Density matrix modelling of Ge/GeSi bound-to-continuum terahertz quantum cascade lasers

T. V. Dinh, A. Valavanis, L. J. M. Lever, Z. Ikonic, and R. W. Kelsall*
Institute of Microwaves and Photonics, School of Electronic and Electrical Engineering,
University of Leeds, Leeds LS2 9JT, United Kingdom
e-mail: r.w.kelsall@leeds.ac.uk

In addition to the mainstream III-V quantum cascade lasers (QCLs), Si-based QCLs have attracted considerable research interest in recent years, due to their significant potential advantages including a mature Si processing technology, prospect of integration with Si microelectronics, superior thermal performance to that of III–V devices and absence of optical absorption in the Reststrahlen band [1–3]. Amongst various proposed designs, (001) oriented n-type Ge/GeSi structures utilising L-valley intersubband transitions appear to be the most promising due to a small quantisation effective mass, and hence large optical matrix elements and practically feasible layer widths [4]. All previous simulations for group IV-based QCLs followed the rate equation approach, which is considered not to be accurate enough for predicting the performance of terahertz QCLs, due to its limitation in describing coherent transport [5, 6]. Therefore, a quantum-mechanics approach such as non-equilibrium Green's function or density matrix is required. Although the former is more accurate, its complexity and computational burden make it difficult to be implemented as a simulation tool. In this work, a density matrix (DM) model for Ge/SiGe QCL simulation has been developed. The existing models have used a reduced set of basis states, leaving out some coherences, which was justified for the particular structures they were used for, but potentially limits their generality and accuracy. In this work, we present an extended DM model, which considers all basis states involved in transport between periods of a QCL. The simulator based on it is sufficiently general to be able to simulate a QCL with any number of states and tight-binding modules per period. This is useful for investigating various QCL structures without modifying the code. It also includes multiple scattering mechanisms existing in Si and Ge quantum wells [4], i.e. intravalley scattering due to interface roughness, alloy disorder, ionized impurities, electron-electron, electron-acoustic phonon and optical phonon interactions, and intervalley phonon scattering. Since the simulator is still quite fast, it was used, in conjunction with a semi-automated optimization algorithm, to improve the predicted performance of bound-to-continuum QCLs, and to compensate for the gain-reduction associated with diffuse Ge/GeSi interfaces.

Figs.1-4 show some examples of the designed bound-to-continuum Ge/GeSi QCLs, and simulation results.

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REFERENCES

[1] K. Driscoll and R. Paiella, *Silicon-based injection lasers using electronic intersubband transitions in the L-valleys*, Appl..Phys. Lett, **89**, 191110 (2006).
[2] L. Lever, A. Valavanis, Z. Ikonic, and R. W. Kelsall, *Simulated [111] Si-SiGe terahertz quantum cascade laser*, Appl. Phys. Lett, **92**, 021124 (2009).
[3] Y. Busby et al., *Near- and far-infrared absorption and electronic structure of Ge-SiGe multiple quantum wells*, Phys. Rev. B, **82**, 205317, 2010.
[4] A. Valavanis, T. V. Dinh, L. J. M. Lever, Z. Ikonic, and R. W. Kelsall, *Material configurations for n-type silicon-based terahertz quantum cascade lasers*, Phys. Rev. B, **83**, 195321 (2011).
[5] H. Callebaut and Q. Hu, *Importance of coherence for electron transport in terahertz quantum cascade lasers*, J. Appl. Phys, **98**, 104505 (2005).
[6] J. B. Khurgin, Y. Dikmelik, P. Q. Liu, A. J. Hoffman, M. D. Escarra, K. J. Franz, and C. F. Gmachl, *Role of interface roughness in the transport and lasing characteristics of quantum-cascade lasers*, Appl. Phys. Lett, **94**, 091101 (2009).

