
Published paper

Valavanis, A., Ikonic, Z., Lever, L., Evans, C.A. and Kelsall, R.W. (2008) *Substrate orientation and alloy composition effects in n-type SiGe quantum cascade structures.* In: 2008 5th IEEE International Conference on Group IV Photonics. Group IV Photonics, 2008 5th IEEE International Conference on, 17-19 Sept. 2008, Sorrento, Italy. IEEE , pp. 251-252.

http://ieeexplore.ieee.org/xpls/abs_all.jsp?arnumber=4638162

doi: 10.1109/GROUP4.2008.4638162

Substrate orientation and alloy composition effects in n-type SiGe quantum cascade structures

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***Abstract*—We show using a theoretical self-consistent effective mass/rate equation approach that n-type SiGe-based quantum cascade lasers are potentially made viable by either using the (111) orientation or a Ge-rich substrate.**

I. INTRODUCTION

Quantum cascade lasers (QCLs) are well established as compact sources of mid-infrared and THz frequency radiation, but remain restricted to III–V materials systems. Extending the range of usable materials to include group-IV alloys would offer many potential advantages, including reduced processing costs due to the maturity of CMOS technology, and a possible route to photonic integrated circuit applications [1]. The large thermal conductivity of Si, combined with the absence of polar LO-phonon interactions is also expected to increase the maximum QCL operating temperature.

Although electroluminescence has been observed from p-type, (001) oriented Si/SiGe quantum cascade structures [2], lasing has not yet been achieved. The design of such structures is challenging, as the mixing of light- and heavy-hole subband states leads to large variations in intersubband transition energies with in-plane wave vector, and the creation of undesirable nonradiative current paths [3].

In n-type systems, these complications are absent due to the large separation between conduction bands and the almost parabolic dispersion of the band minima. Such systems have generally been overlooked because of the large quantisation effective mass in (001) oriented Si, 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, using an effective mass/rate equation approach that n-type SiGe-based lasers are viable, by either 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.

II. STRAIN DEPENDENT BANDSTRUCTURE

Depending on the crystal orientation, the quantisation effective mass may vary between the valleys at the conduction band edge. For Si-rich quantum wells (Ge fractions under

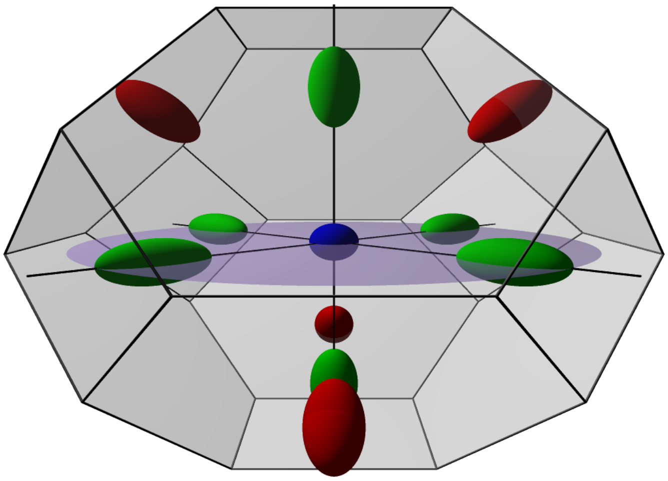

Fig. 1. The quantisation effective mass is identical for all L valleys (red) in the (001) orientation, while the Δ valley (green) masses vary.

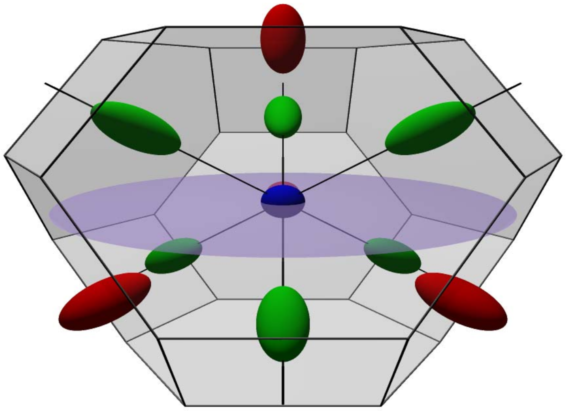

Fig. 2. The quantisation effective mass is identical for all Δ valleys (green) in the (111) orientation, while the L valley (red) masses vary.

