Alloy disorder effects in $GaBi_xAs_{1-x}$/GaAs Single Quantum Wells

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Dilute bismide alloys, such as $GaBi_xAs_{1-x}$, are promising candidates for the design of highly efficient and temperature-stable optoelectronic devices working at telecom wavelengths[1]. Replacing a small fraction of As by Bi in GaAs leads to a large reduction of band-gap energy (E_g), accompanied with a rapid increase in spin-orbit-splitting energy (Δ_{SO}), thereby leading to $\Delta_{SO} > E_g$ regime[2] which is technologically improrant for the supression of Auger loss mechanism[3]. In order to efficiently exploit the beneficial properties of bismide alloys, a comprehensive understanding of their electronic structure is crucial. In this regard, one critical aspect is to analyse alloy randomness effects which in recent experimental measurements has been identified as a source of strong band-edge broadening[4,5]. While conituum models fail to capture alloy fluctuation effects, we apply atomistic tight-binding approach[2] to study inhomogenous broadening of band edge energies and inter-band optical transitions in $GaBi_xAs_{1-x}$/GaAs single quantum wells[6].

Our study was based on fully atomistic simulations of 8 nm wide $GaBi_xAs_{1-x}$ QWs, with GaAs barriers being 8 nm both above and below the QW region. Thus the simulated supercells were very large consisting of 24576 atoms, with 8192 atoms only in the $GaBi_xAs_{1-x}$ QW region. A large supercell size with more than 4096 atoms is citical to correctly capture the alloy randombess effects[7]. The alloy fluctuation effects were modeled by randomly replacing As atoms with Bi atoms in the QW. We simulated twenty different random distributions of the Bi atoms to average out the effect of localized variations in the Bi configurations.

Our detailed calculations concluded that while the conduction band states were largely unaffected by the alloy disorder, the valence band states were strongly perturbed leading to a large inhomogenous energy broadening and significant distortion of wave functions in particular at lower Bi fractions. The inhomogenous broadening in the FWHM of the ground state optical transition was calculated as ~33 meV at 3.125% Bi which reduces to ~23.5 meV at 12.5% Bi in the QW. Furthermore, the symmetry breaking allowed transitions between the lowest conduction band state and a wide range of valence band states, leading to a further contribution to the inhomogenous broadening of the absorption spectra. Our study also concluded that the disorder related effects are stronger for large QW widths. Overall, our calculations clearly demostrated the critical importance of taking alloy fluctuations into account for the analysis and design of optoelectronic devices based on this new class of III-V materials.

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[1] S.J. Sweeney *et al*., 13th International Conference on Transparent Optical Networks, Stockholm, Sweden, 2011.
[2] M. Usman, C.A. Broderick, A. Lindsay, and E.P. O'Reilly, Phys. Rev. B 84, 245202, 2011.
[3] C.A. Broderick, M. Usman, S.J. Sweeney, E.P. O'Reilly, Semicond. Sci. Technol. 27, 094011, 2012.
[4] S. Imhif *et al*., Appl. Phys. Lett. 96, 131115, 2010.
[5] C. Gogineni *et al*. Appl. Phys. Lett. 103, 041110, 2013.
[6] M. Usman and E. P. O'Reilly, Applied Physics Letters 104, 071103, 2014.
[7] M. Usman *et al*. Phys. Rev. B 87, 115104, 2013.