Intervalley mixing and intersubband transitions in n-type Si/SiGe quantum wells

A. Valavanis, Z. Ikonić and R. W. Kelsall
Institute of Microwaves and Photonics
School of Electronic and Electrical Engineering
University of Leeds
Leeds LS2 9JT
Email: a.valavanis05@leeds.ac.uk

The Si/SiGe materials system offers the prospect of excellent integration between CMOS technology and optoelectronics, employing well-established fabrication technology at low cost. Whilst the indirect bandgap means that interband lasing is challenging, stimulated emission from intersubband transitions offers a route to long wavelength Si based lasers. In bulk silicon, the conduction band minima are located in six degenerate valleys near the Brillouin zone edge in the Δ directions. In a two-dimensional system however, uniaxial strain effects split the degeneracy of the valleys into two sets — two Δ_z valleys perpendicular to the heterostructure interfaces and four Δ_{xy} valleys in the growth plane.

Atomistic simulation methods have shown that the two degenerate valley sets are sufficiently separated from each other to be considered independently within an effective mass approximation (EMA) model. Electrons emanating transversely from each of the Δ_{xy} valleys contribute identically to the z-varying component of the wavefunction, resulting in four degenerate states. In the case of the Δ_z valleys however, the electrons have different wavevector components in the z-direction. Quantum confinement yields interference between these basis functions and two distinct solutions to Schrödinger's equation exist at separate energies, *i.e.* the degeneracy of Δ_z states is split. The effect has been observed experimentally in Schubnikov-de Haas oscillations in high magnetic fields.[1] It is therefore important to consider the mixing effect between the Δ_z valleys when determining states in a quantum confined system.

Whilst atomistic simulation methods such as the tight-binding approximation implicitly take intervalley mixing into account,[2] the computation is considerably slower than the effective mass approximation — particularly in the case of large complicated structures such as a quantum cascade laser (QCL). A Double Valley Effective Mass Approximation (DVEMA) is therefore desirable as it offers the rapid computation of the EMA whilst including intervalley mixing effects explicitly. Such a model was derived for a square quantum well by Ting and Chang.[3] The energy splitting in the lowest states is shown to be a decaying oscillatory function of well width. The present work details the expansion of the DVEMA model to a general symmetric envelope potential.

In SiGe molecular beam epitaxy (MBE), interdiffusion of Ge between heterolayers prevents abrupt interfaces from existing in the envelope potential. By considering a number of structures with more realistic interfaces than previous studies, the surface segregation effect is shown to reduce valley splitting slightly. Although the DVEMA applies only to symmetric structures, the present studies show that the model often remains reliable for slightly asymmetric structures.

Using the DVEMA model, the effect of valley splitting upon realistic Si/SiGe intersubband optical devices has been investigated. The optical matrix elements for valley split intersubband transitions are shown to be almost identical, whilst their energies may differ by up to 10 meV. The emission spectrum is therefore expected to exhibit transition doublets when the valley splitting becomes large. It is shown that through careful design, the valley splitting may be minimized; although there is scope for exploiting intervalley scattering effects to achieve population inversion in an intersubband laser.

References

[1] K. Lai, W. Pan, D. C. Tsui, S. Lyon, M. Mühlberger, and F. Schäffler, "Intervalley gap anomaly of two-dimensional electrons in silicon," *Phys. Rev. Lett.*, vol. 96, p. 076805, Feb. 2006.

[2] T. B. Boykin and G. Klimeck, "The discretized Schrödinger equation for the finite square well and its relationship to solid-state physics," *European J. Phys.*, vol. 26, pp. 865–881, Jul. 2005.

[3] D. Z. Y. Ting and Y.-C. Chang, "L-valley-derived states in (001) GaSb/AlSb quantum wells and superlattices," *Phys. Rev. B*, vol. 38, no. 5, pp. 3414–3422, Aug. 1988.