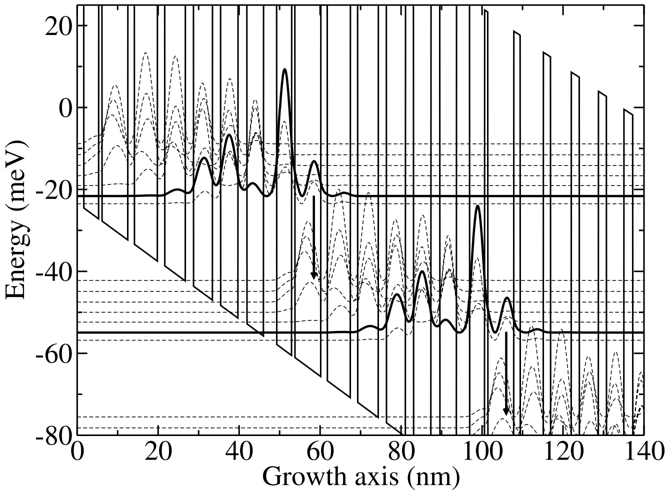

Fig. 3. A seven-well bound-to-continuum QCL using Δ valley transitions in the (111) orientation, with an applied electric field of $7\,\mathrm{kVcm}^{-1}$. The lower laser level is shown in bold, and the lasing transition to the miniband is shown with an arrow.

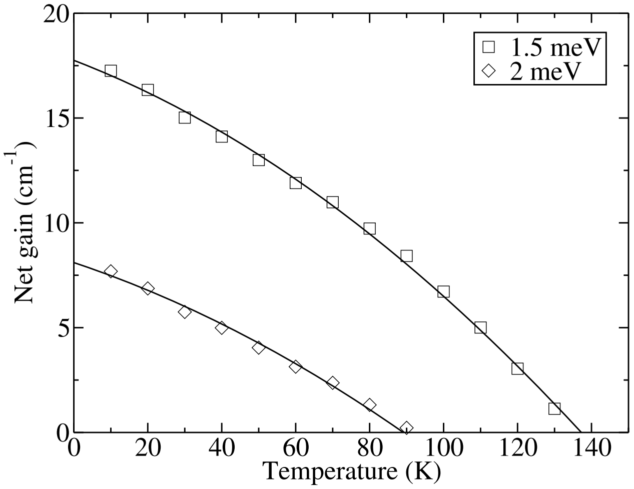

Fig. 4. Net gain for the (111) oriented Δ valley system in Fig. 3, for transition linewidths of 1.5 and 2.0 meV. Waveguide losses were calculated for a $15\,\mu$m thick active region with a double metal waveguide.

around 85%), the Δ valleys contain the lowest energy states and therefore most relevance to device behaviour, while L valleys contain the lowest energy states in Ge-rich systems.

In (001) orientation Si-rich systems (Fig. 1), two Δ valleys are aligned perpendicular to the growth plane while the other four Δ valleys are aligned in the growth plane. The quantisation effective mass for the perpendicular valleys is therefore large, while that of the in-plane valleys is small. Conversely, Fig. 2 shows that in the (111) orientation, the cross-section pependicular to the growth plane, and hence the quantisation effective mass is identical for all the Δ valleys.

Similar arguments show that uniaxial strain breaks the degeneracy of the Δ valley subbands in the (001) orientation, but not in the (111) orientation. [4] The opposite situation applies for L valleys in Ge-rich systems, whose subband energies and quantisation effective masses are split in the (111) orientation but not in the (001) orientation.

We show using a model solid approximation that quantum cascade structures using either L valley subbands in the (001) orientation or Δ valley subbands in the (111) orientation minimise the quantisation effective mass in the low energy subbands. Undesirable nonradiative intervalley scattering pathways are also avoided as subband degeneracy is preserved. For the example (111) Δ valley bound-to-continuum QCL design in Fig. 3, a quantisation effective mass of 0.26 and a conduction band offset of 150 meV were calculated.

III. TRANSPORT CALCULATIONS

The gain coefficient for an intersubband radiative transition is dependent upon the square of the dipole matrix element [5], which in turn reduces rapidly as the quantisation effective mass increases. Therefore, by minimising the effective mass of the lowest energy subbands, we maximise the gain coefficient.

We use time-independent perturbation theory to calculate all the principal intervalley and intravalley scattering rates and determine subband populations using a self-consistent, energy balance/rate equation approach. We then determine the gain coefficient and temperature dependent linewidth for optical transitions within a structure. We show that net gain is achievable for the two optimal systems described above, while the (001) orientation for Δ valleys and (111) orientation for L valleys yield a net loss. For the bound-to-continuum (111) Δ valley system described above, Fig. 4 shows that net gain is achievable up to lattice temperatures of 90 K with a $15\,\mu$m thick active region and a double-metal waveguide.

ACKNOWLEDGMENTS

This work is supported by EPSRC Doctoral Training Allowance funding and DTI-MNT contract 491: “Fast THz Cameras”.

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