## Theoretical modeling of quantum-well structures in dilute bismide optoelectronics

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Dilute III-V-bismide alloys are promising candidates for developing high-power and high-efficiency midwave infrared (MWIR) optoelectronic devices. Currently, this spectral range is dominated by quantum and interband cascade lasers (QCLs and ICLs). However, these structures are very complicated and suffer from high temperature sensitivity due to Auger recombination. Bismide alloys allow for uniquely large spin-orbit split-off energies [1], which suppresses Auger recombination and thus temperature sensitivity. Additionally, the 3-4 µm waveband remains difficult to achieve with existing technologies. The quaternary alloy  $In_yGa_{1-y}As_{1-x}Bi_x$  shows promise in filling this spectral gap with quantum-well devices based on the mature InP platform.

Introducing bismuth to III–V alloys dramatically raises the valence band due to a valence band anti-crossing (VBAC) interaction [2]. To accurately model these alloys, we utilize a 12-band  $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian [3]. This model allows for numerically efficient calculation of the alloys' band structures given a small number of parameters. As an example, Fig. 1 shows the bulk band structure of In<sub>0.50</sub>Ga<sub>0.50</sub>As<sub>0.92</sub>Bi<sub>0.08</sub> calculated with this model and Fig. 2 shows calculated bandgaps for differing compositions of the alloy.

Two challenges with bismide alloys are the difficulty of incorporating large amounts of bismuth and managing the strain introduced to the system. To increase the emission wavelength of the device without raising the required bismuth concentration, one can increase the width of the quantum well. However, if the well material is strained, there is a restriction on how wide the well can be before relaxation occurs. These challenges can be overcome by using a graded quantum-well structure. One such example that we have explored is shown in Fig. 3. The barrier layers and outer-well layers are lattice-matched to the InP substrate, while the center layer is compressively strained. This center layer is sufficiently thin to avoid relaxation. The outer-well layers widen the well and lower the energy of bound electron states, while the center layer confines holes at a higher energy. These effects combine to reduce the energy gap of the well and increase the emission wavelength of the device. Fig. 4 shows the band diagram of this structure, with a calculated emission wavelength of  $3.4 \mu m$ .

In conclusion, this work aims to accurately model optoelectronic devices implementing III–V-bismide alloys. Additionally, we aim to develop devices that can detect and emit light in the difficult 3–4  $\mu$ m waveband. Preliminary results suggest this is possible with bismuth concentrations of less than 10% and strain of less than 1% by utilizing a graded quantum-well structure.

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## References

- [1] S. Jin and S. J. Sweeney, *InGaAsBi alloys on InP for efficient near- and mid-infrared light emitting devices*, Journal of Applied Physics **114**, 213103 (2013).
- [2] K. Alberi, J. Wu, W. Walukiewicz, K. M. Yu, O. D. Dubon, S. P. Watkins, C. X. Wang, X. Liu, Y. J. Cho, and J. Furdyna, *Valence-band anticrossing in mismatched III–V semiconductor alloys*, Phys. Rev. B **75**, 045203 (2007).
- [3] C. A. Broderick, M. Usman, and E. P. O'Reilly, *Derivation of 12- and 14-band k · p Hamiltonians for dilute bismide and bismide-nitride semiconductors*, Semiconductor Science and Technology 28, 125025 (2013).



Fig. 1. Bulk band structure of  $In_{0.50}Ga_{0.50}As_{0.92}Bi_{0.08}$  on InP calculated using a 12-band  $\mathbf{k} \cdot \mathbf{p}$  Hamiltonian near the  $\Gamma$  point. Note the small bandgap and large spin-orbit split-off energy.



Fig. 3. Quantum-well structure explored in this work. The  $In_{0.53}Ga_{0.47}As$  barrier layers and  $In_{0.40}Ga_{0.60}As_{0.92}Bi_{0.08}$  well layers are lattice-matched to the InP substrate, while the  $In_{0.50}Ga_{0.50}As_{0.92}Bi_{0.08}$  well layer is compressively strained.



Fig. 2. Calculated bandgap (in eV) of bulk  $In_xGa_{1-x}As_{1-y}Bi_y$  on InP. Solid lines show constant energy compositions and the dashed line shows lattice-matched compositions.



Fig. 4. Band diagram of the explored quantum-well design. Theoretical emission wavelength of  $3.4 \ \mu m$  with less than 1% strain in the 5 nm well.