Strain-balanced type-II superlattices on GaAs: novel heterostructures for photonics and photovoltaics

Christopher A. Broderick[1,2,*], Wanshu Xiong[2], Shirong Jin[3], Igor P. Marko[3], Zoe L. Bushell[3], Konstanze Hild[3], Peter Ludewig[4], Wolfgang Stolz[4], Kerstin Volz[4], Judy M. Rorison[2], Stephen J. Sweeney[3], and Eoin P. O'Reilly[1,5]

[1]Tyndall National Institute, Lee Maltings, Dyke Parade, Cork T12 R5CP, Ireland
[2]Department of Electrical and Electronic Engineering, University of Bristol, Bristol BS8 1UB, U.K.
[3]Advanced Technology Institute and Department of Physics, University of Surrey, Guildford GU2 7XH, U.K.
[4]Materials Science Center and Faculty of Physics, Philipps-Universität Marburg, 35032 Marburg, Germany
[5]Department of Physics, University College Cork, Cork T12 YN60, Ireland

Abstract—**We present a theoretical analysis of the optoelectronic properties of type-II $GaAs_{1-x}Bi_x/GaN_yAs_{1-y}$ quantum wells (QWs) grown on GaAs substrates. We eludicate the broad scope for band structure engineering in these novel heterostructures, demonstrating that they offer emission and absorption out to mid-infrared wavelengths in structures which can be grown with little or no net strain relative to GaAs. We confirm our analysis by comparing to experiments on a prototype $GaAs_{0.967}Bi_{0.033}/GaN_{0.062}As_{0.938}$ structure, which show room temperature photoluminescence (PL) and absorption at a wavelength of 1.72 μm (one of the longest achieved to date from a pseudomorphic GaAs-based heterostructure). Overall, we demonstrate that this new class of type-II QWs has significant promise for (i) extending the wavelength range accessible to the GaAs material platform, and (ii) the development of long-wavelength photonic devices and highly efficient solar cells.**

I. INTRODUCTION

Significant effort has been dedicated to developing long-wavelength photonic devices on GaAs substrates, in order to overcome the limitations associated with the InP and GaSb material platforms upon which existing technologies are traditionally based. These efforts have been driven by the superior properties of GaAs-based materials and the potential to exploit vertical-cavity architectures, and have included the development of quantum dots, dilute nitride, metamorphic and, more recently, dilute bismide heterostructures. While these approaches have had varying degrees of success, their limitations have prevented widespread adoption and there remains a need to develop GaAs-based devices at and beyond 1.55 μm.

In parallel, significant advances have been made in the development of high-efficiency photovoltaics based on multi-junction solar cells (MJSCs). While these advances have been enabled by combinations of III-V alloys having both tunable band gaps and small lattice mismatch with respect to GaAs, the requirement for these properties constrains the development of new approaches to drive towards and beyond 50% efficiency in MJSCs. This has created a strong need for new material concepts offering tunable band structures in addition to being compatible with growth on GaAs (or Ge) substrates.

We have recently proposed and demonstrated [1] that type-II $GaAs_{1-x}Bi_x/GaN_yAs_{1-y}$ QWs – based on the highly-mismatched dilute bismide and nitride alloys $GaAs_{1-x}Bi_x$ and GaN_yAs_{1-y} – are a promising new class of GaAs-based heterostructures for the development of near- and mid-infrared photonic devices, supplementing their noted potential for applications in photovoltaics [2]. We take advantage of recent developments in the theory of dilute bismide heterostructures [3] to quantitatively (i) elucidate the properties and potential of $GaAs_{1-x}Bi_x/GaN_yAs_{1-y}$ type-II QWs for applications in semiconductor lasers and MJSCs, (ii) provide strict criteria for the growth of structures which are strain-balanced with respect to GaAs, and (iii) outline the design of structures having optimised optical emission/absorption across a broad spectral range.

Our analysis is validated by comparison to experimental measurements performed on a prototype $GaAs_{0.967}Bi_{0.033}/GaN_{0.062}As_{0.938}$ structure; the first growth and demonstration of this new class of QWs [1]. Experimental analysis verifies that this prototype structure has high structural quality, in addition to observable PL and optical absorption at a long wavelength of 1.72 μm at room temperature, in good agreement with theory. Overall, our analysis quantifies the potential of this new class of QW heterostructures for applications in photonics and photovoltaics, and outlines routes towards the development of optimised device structures.

