Title:

Theory of the electronic structure of dilute bismide and bismide-nitride alloys of GaAs: Tight-binding and **k.p** models

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Abstract:

The highly mismatched semiconductor alloy $GaBi_xAs_{1-x}$, comprised of dilute concentrations of bismuth (Bi) incorporated in GaAs, is an attractive candidate for the design of highly efficient mid- and far-infrared optical [1] and spintronic [2] devices. It has been shown both experimentally [3] and theoretically [4] that isovalent substitution of a small fraction of Bi atoms in GaAs drastically reduces the band gap (E_g) by ~90 meV/% Bi replacing As. A giant bowing of the spin-orbit-splitting energy (Δ_{SO}) has also been observed in $GaBi_xAs_{1-x}$, leading to the onset of an $E_g < \Delta_{SO}$ regime. This characteristic is of fundamental importance as it opens up the possibility to suppress the dominant CHSH Auger recombination losses suffered by conventional III-V optical devices operating at high temperatures. Therefore, an understanding of the electronic structure of $GaBi_xAs_{1-x}$ is crucial both from a fundamental perspective, as well as for potential device applications.

We have developed a nearest neighbor sp^3s^* tight binding (TB) Hamiltonian to investigate the electronic structure of dilute bismide alloys of GaP and GaAs [4]. By applying our model to large $GaBi_xY_{1-x}$ (Y=As,P) supercells, we demonstrate that isovalent Bi substitution introduces Bi-related defect states which interact with the host GaY (Y=As,P) matrix valence band edge via a Bi composition dependent band anti-crossing (BAC) interaction. Our calculations show that the observed strong variations in E_g and Δ_{SO} can be well explained in terms of a BAC model, with the change in E_g also having a significant contribution from a conventional alloy reduction in the conduction band edge energy. Our calculated E_g and Δ_{SO} are in good agreement with experimental measurements throughout the investigated composition range ($x \leq 13\%$), in particular reproducing the $E_g < \Delta_{SO}$ crossover at x ~10.5% in free-standing $GaBi_xAs_{1-x}$.

We further extend our TB model to the dilute bismide-nitride alloys ($GaBi_xN_yAs_{1-x-y}$) and derive **k.p** Hamiltonians both for $GaBi_xAs_{1-x}$ and $GaBi_xN_yAs_{1-x-y}$. We demonstrate that the impacts of Bi and N incorporation on the GaAs electronic structure are largely independent of each other, with N-related defect states mainly perturbing the conduction band edge according to well understood BAC model. The large band gap reduction with N composition in GaN_yAs_{1-y}, is significantly enhanced by presence of Bi, leading to a giant E_g bowing in $GaBi_xN_yAs_{1-x-y}$ [5]. Since N weakly perturbs the GaAs valence band structure, the bowing of Δ_{SO} in $GaBi_xN_yAs_{1-x-y}$ is similar to that in $GaBi_xAs_{1-x}$.

Co-alloying of Bi and N in GaAs also allows the possibility of precise strain control in $GaBi_xN_yAs_{1-x-y}$ thereby opening up a large and flexible parameter space for band structure engineering. This is of significant importance for the design of highly efficient optoelectronic devices operating with reduced temperature sensitivity at telecommunication wavelengths, a key requirement for future 'green' commercial telecommunication networks.

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