Self-Consistent Quantum Transport Theory: Applications and Assessment of Approximate Models

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In this paper, we present fully self-consistent non-equilibrium Green's function (NEGF) calculations of resonant tunneling diodes and quantum cascade laser structures and a careful assessment of commonly used approximations in the NEGF scheme [1,2].

METHOD

In the present implementation of the NEGF formalism, we take into account acoustic and polar-optical phonon scattering as well as impurity scattering, both within the self-consistent Born approximation. The momentum and energy dependence of all scattering mechanisms is fully accounted for. The electron-electron scattering is incorporated self-consistently within the Hartree approximation. The coupling between the lesser and the retarded Green's function is fully taken into account. In this way, the scattering states, the transition probabilities between them, and their occupations are calculated self-consistently. The Ohmic leads supply electrons with a density of states that is matched to that of the device region near the interface to avoid quantum mechanical reflections. The occupancy of the lead states is represented by a drifted Fermi distribution such that device charge neutrality and current conservation is preserved.

RESONANT TUNNELING DIODE

In Fig. 1, we depict a 40 nm $GaAs/Al_{.3}Ga_{.7}As$ resonant tunneling diode with two 3 nm wide $Al_{.3}Ga_{.7}As$ barriers and a 4 nm quantum well in the center. To the left and right of the barriers, there is a 3 nm intrinsic region and a 12 nm n-doped region with $n=2\times10^{17}$ cm^{-3}, respectively. In order to assess the adequacy of approximate quantum transport models, Fig. 2 shows a comparisin of the full NEGF calculation (circles) with a simplified model (diamonds) that neglects all inelastic and off-diagonal phonon scattering processes ($\Sigma(z,z') \propto \delta_{z,z'}$) at 300 K. Computationally, the latter approach is orders of magnitudes faster. However, the strong inelastic scattering causes the triangular quasi-bound state in front of the left barrier to get filled with electrons. Then, the peak current occurs at a voltage where this quasi-bound state energy is in resonance with the resonant quantum well state [3]. This is a radically different physical situation as in the elastic model where artificial energy conservation prevents the electrons to occupy the quasi-bound state in front of the left barrier.

QUANTUM CASCADE LASER STRUCTURE

In Fig. 3, we show the potential profile and the energy resolved electron density, defined by $\rho(z,E) \propto \mathrm{Im}\int d^2kG^<(z,z,k,E)$, in the active region of a $GaAs/Al_{.15}Ga_{.85}As$ quantum cascade laser structure. The geometry and doping of the structure has been taken from Ref. [4]. The results show clearly the necessity to treat coherent and incoherent quantum transport on an equal footing. The inverted occupation of the two resonance levels in the central double quantum well is clearly visible. The calculated photon emission energy is 17.5 meV (exp: 14.2 meV). The inelastic LO phonon emission (35 meV) across the last barrier on the right hand side efficiently empties the lower of the double quantum well levels, in accord with the data.

ACKNOWLEDGEMENT

Financial support by Deutsche Forschungsgemeinschaft (SFB 631) is gratefully acknowledged.

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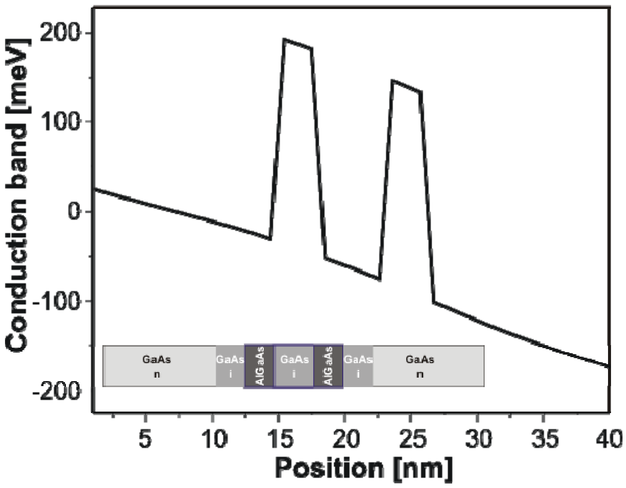

Fig. 1. Conduction band energy of the GaAs/$Al_{.3}Ga_{.7}As$ resonant tunneling structure described in the text, at a bias voltage of 200 mV.

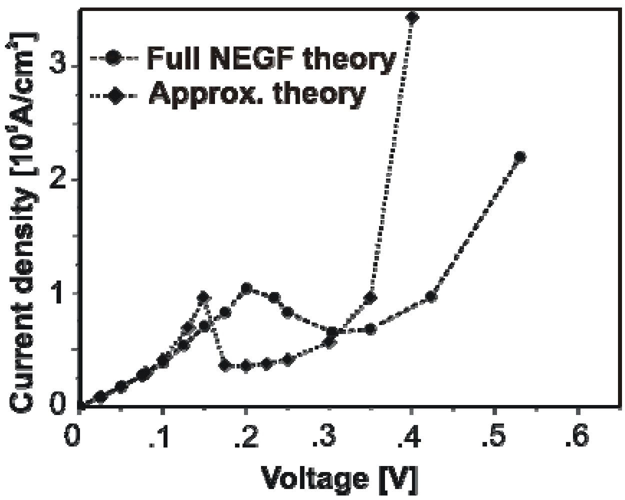

Fig 2. Calculated current density in the GaAs/$Al_{.3}Ga_{.7}As$ resonant tunneling structure of Fig. 1 with (circles) and without (diamonds) off-diagonal inelastic scattering. The connecting lines are only meant to guide the eye.

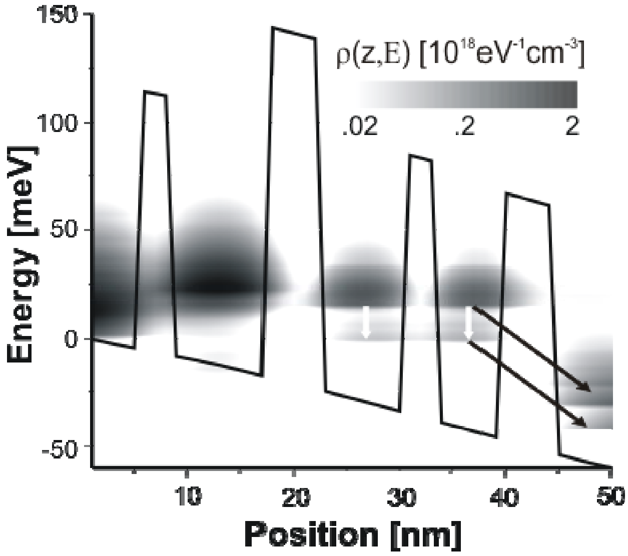

Fig. 3. Potential profile of 50 nm GaAs/$Al_{.15}Ga_{.85}As$ quantum cascade laser structure from Ref. [4] at a bias voltage of 60 mV. The energy resolved electron density is shown as contour plot. The arrows are only meant to guide the eye and show the calculated emission energies (white = photons, black = phonons).