II. RESULTS

Incorporation of dilute concentrations of N in GaAs is known to strongly perturb the conduction band (CB) structure, bringing about an extremely large reduction of the band gap and leading to large CB offsets in QW structures [4]. Similarly, incorporation of dilute concentrations of Bi is known to strongly perturb the valence band (VB), again bringing about a large band gap reduction but leading instead to large VB offsets [3], [4]. Furthermore, since N (Bi) is significantly smaller (larger) than the As atoms it replaces, GaN_yAs_{1-y} ($GaAs_{1-x}Bi_x$) alloys are under tensile (compressive) strain when grown pseudomorphically on GaAs. Combining these unique properties provides broad scope for band structure engineering, allowing for readily tunable band gaps and band offsets in a large number of strain-balanced configurations, covering a continuous spectral range starting below the GaAs band gap and extending into the mid-infrared [1].

This work was supported by Science Foundation Ireland (SFI; 15/IA/3082), and by the Engineering and Physical Sciences Research Council, U.K. (EPSRC; EP/K029665/1, EP/H005587/1 and EP/H050787/1).

*Email: `c.broderick@umail.ucc.ie`

978-1-5090-5323-0/17/$31.00 ©2017 IEEE

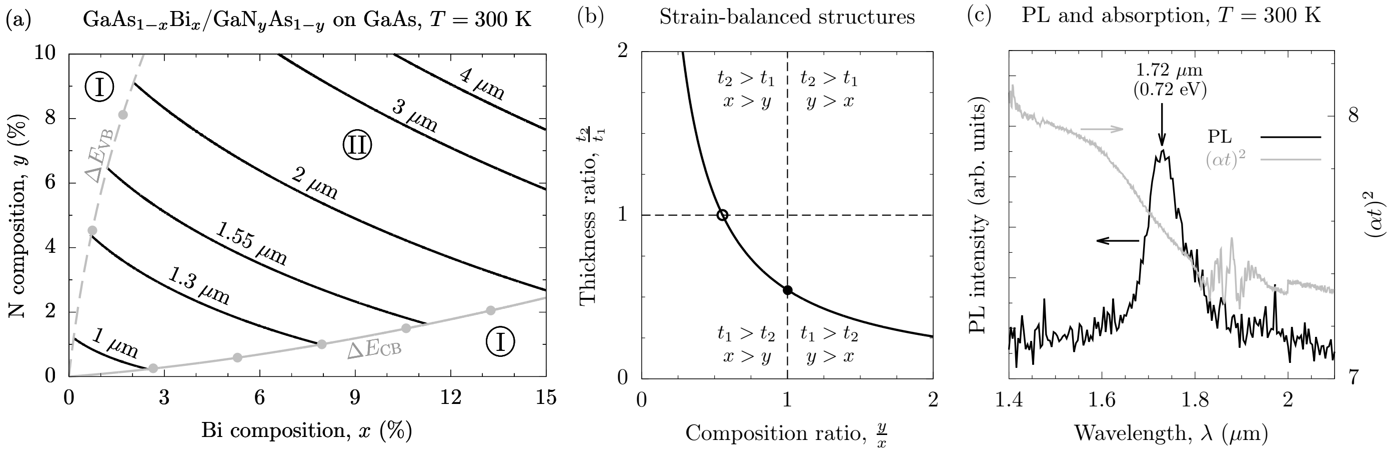

Fig. 1. (a) Composition space map describing the variation of the band gap and band offsets in $\mathrm{GaAs}_{1-x}\mathrm{Bi}_x/\mathrm{GaN}_y\mathrm{As}_{1-y}$ type-II QWs. The solid (dashed) grey line denotes Bi and N compositions x and y for which the CB (VB) offset ΔE_{CB} (ΔE_{VB}) is equal in the $\mathrm{GaAs}_{1-x}\mathrm{Bi}_x$ and $\mathrm{GaN}_y\mathrm{As}_{1-y}$ layers, describing the transition from a type-I (regions Ⓘ) to type-II (region Ⅱ) band gap. Black lines denote Bi and N compositions x and y for which the type-II band gap – between the $\mathrm{GaN}_y\mathrm{As}_{1-y}$ CB and $\mathrm{GaAs}_{1-x}\mathrm{Bi}_x$ VB – is constant, showing that long-wavelength emission/absorption can be readily achieved. (b) Criteria for the growth of strain-balanced structures: the thicknesses t_1 and t_2 and alloy compositions x and y of adjacent $\mathrm{GaAs}_{1-x}\mathrm{Bi}_x$ and $\mathrm{GaN}_y\mathrm{As}_{1-y}$ layers must lie on or close to the curve described by the solid line, in order to achieve a strain-balanced structure. (c) Experimental measurements of the room temperature PL and absorption spectra undertaken on a prototype structure containing five repeats of a strain-compensated $\mathrm{GaAs}_{0.967}\mathrm{Bi}_{0.033}/\mathrm{GaN}_{0.062}\mathrm{As}_{0.938}$ type-II QW [1].

