Multi-scale modelling of the electronic structure of dilute bismide alloys

Christopher A. Broderick[a,b], Muhammad Usman[a] and Eoin P. O'Reilly[a,b]
[a] Tyndall National Institute, Lee Maltings, Dyke Parade, Cork, Ireland
[b] Department of Physics, University College Cork, Cork, Ireland

Dilute bismide alloys, such as $GaBi_xAs_{1-x}$, in which a small fraction x of the group-V atoms in GaAs are replaced by bismuth (Bi), have been identified as a promising material system for the realisation of highly efficient, temperature stable semiconductor lasers operating at telecom wavelengths. Experimental and theoretical investigations have shown that with increasing x the band gap (E_g) decreases rapidly, accompanied by a large increase in the spin-orbit-splitting energy (Δ_{SO}),[1,2] leading to $E_g < \Delta_{SO}$ for $x >$ 10%.This band structure condition is of particular interest for semiconductor laser operation, as the dominant non-radiative Auger recombination pathway is suppressed by conservation of energy.[3,4]

We outline here our theoretical models of the electronic structure of $GaBi_xAs_{1-x}$ and related alloys. We present a multi-scale approach ranging from atomistic electronic structure models to continuum band structure models suited to device calculations.

We first formulate an atomistic tight-binding model for large supercell calculations, which is in good agreement with a range of experimental measurements, accurately describing the main features of the $GaBi_xAs_{1-x}$ electronic structure.[5] Using this model we demonstrate how the evolution of the electronic structure with increasing x is influenced by the Bi-related impurity states that are formed as a result of the chemical and size differences between Bi and the As atoms, as well as by alloy disorder.[6]

Next, we outline the derivation of a continuum 12-band **k.p** model for $GaBi_xAs_{1-x}$. The model is derived explicitly from ordered supercell calculations using the tight-binding model, and provides a description of the band structure in terms of an anti-crossing interaction between the extended states of the GaAs host matrix and localised Bi-related states which are resonant with the GaAs valence band.[7] The models we present are useful for understanding both the fundamental physics and device properties of dilute bismide alloys.

[1] Z. Batool, K. Hild, T. J. C. Hosea, X. Lu, T. Tiedje and S. J. Sweeney, *J. Appl. Phys.* **111**, 113108 (2012)

[2] C. A. Broderick, M. Usman and E. P. O'Reilly, *"Theory of the electronic structure of dilute bismide alloys: Tight-binding and **k.p** models"*, Chapter 3 in Bismuth-Containing Compounds, Springer Series in Materials Science Volume 186, pp. 55 – 88 (2013)

[3] S. J. Sweeney, Z. Batool, K. Hild, S. R. Jin and T. J. C. Hosea, *"The potential role of bismide alloys in future photonic devices"*, in Proceedings of the 13th International Conference on Transparent Optical Networks (ICTON), Stockholm (2011)

[4] C. A. Broderick, M. Usman, S. J. Sweeney and E. P. O'Reilly, *Semicond. Sci. Technol.* **27**, 094011 (2012)

[5] M. Usman, C. A. Broderick, A. Lindsay and E. P. O'Reilly, *Phys. Rev. B* **84**, 245202 (2011)

[6] M. Usman, C. A. Broderick, Z. Batool, K. Hild, T. J. C. Hosea, S. J. Sweeney and E. P. O'Reilly, *Phys. Rev. B* **87**, 115104 (2013)

[7] 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", Semicond. Sci. Technol.* **28**, 125025 (2013)