Strain-balanced $GaAs_{1-x}Bi_x/GaN_yAs_{1-y}$ W-type quantum wells for GaAs-based 1.3–1.6 μm lasers

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***Abstract*—Highly-mismatched alloys constitute a promising approach to extend the operational range of GaAs-based quantum well (QW) lasers to telecom wavelengths. This is challenging using type-I QWs due to the difficulty to incorporate sufficient N or Bi via epitaxial growth. To overcome this, we investigate a novel class of strain-compensated type-II QWs combining electron-confining, tensile strained GaN_yAs_{1-y} and hole-confining, compressively strained $GaAs_{1-x}Bi_x$ layers. We systematically analyse the optoelectronic properties of W-type $GaAs_{1-x}Bi_x/GaN_yAs_{1-y}$ QWs, and identify paths to optimise their threshold characteristics. Solving the multi-band k·p Schrödinger equation self-consistently with Poisson's equation highlights the importance of electrostatic confinement in determining the optical and differential gain of these QWs. Our calculations demonstrate that $GaAs_{1-x}Bi_x/GaN_yAs_{1-y}$ QWs offer broad scope for band structure engineering, with W-type structures presenting the possibility to combine high long-wavelength gain with the intrinsically low non-radiative Auger recombination rates of type-II QWs.**

I. Introduction

The performance of InP-based 1.3–1.6 μm lasers is impaired by the presence of strong non-radiative Auger recombination, which reduces efficiency and temperature stability. This persistent issue, linked fundamentally to the band structure of the materials forming the laser active region, has motivated several approaches to develop GaAs-based lasers with the aim of achieving highly efficient, temperature stable operation. One promising route to achieve this is the use of highly-mismatched dilute nitride (N-containing) and bismide (Bi-containing) alloys. The giant band gap reduction associated with N or Bi incorporation in (In)GaAs (cf. Fig. 1(a)) allows to reach 1.3–1.6 μm wavelengths in pseudomorphically strained QWs, while the increase in spin-orbit splitting energy in $GaAs_{1-x}Bi_x$ promises suppression of the dominant, hot hole-producing Auger recombination pathway in type-I QWs [1].

While progress has been made towards realising 1.3–1.6 μm GaAs-based dilute nitride and bismide QW lasers, achieving performance competitive with InP-based lasers has proved challenging due to the difficulty to incorporate sufficient N or Bi while maintaining low defect density in epitaxial growth. To overcome this, we investigate a novel class of type-II QWs which simultaneously exploit the band gap reduction of GaN_yAs_{1-y} and $GaAs_{1-x}Bi_x$ [2]. While N incorporation in GaAs strongly perturbs the conduction band (CB) structure, Bi incorporation strongly perturbs the valence band (VB) structure. The strong reduction (increase) in CB (VB) edge energy in GaN_yAs_{1-y} ($GaAs_{1-x}Bi_x$) provides strong confinement of electrons (holes), allowing to form so-called "W-type" QWs in which long emission wavelengths can be readily achieved [2], [3]. Auger recombination is expected to be intrinsically suppressed in type-II QWs [4], suggesting potential to design highly-efficient GaAs-based telecom lasers.

We present a systematic theoretical analysis of the properties and performance of 1.3–1.6 μm W-type QWs, in which a central hole-confining $GaAs_{1-x}Bi_x$ layer is surrounded by electron-confining GaN_yAs_{1-y} layers. Originally investigated for applications in mid-infrared emitters, W-type QWs are of increasing interest for telecom wavelengths due to the flexibility they offer to tune recombination rates and optimise performance. Compared to $In_xGa_{1-x}As/GaAs_{1-y}Sb_y$ W-type QWs [5], $GaAs_{1-x}Bi_x$ (GaN_yAs_{1-y}) is compressively (tensile) strained when grown on (001) GaAs, providing scope for strain engineering and to circumvent critical thickness limitations via strain compensation [2]. Our calculations reveal that strain and band gap/offset engineering of $GaAs_{1-x}Bi_x/GaN_yAs_{1-y}$ W-type QWs leads to impressive threshold characteristics, making this novel class of heterostructures a promising new approach to achieve the long-held goal of highly-efficient and temperature stable GaAs-based telecom lasers.

