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Intersubband transitions in n-type group IV quantum cascade lasers

Alex Valavanis,* **Z. Ikonić**, and **R.W. Kelsall**
Institute of Microwaves and Photonics, School of Electronic and Electrical Engineering, University of Leeds, Leeds LS2 9JT, United Kingdom

Abstract: In a theoretical investigation of intersubband transport in SiGe based quantum cascade structures, we show that low effective mass and a large confining potential may be achieved with either (001) oriented Ge-rich or (111) orientated Si-rich structures. Using a self-consistent time-independent perturbation/rate equation approach, we predict net gain in both systems and compare their maximum operating temperatures.

Despite the great success of quantum cascade lasers (QCLs) as compact sources of mid-infrared and terahertz frequency radiation, existing devices are restricted to III-V compound semiconductors. Group IV alloys however offer many potential advantages.[1] Mature CMOS processing technology may reduce fabrication costs and the absence of polar LO-phonon interactions, combined with the higher thermal conductivity of silicon, may allow higher temperature operation.

Electroluminescence has been observed in quantum cascade structures based on (001) oriented p-type Si/SiGe,[2] but laser action in these systems has proved elusive. This is possibly due to the coexistence of light-hole and heavy-hole subbands and associated subband mixing, which can cause large variations in transition energy with in-plane wave vector and open up rapid nonradiative scattering channels.[3]

These complications are avoided in n-type systems, due to the large separation between conduction bands and the almost parabolic dispersion of the band minima. Despite its advantages, n-type SiGe has generally been overlooked, as bound states in (001) oriented systems have large effective mass, which reduces the dipole matrix element between states. As the gain coefficient is proportional to the square of the dipole matrix element, it was previously thought that the prospects of developing a successful laser were limited.

We show however, in a theoretical study of intersubband transitions in SiGe heterostructures that n-type group IV QCLs are viable. We show that a low effective mass is achievable either by moving to the (111) crystal orientation or by using Ge-rich systems. Concerns about the difficulty of modulation doping have also been addressed by recent improvements in SiGe epitaxial growth technology.

As $Si_{1-x}Ge_x$ alloys are indirect bandgap materials, the conduction band minima are located at nonzero wavevectors, and form degenerate sets in bulk alloys. In Si rich systems ($x < 0.85$), the conduction band edge lies in six degenerate minima close to the X symmetry points in the Δ directions, while the band edge in Ge rich systems lies in eight half-valleys at the L points. Each set of conduction band minima offers a possible route to the realisation of Si/SiGe QCLs, and designs have been presented for devices using both the Δ[4] and L[5] valleys.

Each valley forms an ellipsoidal equipotential surface in reciprocal space, in which electrons have anisotropic effective mass. Combined with strain effects, this breaks subband degeneracy within the Δ valley set in (001) oriented systems, and the higher energy subbands can prevent population inversion by providing parasitic current pathways. We show however, that subband degeneracy within valleys is preserved by selecting the (111) crystal orientation for Δ valleys or the (001) orientation for L valleys.

By calculating intersubband scattering rates for each of the principal mechanisms in a self-consistent rate-equation model, we show that population inversion and large active region gain are achievable for both systems. By studying the effect of temperature on intersubband transition linewidth, we compare the maximum operating temperature of each device.

[1] R. W. Kelsall, Z. Ikonić, P. Harrison, S. A. Lynch, *et al.* vol. 93 of *NATO Science Series II: Mathematics, Physics and Chemistry*, 367–382 (Kluwer Academic Publishers, Dordrecht, 2003).
[2] G. Dehlinger, L. Diehl, U. Gennser, H. Sigg, *et al.* Science **290**, 2277 (2000).
[3] Z. Ikonić, P. Harrison, and R. W. Kelsall. Phys. Rev. B **64**(24), 245311 (2001).
[4] L. Lever, A. Valavanis, Z. Ikonić, and R. W. Kelsall. Appl. Phys. Lett. **92**(2), 021124 (2008).
[5] K. Driscoll and R. Paiella. Appl. Phys. Lett. **89**(19), 191110 (2006).

*Electronic address: `a.valavanis05@leeds.ac.uk`