

Studies on III-V Dilute Nitride, Bismuth and Antimonide Alloys Using k.p Hamiltonian

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This dissertation investigates the electronic band structure and optical properties of strained GaSbBi/GaAs and GaAsSbN/GaAs heterostructures using extended $k \cdot p$ Hamiltonian models. A 14-band $k \cdot p$ Hamiltonian based on the Valence Band Anticrossing (VBAC) model analyzes GaSbBi alloys, while a 16-band $k \cdot p$ Hamiltonian combining VBAC and Conduction Band Anticrossing (CBAC) models examines GaAsSbN alloys. The research focuses on band gap engineering, spin-orbit splitting, carrier effective masses, band offsets, and optical gain for optoelectronic applications in mid-infrared and telecommunication wavelength regions.

GaSbBi/GaAs Type-II Heterostructures In bulk $\text{GaSb}_{0.987}\text{Bi}_{0.013}$, incorporating 1.3% Bi reduces the band gap by 51 meV (~ 39 meV/%Bi) through a 36 meV downward shift of the conduction band minimum and a 15 meV upward shift of the valence band maximum. The spin-orbit split-off band moves upward by 10.3 meV, increasing spin-orbit splitting by ~ 27 meV. Strain dramatically alters these properties in GaSbBi/GaAs quantum wells (QWs). The 7.3% compressive strain splits the light hole (LH) and heavy hole (HH) bands by 373 meV and shifts the conduction band upward, increasing the band gap to 1.12 eV—opposite to the bulk reduction. The spin-orbit split-off band E_{SO+} moves downward by 230 meV, significantly increasing the spin-orbit splitting energy to 1.217 eV. This Type-II band alignment enhances electron-hole envelope function overlap compared to Type-I GaAsBi structures. Optical gain calculations for 10 nm QWs show peak gain shifts toward lower wavelengths as well width decreases. Dispersion relations reveal the spin-orbit split-off band is isotropic, while LH and HH bands maintain p-like anisotropy.

GaAsSbN/GaAs Quaternary Alloys The 16-band model accounts for N-related states interacting with the conduction band and Sb-related states with the valence band. For $\text{GaAs}_{0.931}\text{N}_{0.019}\text{Sb}_{0.05}$ alloys, a band gap reduction of 330 meV results from a 281 meV decrease in the conduction band minimum (CBM) and a 49 meV increase in the valence band maximum (VBM). The CBM lowering contributes approximately 90% of the total reduction due to the large coupling parameter C_N . The alloy achieves lattice matching to GaAs at an N-to-Sb ratio of 0.38, with band gaps as low as 1 eV. Increasing Sb concentration enhances spin-orbit splitting by ~ 22 meV per $y=0.01$. A crossover where spin-orbit splitting energy Δ_{SO} exceeds band gap E_g occurs at Sb=27% and N=10%, creating an $E_g < \Delta_{SO}$ regime critical for suppressing Auger recombination losses in optoelectronic devices. Band offset calculations show the conduction band offset (CBO) is significantly larger than the valence band offset (VBO). For QWs, the CBO increases non-linearly and is nearly ten times greater than the VBO, providing strong electron confinement. Unlike typical dilute nitrides, electron effective mass calculations indicate electron mobility increases for Sb concentrations above 3%, while hole mobility decreases with increasing Sb. Strain effects in QWs produce distinct behaviors. Tensile strained $\text{GaAs}_{0.94}\text{N}_{0.05}\text{Sb}_{0.01}/\text{GaAs}$ QWs exhibit a band gap of 0.75 eV with large LH-HH splitting of 0.75 eV. Compressive strained $\text{GaAs}_{0.94}\text{N}_{0.01}\text{Sb}_{0.05}/\text{GaAs}$ QWs show a higher band gap of 1.22 eV with less significant LH-HH splitting.

Conclusion GaSbBi/GaAs QWs are suitable for 2–5 μm mid-infrared applications due to enhanced spin-orbit splitting and Type-II alignment. The GaAsSbN/GaAs system is a promising

candidate for 1.3–1.55 μm telecommunication lasers, offering tunable band gaps and reduced Auger recombination through band offset engineering.