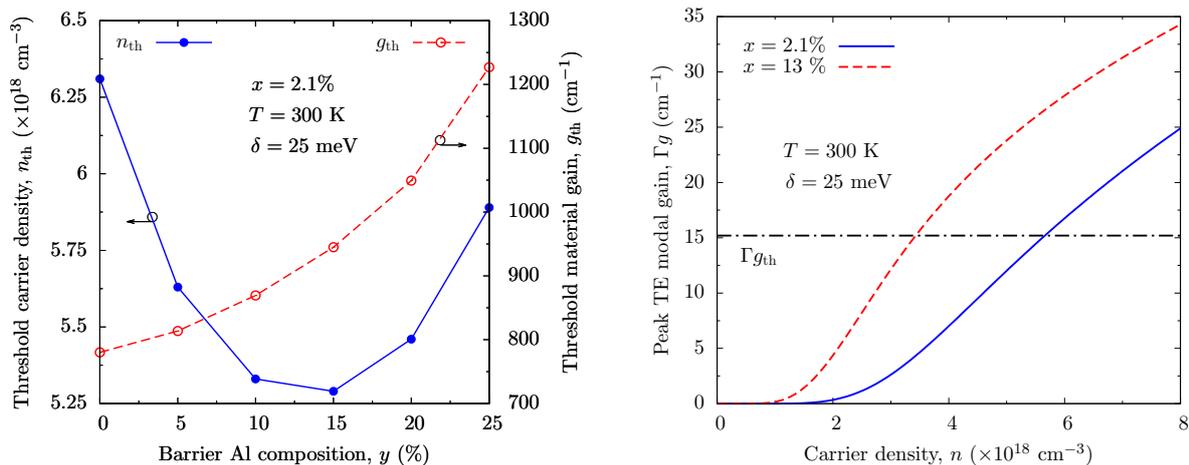
Figure 2: Left – Optimisation of threshold carrier density (closed blue circles) in GaBi$_{0.021}$As$_{0.979}$ QWs having Al$_y$Ga$_{1-y}$As barriers, by varying y to control the trade-off between the carrier and optical confinement [6]. The calculated variation of the threshold material gain is also shown (open red circles). Right – Calculated modal gain as a function of carrier density for GaBi$_{0.021}$As$_{0.979}$/AlGaAs (solid blue line) and GaBi$_{0.13}$As$_{0.87}$/GaAs (dashed red line) QWs, with the latter designed to emit at 1.55 μm. Despite reduced optical confinement at longer wavelengths, the QW with higher Bi composition has improved gain characteristics due to enhanced carrier confinement and the impact of compressive strain on the band structure [6].

B. InP-based dilute bismide alloys and mid-infrared semiconductor lasers

We have used our theoretical model to analyse the band structure of InGaBiAs alloys grown on InP. The results of this analysis are summarised in Fig. 3 (left), where the dashed black, solid blue and solid red lines denote, respectively, alloy compositions for which the in-plane strain, band gap, and difference between the band gap and spin-orbit-splitting energy are constant. Alloys lying above the $E_g = \Delta_{SO}$ contour have $\Delta_{SO} > E_g$, so that the dominant Auger and IVBA loss mechanisms are suppressed [12]. Our analysis indicates that emission at wavelengths > 3 μm can be achieved for modest Bi compositions ($\approx$ 5%) and compressive strains (< 1.5%) [11]–[13]. Our calculations further predict that alloys with $\Delta_{SO} > E_g$ have large type-I band offsets with respect to unstrained InGaAs. InGaBiAs QWs should therefore – in addition to enabling suppression of the dominant Auger recombination and IVBA mechanisms – mitigate carrier leakage, and hence provide efficient, temperature stable laser operation without the need to resort to complicated cascade structures, or metamorphic, type-II or Sb-containing QWs, to facilitate the growth on InP of heterostructures emitting at > 3 μm [8].

We have also performed a systematic analysis of InGaBiAs QW lasers designed to emit at 3 – 5 μm [8]. The available parameter space for the design of such structures is extremely large, encompassing wide ranges of alloy compositions, QW thicknesses and epitaxial strains. In order to facilitate the identification of trends in the device performance we have restricted our attention at each wavelength to two sets of laser structures, having: (i) variable QW thickness and fixed strain, and (ii) variable strain and fixed QW thickness. In this manner we are able to directly identify key material trends and their contribution to the overall device performance, and also to quantify the potential to use alloy, heterostructure and strain engineering to optimise the laser performance at a given wavelength. In particular, we focus on the gain characteristics in order to optimise the carrier density and differential gain at threshold – which we seek to minimise and maximise, respectively – and on this basis identify laser structures that should deliver high-speed performance at low injection currents. Figure 3 (right) shows an example of the calculated variation of the sheet carrier density and differential gain at threshold for a series of 1.5% compressively strained InGaBiAs QW laser structures designed to emit at 3.5 μm, demonstrating (i) the potential of InGaBiAs alloys to deliver high performance mid-infrared laser diodes, and (ii) that there is much scope for optimisation of the properties and performance of this class of laser structures [8].

