Simulation of Room-Temperature Terahertz Quantum Cascade Lasers with Varying Degrees of Transverse Confinement

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Abstract

The transport and scattering of electrons through quantum wire aluminium gallium arsenide (AlGaAs)/GaAs heterostructures were simulated for various diameters. The effects of transverse confinement on non-radiative electron transitions were studied in an attempt to improve lasing efficiency at room-temperature.

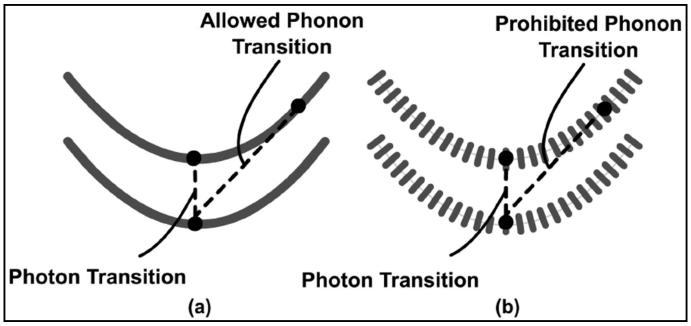

Figure 1: Energy bands; (a) without transverse confinement, and (b) with transverse confinement.

The focus of this project lay in qualitatively determining the efficacy of transverse confinement in improving the radiative efficiency of a terahertz QCL operating at room-temperature. We designed a heterostructure that possessed desirable spacings and resonances between energy eigenstates. This was followed by the simulation of the transport and scattering of electrons through quantum wires of various diameters with this heterostructure, using a quasi-three-dimensional non-equilibrium Green's function (NEGF) simulator entitled "Schrödinger Equation Monte Carlo 3D" (SEMC3D). Only scattering by phonon emission was considered. Reductions in non-radiative phonon transition rates were associated with increased radiative photon transition rates, and vice versa. Transitions triggered by phonon absorption were ignored.

Introduction

Quantum cascade lasers (QCLs) emit radiation when electrons passing through a layered heterostructure undergo transitions between energy eigenstates and then emit photons. Currently, terahertz QCLs only operate at very low temperatures, as electrons absorb thermal energy and rise in energy bands associated with dimensions transverse to the direction of transport, undergoing transitions to lower eigenstates by emitting LO-phonons instead of photons (Figure 1a). LO-phonons are bosons that correspond to high-frequency longitudinal lattice vibrations. Applications of terahertz QCLs would be significantly economized by successfully achieving room-temperature operation. Theoretically, transverse confinement of the superlattice in quantum wires would discretize energy bands associated with dimensions transverse to the transport direction. This would obstruct the absorption of thermal energy by electrons, and subsequent transitions between eigenstates would result in the radiative emission of photons instead of the non-radiative emission of phonons (Figure 1b).

Method

We found the energy eigenstates of a potential profile using a shooting-point eigenvalue solver. The profile consisted of wells and barriers that corresponded to the GaAs/AlGaAs heterostructure of a single QCL module, over which a potential drop of 46 meV was applied. The widths of the wells and barriers were adjusted and the effective mass of each region was tuned until desirable spacings and resonances between energy eigenstates were obtained.

Figure 2 displays the final heterostructure designed, along with the energy eigenstates superposed with their probability densities. E_5's wavefunction was concentrated in the first two wells to ensure that electrons injected into this level would fall to E_4 or E_3 within these wells, preferably by emitting a photon. Population inversion was promoted by evenly spreading out the probability densities of E_4 and E_3 between all three wells to provide rapid tunneling, and by setting the energy gap between

