Density Matrix Model Applied to GaAs and GaN-based Terahertz Quantum Cascade Lasers

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Introduction

Quantum cascade lasers (QCLs) are compact sources of coherent radiation that can emit in the terahertz (THz) region of the electromagnetic spectrum. However, room temperature operation has not yet been achieved in THz QCLs; the current highest temperature operation is 199.5 K at 3.22 THz using an AlGaAs/GaAs stucture [1]. Advances in theoretical modelling have contributed to the development of such optimized and novel devices and both Monte Carlo and rate-equation models of QCLs can give good agreement with experimental results [2]. However, these semi-classical models do not account for coherent transport which is thought to be important in THz QCLs due to the typically thick injection barriers and can predict unrealistic results. Like non-equilibrium Green's functions (NEGF), density matrix (DM) modelling accounts for tunnelling but is less computationally intensive which allows for its use as a simulation tool. To reach higher temperatures, it is necessary to suppress the performance degradation mechanisms which occur. These include thermal backfilling and thermally activated LO phonon scattering which occurs as electrons gain enough in-plane kinetic energy to emit an LO phonon and relax to the lower laser level non-radiatively. Therefore, we aim to investigate and then apply the DM approach to the AlGaN/GaN system which has been considered promising due to its higher LO phonon energy (92 meV) compared to that of GaAs (36 meV) [3].

Method

The density matrix method outlined in Ref. 4 allows for coherent modelling of a QCL structure with any number of states. Additionally, the Hamiltonian in the Liouville equation can be be altered to include further submodules in each period so that intra-period transport is modelled coherently. We first model a GaAs structure measured experimentally in Ref. 5 to compare gain/current vs applied field using the rate equation approach, the DM approach, and the DM approach with two submodules per period [6]. The Armadillo C++ linear algebra library [7] is used to solve the Liouville equation in the DM calculations. In the first implementation of the DM approach (Figs. 1 and 4) tunnelling transport only through the injection barrier is considered. Fig. 2 illustrates the unrealistic spikes in current density and gain when electrons scatter between spatially extended subbands (as in Fig. 3) using the rate equation approach.

The formalism is then applied to InAlGaN/GaN (Fig. 5) and AlGaN/GaN THz QCLs with polarization fields included. To calculate tight-binding energies, wavefunctions and coupling strengths it is necessary to remove pyro- and piezo-electric fields from the isolating barriers to maintain periodicity of the bandstructure. Optimizations are limited to diagonal transition designs to account for an enhanced Frölich interaction which is thought to suppress gain in nitride systems [8].

Acknowledgement

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References

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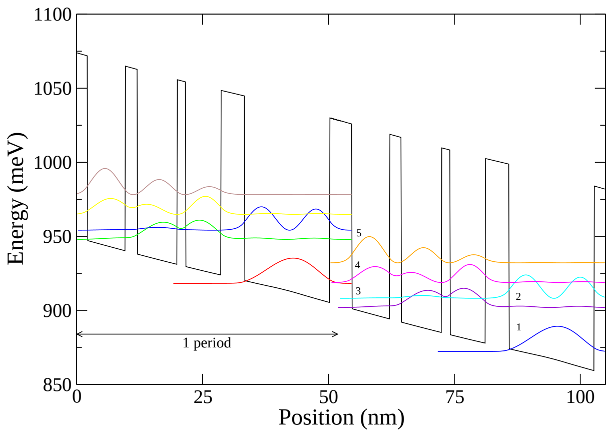

Fig. 1. Energy-band diagram of the ambipolar THz QCL in Ref. 5 at 9 kV/cm. The lasing transition is from state 4 to 3.

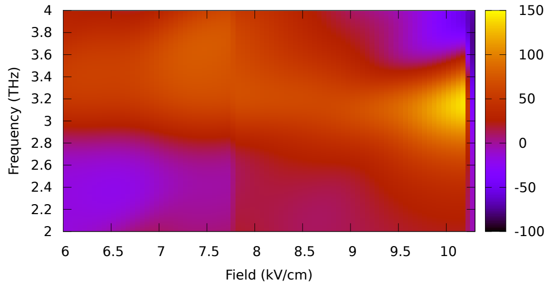

Fig. 4. Simulated gain (or negative absorption) per cm for the ambipolar THz QCL in Ref. 5 at 80 K with an excess electron temperature of 10 K using the density matrix approach.

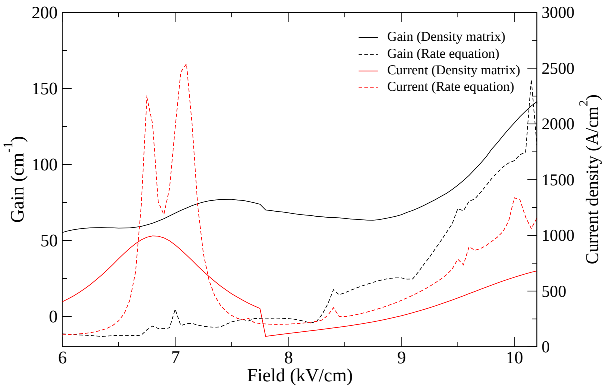

Fig. 2. Current density and gain as a function of forward bias for the ambipolar THz QCL in Ref. 5 at 80 K with an excess electron temperature of 10 K.

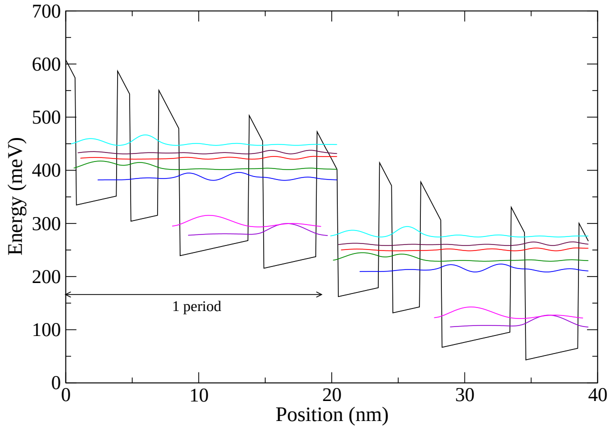

Fig. 5. Energy-band diagram of the GaN THz QCL in Ref. 8 at a forward bias of 80 kV/cm with the tight-binding scheme to obtain the localized wavefunctions shown.

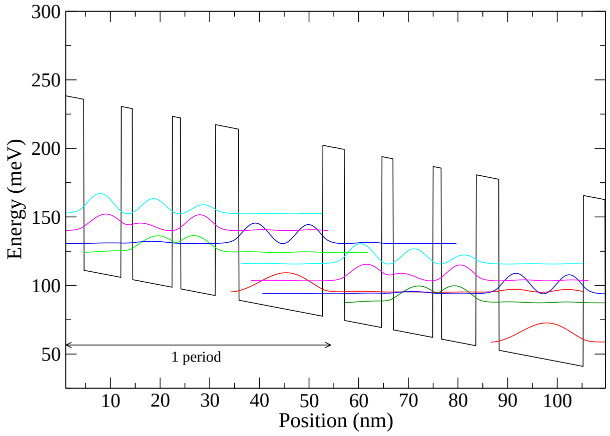

Fig. 3. Energy-band diagram of the ambipolar THz QCL in Ref. 5 at 7 kV/cm without the tight-binding approach. This leads to an extended state 1 wavefunction providing an unrealistic resonant LO phonon current path.