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Density matrix modelling of Ge/GeSi quantum cascade terahertz lasers

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The prospect of making silicon-based quantum cascade lasers (QCLs) has attracted considerable research interest in recent years, due to their significant potential advantages including a mature Si processing technology, the prospect of integration with Si microelectronics, and superior thermal performance to that of III–V devices. Amongst various proposed designs, with different material compositions and substrate orientations, (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 realisable layer widths. While all the previous simulations for group IV-based QCLs used the rate equation model, this neglects the coherence effects and is of limited usefulness for predicting QCL performance, particularly in the terahertz range. In this work, a quantum-mechanics transport model for Ge/SiGe QCL simulation has been developed, using the density matrix (DM) approach. In contrast to the existing DM formulations which have been used to simulate III-V based QCLs, the present model accounts for the role of all the QCL states in coherent transport, or in optical transitions, or both. The simulator includes all the principal scattering mechanisms in Ge/SiGe heterostructures: intravalley scattering due to interface roughness, alloy disorder, ionized impurities, electron-acoustic phonon and optical phonon interactions, and intervalley phonon scattering. It was used in conjunction with a semi-automated optimization algorithm to identify heterostructure designs for bound-to-continuum Ge/GeSi QCLs, and to compensate for the gain-reduction associated with diffuse Ge/GeSi interfaces.