II. Theoretical model

Our theoretical analysis of the electronic and optical properties of type-II $GaAs_{1-x}Bi_x/GaAs_{1-y}N_y$ QWs is based on a 14-band **k**·**p** Hamiltonian and plane wave expansion method. This extended-basis Hamiltonian incorporates Bi (N) composition-dependent band-anticrossing interactions – fully parametrised via atomistic electronic structure calculations [6] – between the extended VB (CB) edge states of GaAs and localised Bi- (N-) related impurity states. To account for electrostatic confinement effects we compute the QW electronic structure self-consistently by solving the 14-band **k**·**p** Schrödinger (envelope function) equation coupled to Poisson's equation for the net electrostatic potential generated by injected electron and hole populations (under the assumptions of net charge neutrality and quasi-thermal equilibrium). The heterostructure eigenstates obtained from these self-consistent calculations are then employed directly to compute carrier density-dependent optical matrix elements, which are in turn employed to compute optical gain spectra and differential gain.

III. Results

$GaAs_{1-x}Bi_x/GaN_yAs_{1-y}$ type-II QWs provide broad scope for heterostructure design [2]. N and Bi incorporation allow to independently adjust the CB and VB offsets ΔE_{CB} and ΔE_{VB} in GaN_yAs_{1-y} and $GaAs_{1-x}Bi_x$ layers, respectively. To identify key trends, we select structures for