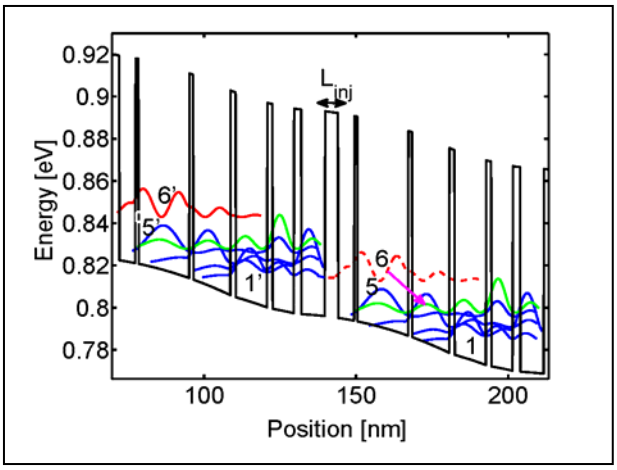

Fig. 1. Band structure and electron probability densities for two periods of an optimized 6-well bound-to-continuum QCL based on $Ge/Si_{0.15}Ge_{0.85}$.

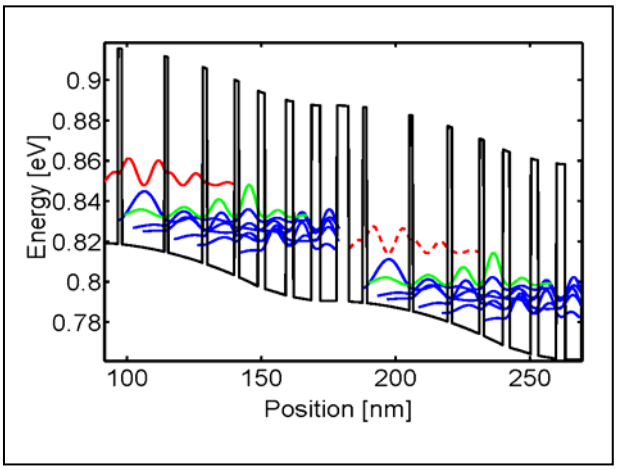

Fig. 2. As in Fig.1, but for an 8-well bound-to-continuum structure.

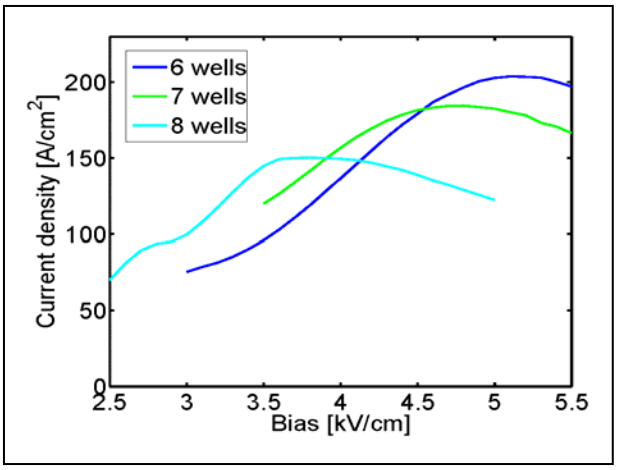

Fig. 3. The calculated current density vs. bias dependence for the designed 3.8 THz QCLs with varying number of quantum wells.

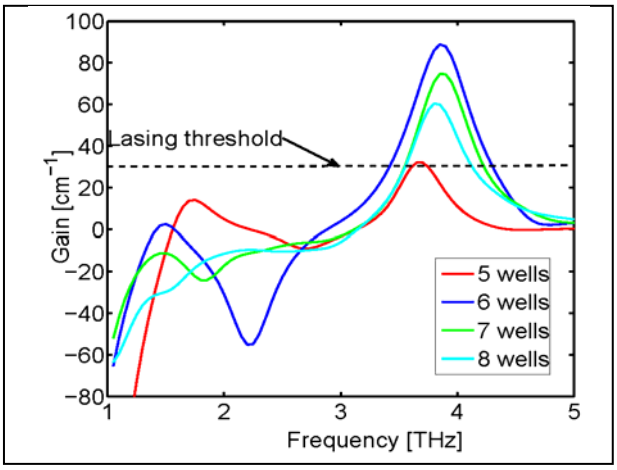

Fig. 4. The calculated small-signal gain spectrum for structures with varying numbers of wells. The dashed horizontal line is the indicative figure for threshold gain.