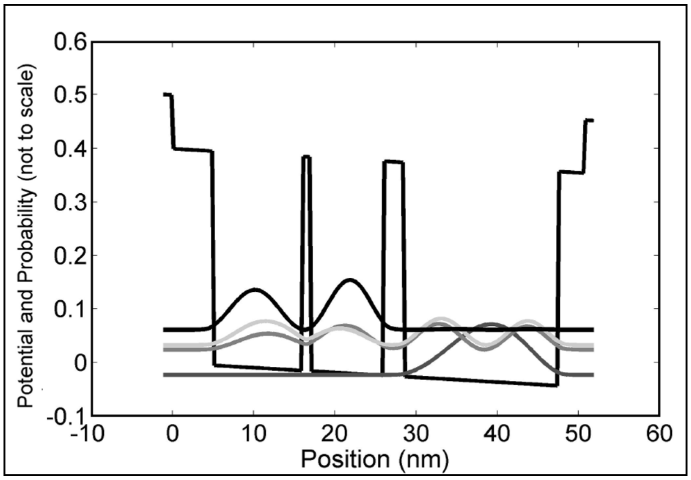

Figure 2: Potential profile with energy eigenstates and probability densities.

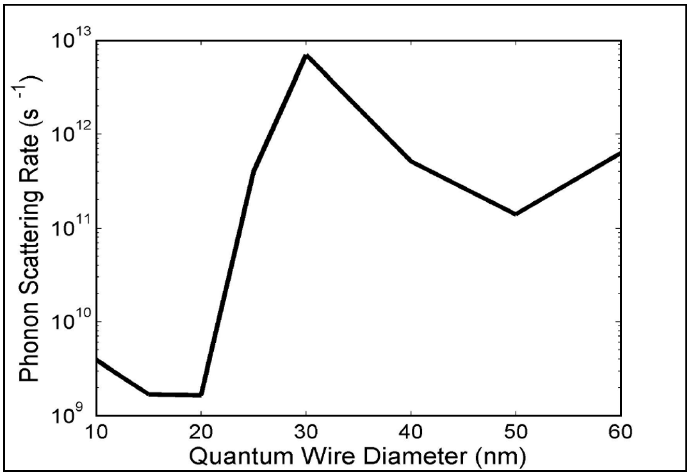

Figure 3: Variation of non-radiative phonon scattering rate with diameter.

E_3 and E_2 to roughly equal the LO-phonon energy of GaAs, as this would encourage rapid transitions between these levels by phonon scattering.

We built three-dimensional potential fields corresponding to quantum wires of different diameters using this heterostructure, to be loaded into SEMC3D. However, since the heterostructure would no longer be isolated from the “outside world,” a slight offset in the spacings between the energy eigenstates as calculated by SEMC3D was expected. To discover the true spacings between the eigenstates, we configured SEMC3D to inject electrons into the profile over a range of energies, and calculated the transmission probability (i.e., the likelihood that an injected electron would traverse the entire length of the module). Energies for which there was a spike in the transmission probability corresponded to the now quasi-bound eigenstates.

To ensure the qualitative accuracy of the simulation, we varied the LO-phonon energy until the electron scattering rate by the emission of phonons in the third well was maximized. This was vital to ensure rapid depopulation of E_4 and E_3, promoting population inversion. The LO-phonon energy settled upon was 36.263 meV. For each quantum wire diameter, we used SEMC3D to calculate the energies and wavefunctions of the two-dimensional transverse energy subbands. We followed this by injecting electrons into E_5 for each of these subbands. In each case, the average phonon scattering rate in the first two wells was calculated using the average self energy. A Fermi-weighted average of the subbands’ scattering rates was used at 300 K to understand the effects of transverse confinement on scattering by phonon emission at room-temperature. We performed this procedure for quantum wires with diameters of 10 nm, 15 nm, 20 nm, 25 nm, 30 nm, 40 nm, 50 nm and 60 nm.

Results

The phonon scattering rate decreased precipitously for wires with diameters below 30 nm (Figure 3). The peak in scattering rate observed for 30 nm was attributed to resonances between the transverse subbands. The lowest scattering rate was achieved at a diameter of 20 nm. Further reduction in diameter led to an increase in the scattering rate. This was attributed to an increase in the overlap between the initial and final carrier states between the ground states of E_5, and E_3 and E_4.

Conclusion

We have qualitatively demonstrated that the discretization of energy bands by transverse confinement decreases the likelihood of non-radiative scattering by phonon emission. New methods for the construction of quantum wire heterojunctions may provide a means to implement transverse confinement in terahertz QCLs, enabling room-temperature operation.

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