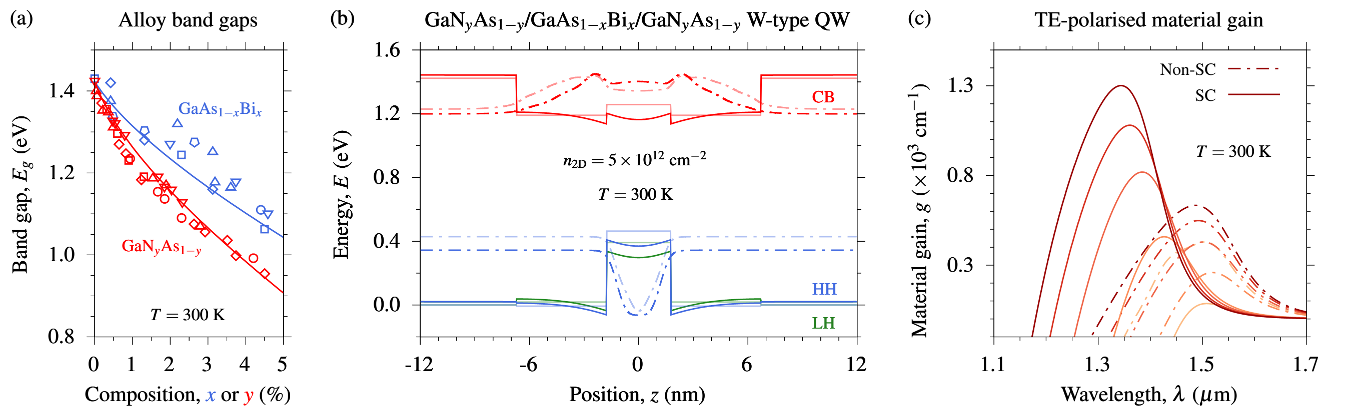

Fig. 1. (a) Calculated (lines) and measured (symbols) band gap vs. composition for $GaAs_{1-x}Bi_x$ (blue) and GaN_yAs_{1-y} (red) alloys grown pseudomorphically on (001) GaAs. (b) Band offsets of an exemplar strain-balanced 1.55 μm $GaN_yAs_{1-y}/GaAs_{1-x}Bi_x/GaN_yAs_{1-y}$ W-type QW having band offset ratio $\Delta E_{\text{VB}} = 2\,\Delta E_{\text{CB}}$, in the absence of injected carriers (light colours) and at an injected carrier density $n_{2D} = 5 \times 10^{12}$ cm^{-2} (full colours). (c) Non-self-consistent (dashed lines) and self-consistent (solid lines) calculated optical gain spectra at $n_{2D} = 2, 4, 6, 8$ and 10×10^{12} cm^{-2} (darkening colours) for the W-type QW of (b).

analysis by imposing two conditions. Firstly, we consider W-type QWs in which a central $GaAs_{1-x}Bi_x$ layer of thickness t_x is surrounded by GaN_yAs_{1-y} layers of thickness $\frac{t_y}{2}$ (total thickness t_y). Imposing strain balancing allows to relate the layer thickness ratio $\frac{t_y}{t_x}$ to the composition ratio $\frac{y}{x}$ [2]. Secondly, the Auger recombination rate in type-II QWs is a strong function of the VB to CB offset ratio $\frac{\Delta E_{\text{VB}}}{\Delta E_{\text{CB}}}$ [4]. Imposing a fixed band offset ratio, while requiring a specific emission wavelength, then allows to fully specify layer thicknesses and compositions. We analyse the performance of strain-balanced QWs having (i) fixed band offset ratio and variable thickness, and (ii) fixed thickness and variable band offset ratio.

In the presence of injected carriers, self-consistent (SC; Schrödinger-Poisson) calculations reveal that electrostatic attraction of electrons by strongly-confined holes in the central $GaAs_{1-x}Bi_x$ layer strongly enhances electron-hole spatial overlap (so-called "band bending"; cf. Fig. 1(b)). This high electron-hole overlap is facilitated by the chosen layer ordering: while the band gap reduction in GaN_yAs_{1-y} results almost entirely from a reduction in CB edge energy, in $GaAs_{1-x}Bi_x$ $\approx \frac{1}{3}$ of the band gap reduction results from a reduction in CB edge energy. At the composition ratios $x > y$ producing the large band offset ratios $\frac{\Delta E_{\text{VB}}}{\Delta E_{\text{CB}}} \approx$ 2–4 that minimise Auger recombination [4], this produces a low central CB potential barrier (cf. Fig. 1(b)), allowing significant penetration of electron probability density into the central $GaAs_{1-x}Bi_x$ layer.

As shown in Fig. 1(c) for an exemplar QW having $\Delta E_{\text{VB}} = 2\,\Delta E_{\text{CB}}$ and a 1.55 μm ground state band gap in the absence of injection (non-SC, "flat band"), these unique band characteristics have significant and beneficial implications for optical gain. Firstly, electrostatic confinement of electrons strongly enhances material gain at fixed carrier density in SC calculations (solid lines) compared to equivalent non-SC (dashed lines) calculations. Secondly, material gain in excess of 10^3 cm^{-1} can be achieved, despite the presence of spatially "indirect" electron-hole recombination. Overall, our systematic analysis identifies pathways to minimise (maximise) threshold carrier density (differential gain at threshold), identifying promising prototype structures for growth and experimental investigation.

IV. Conclusion

We have established predictive theoretical calculations of the electronic and optical properties of GaAs-based, strain-compensated type-II QWs based on the highly-mismatched alloys GaN_yAs_{1-y} and $GaAs_{1-x}Bi_x$. Our analysis indicates that $GaAs_{1-x}Bi_x/GaN_yAs_{1-y}$ QWs offer broad scope for band structure engineering, allowing to precisely tune strain and carrier confinement to achieve telecom-wavelength structures offering impressive predicted performance. This novel class of heterostructures represents a new approach to target the long-held goal of achieving telecom-wavelength GaAs-based semiconductor lasers displaying reduced non-radiative losses.

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