4. SUMMARY AND CONCLUSIONS

We have developed a detailed theoretical approach to study the electronic and optical properties of dilute bismide alloys, and have applied our model to analyse the performance of near- and mid-infrared dilute bismide QW lasers grown respectively on GaAs and InP substrates. Our analysis has (i) elucidated the impact of Bi incorporation on the electronic and optical properties, (ii) identified and quantified key trends in the performance of ideal devices as a function of Bi composition, and (iii) provided guidelines for the development of optimised devices emitting across a wide range of wavelengths. We have also compared the results of our calculations to experimental measurements of the SE and optical gain spectra performed on first-generation GaBiAs devices (the first such measurements and comparison for this emerging class of semiconductor alloys). Our calculations are in quantitative agreement with experiment, validating our theoretical approach and demonstrating its applicability to the analysis and design of future photonic and photovoltaic devices incorporating dilute bismide alloys.

As well as confirming the promise of GaBiAs alloys for the development of highly efficient 1.55 μm GaAs-based lasers, our analysis indicates that InGaBiAs alloys can be used to realise type-I QWs emitting

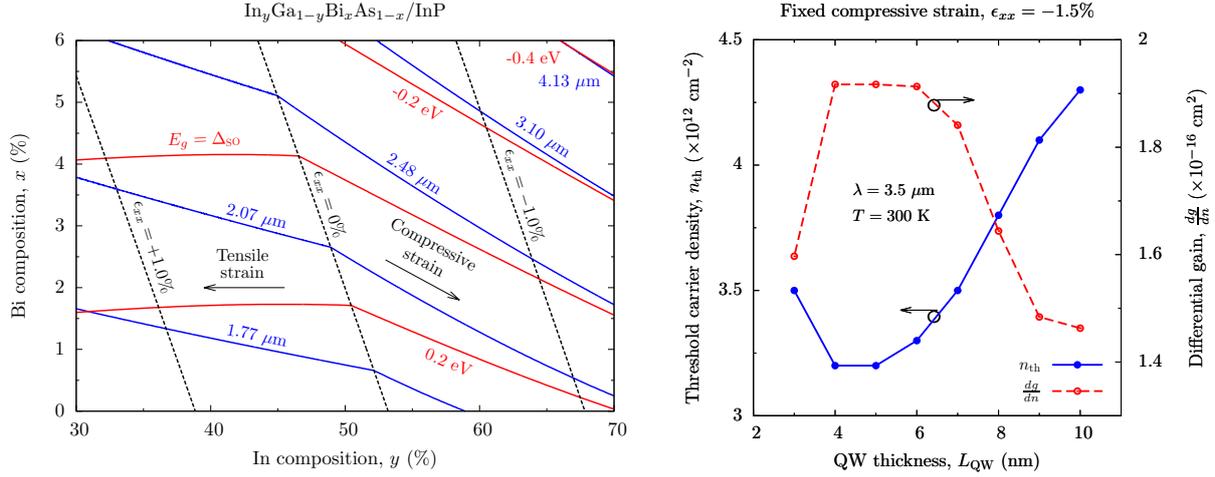*Figure 3: Left – Composition space map showing the variation of the strain (ϵ_{xx}; dashed black lines), band gap (E_g; solid blue lines), and difference between the band gap and spin-orbit-splitting energy ($E_g - \Delta_{SO}$; solid red lines), for $In_yGa_{1-y}Bi_xAs_{1-x}$ alloys grown pseudomophically on InP. Right – Variation of the sheet carrier density (n_{th}; closed blue circles) and differential gain ($\frac{dg}{dn}$; open red circles) at threshold as a function of QW thickness for a series InGaBiAs laser structures designed to emit at 3.5 μm. The InGaBiAs QW alloy compositions were chosen to ensure that (i) the QWs are under 1.5% compressive strain, and (ii) their band structure has $\Delta_{SO} > E_g$ to facilitate Auger and IVBA suppression [8].*

at wavelengths > 3 μm on InP, thereby promising to overcome several limitations associated with current approaches to achieving mid-infrared emission using InP substrates. Overall, our analysis highlights the potential to exploit the impact of Bi incorporation on the (In)GaAs band structure to overcome a number of key limitations associated with existing GaAs- and InP-based near- and mid-infrared semiconductor lasers. Continued work on dilute bismide alloys is therefore expected to deliver a new generation of semiconductor light-emitting devices demonstrating improved performance across a wide range of technologically important wavelengths.

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