The composition space map shown in Fig. 1(a) describes that $\mathrm{GaAs}_{1-x}\mathrm{Bi}_x/\mathrm{GaN}_y\mathrm{As}_{1-y}$ QWs can be grown having type-I or -II band offsets (in the composition regions denoted by Ⓘ and Ⅱ, respectively) with long emission/absorption wavelengths achievable across a wide range of alloy compositions and epitaxial strains (black lines describe compositions for which the type-II band gap, between the $\mathrm{GaN}_y\mathrm{As}_{1-y}$ CB and $\mathrm{GaAs}_{1-x}\mathrm{Bi}_x$ VB, is constant). Furthermore, this can be achieved in QWs having large CB and VB offsets (the solid (dashed) grey line denotes alloy compositions for which the CB (VB) offset is equal in $\mathrm{GaN}_y\mathrm{As}_{1-y}$ and $\mathrm{GaAs}_{1-x}\mathrm{Bi}_x$, with closed grey circles denoting 50 meV increases in the respective band offsets starting from zero at $x = y = 0$). The large design space offered by $\mathrm{GaAs}_{1-x}\mathrm{Bi}_x/\mathrm{GaN}_y\mathrm{As}_{1-y}$ QWs also provides significant freedom to engineer the radiative and non-radiative carrier recombination rates for specific applications.

Analysis of the structural properties of pseudomorphically strained $\mathrm{GaAs}_{1-x}\mathrm{Bi}_x/\mathrm{GaN}_y\mathrm{As}_{1-y}$ QWs shows that, for a given emission/absorption wavelength, a wide range of structures can be grown which are strain-balanced with respect to a GaAs substrate [1]. A simple relationship can be obtained between the layer thicknesses and alloy compositions required to achieve strain-balanced structures: the layer thickness and composition ratios for a strain-balanced structure must lie on or close to the solid black line in Fig. 1(b). The ability to precisely design strain-balanced QWs allows for the growth of superlattices which are unencumbered by strain-thickness limitations, providing enhanced material/structural quality and large active volumes for light emission/absorption [1].

Fig. 1(c) shows measurements of the room temperature PL (black line) and optical absorption (grey line) undertaken on an MOVPE-grown $\mathrm{GaAs}_{0.967}\mathrm{Bi}_{0.033}/\mathrm{GaN}_{0.062}\mathrm{As}_{0.938}$ prototype QW structure, demonstrating light emission/absorption at a wavelength of 1.72 μm – 0.72 eV, in good agreement with the calculated transition energy of 0.74 eV – one of the longest obtained from a pseudomorphic GaAs-based heterostructure.

III. CONCLUSION

We have presented a theoretical analysis of the optoelectronic properties of $\mathrm{GaAs}_{1-x}\mathrm{Bi}_x/\mathrm{GaN}_y\mathrm{As}_{1-y}$ type-II QWs grown on GaAs substrates. Our analysis has elucidated the unique properties of this new class of GaAs-based heterostructures, demonstrating that they offer the potential to achieve optical emission/absorption out to mid-infrared wavelengths in structures that can be grown with no net strain with respect to a GaAs substrate. Based on our analysis we have (i) described the combinations of layer compositions, thicknesses and strains required to achieve emission/absorption at specific wavelengths, (ii) provided strict criteria for the growth of strain-balanced structures, and (iii) identified routes to optimising structures for applications in semiconductor lasers and MJSCs. Our analysis has been validated by experimental measurements performed on an MOVPE-grown prototype structure, highlighting that $\mathrm{GaAs}_{1-x}\mathrm{Bi}_x/\mathrm{GaN}_y\mathrm{As}_{1-y}$ type-II QWs offer broad scope for band structure engineering and significant promise as a new platform for the development of future photonic and photovoltaic devices.

REFERENCES

[1] C. A. Broderick, S. R. Jin, I. P. Marko, K. Hild, P. Ludewig, Z. L. Bushell, W. Stolz, J. M. Rorison, E. P. O'Reilly, K. Volz, and S. J. Sweeney, "$\mathrm{GaAs}_{1-x}\mathrm{Bi}_x/\mathrm{GaN}_y\mathrm{As}_{1-y}$ type-II quantum wells: novel strain-balanced heterostructures for GaAs-based near- and mid-infrared photonics," *Sci. Rep.*, in press, 2017.

[2] J. Hwang and J. D. Phillips, "Band structure of strain-balanced GaAsBi/GaAsN superlattices on GaAs," *Phys. Rev. B*, vol. 83, p. 195327, 2011.

[3] C. A. Broderick, P. E. Harnedy, and E. P. O'Reilly, "Theory of the electronic and optical properties of dilute bismide quantum well lasers," *IEEE J. Sel. Top. Quantum Electron.*, vol. 21, p. 1503313, 2015.

[4] C. A. Broderick, M. Usman, S. J. Sweeney, and E. P. O'Reilly, "Band engineering in dilute nitride and bismide semiconductor lasers," *Semicond. Sci. Technol.*, vol. 27, p. 094011, 2012.