Electronic Structure and Gain Engineering in Type-I $GaBi_xAs_{1-x}$ and $GaBi_xN_yAs_{1-x-y}$ Quantum Well Devices

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It has been recently proposed [1] that by engineering the band structure to achieve the spin-orbit-splitting energy (Δ_{SO}) greater than the band gap energy (E_g), it should be possible to realize laser devices operating at telecomm and longer wavelengths in which the dominant Auger loss mechanism is suppressed. Such band structure engineering is possible by incorporating dilute Bi compositions in GaAs(N). This work reports sp^3s^* tight-binding [2] and k•p [3] models to investigate and engineer the band structure of $GaBi_xN_yAs_{1-x-y}$ alloys as a function of Bi and N composition. Based on an accurate k•p Hamiltonian derived from tight-binding calculations, we further develop models to calculate and optimize the gain in $GaBi_xAs_{1-x}$/GaAs and $GaBi_xN_yAs_{1-x-y}$ /GaAs quantum well devices.

In the first part of our work, we perform 4096-atom tight-binding supercell calculations to develop a detailed understanding of the evolution of the electronic structure of $GaBi_xN_yAs_{1-x-y}$ alloys as a function of Bi and N composition. The key insights gained are that N and Bi largely independently modify the band structure of GaAs; N via a band-anticrossing (BAC) in the conduction band and Bi via a valence band BAC. Therefore co-alloying of Bi and N allows tuning of the wavelength over a very large range. Secondly, $\Delta_{SO} > E_g$ can be achieved by alloy composition engineering, emitting at 1550 nm with approximately 1% compressive strain on a GaAs substrate.

In the second part of our work, we apply 12 and 14-band k•p Hamiltonians to investigate the material gain in $GaBi_xAs_{1-x}$/GaAs and $GaBi_xN_yAs_{1-x-y}$/GaAs QW devices. Our calculations demonstrate that the gain in $GaBi_xAs_{1-x}$/GaAs lasers with low Bi compositions (x) is poor due to shallow conduction band offset, which can be overcome by the use of AlGaAs barriers. We then propose an Al composition to achieve maximum modal gain by simultaneously optimizing both the QW and waveguide. Our results for $GaBi_xAs_{1-x}$/GaAs lasers at higher x (with wavelengths approaching 1550 nm) show that the gain characteristics become intrinsically superior without even using AlGaAs barrier due to a combination of enhanced electron confinement inside the QW and a reduction of the valence band edge density of states arising from larger compressive strain at higher x. We further extend our calculations to analyze gain in $GaBi_xN_yAs_{1-x-y}$/GaAs QW devices, predicting that low y QWs which are compressively strained, or $y \geq x$ QWs with (larger) tensile strain result in optimized gain. Overall, we conclude that dilute bismide alloys are very promising candidates for the design of high efficiency photonic devices with reduced temperature sensitivity.

References:
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