Self-consistent quantum transport theory of carrier capture in heterostructures

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Summary. We present fully self-consistent NEGF calculations for GaAs/InGaAs heterostructures in a regime where multiple scattering, interference, carrier confinement, and carrier capture must be treated on an equal footing. We include the coupling between $G^<$ and G^R within the device self-consistently and take into account scattering within the leads.

1 Introduction

One of the most widely used methods for a realistic prediction of carrier transport in nanodevices is the non-equilibrium Green's function method (NEGF) [1-3]. The seminal paper by Lake *et al.* provided its first detailed numerical implementation for semiconductor devices [4] and provided the basis for the NEMO package [4]. More recently, this method has been applied to several other devices [5-6].

Nevertheless, it has been notoriously difficult to apply this method to resistive nanodevices where scattering is not weak. In Ref. 4, self-consistent coupling between scattering states (represented by the retarded Green's function G^R) and their occupation (represented by the lesser function $G^<$) has been neglected. This effectively violates Pauli blocking. In Ref. 5, these effects have been taken into account, but all scattering self-energies have been taken as momentum-independent scattering. In addition, the leads were treated ballistically in Ref. 4, whereas Ref. 6 considered periodic boundary conditions for the device.

In this paper, we have implemented the NEGF formalism fully self-consistently for resistive open devices were multiple scattering is significant. We take into account acoustic and polar-optical phonon scattering, including their full momentum and energy dependence, and the electron-electron scattering in Hartree approximation. The coupling between $G^<$ and G^R is completely taken into account, thereby preserving Pauli blocking effects. In addition, we include the scattering within the leads self-

consistently with the device regions close to the Ohmic contacts. The structures specifically considered in this paper are assumed to be homogeneous in the lateral (x, y) direction, and to be in contact with two reservoirs at $z = 0$ and $z = L$. The latter are in thermal equilibrium and we assume room temperature throughout. The electrons are described by a single conduction band with effective mass m^*.

2 Theory and Results

We represent all Green's functions in terms of a discrete real space basis along the device direction and in a plane wave basis in the lateral direction. The only remaining major approximation is the neglect of the off-diagonal elements in the inelastic self-energy in real space. For polar-optical phonons, these off-diagonal elements decay as $\Sigma_{\mathrm{po}}(\mathrm{z}, \mathrm{z}') \propto |z - z'|^{-2}$.

In order to illustrate the influence of scattering in a short device where quantum mechanical effects such as interference, carrier confinement, bound state formation, and carrier capture play a significant role, we have performed systematic NEGF calculations for GaAs n-i-n structures with an InGaAs quantum well within the intrinsic region. The total length of the device is 50 nm with 16 nm intrinsic region embedded in between the two 17 nm n-regions with $n = 1 \times 10^{18} cm^{-3}$ each. Within the i-region, there is a 12 nm $In_{.14}Ga_{.86}As$ quantum well of 150 meV depth. The polar optical phonon energy is $\hbar\omega = 35\,\mathrm{meV}$.

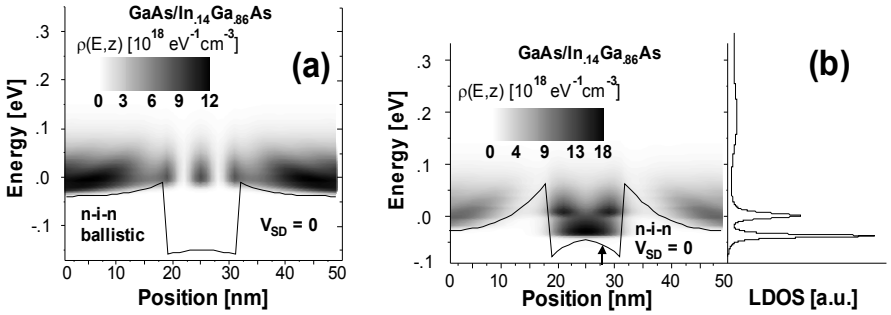

Fig. 1. (a) Contour plot of energy-resolved electron density as a function of energy and position for the GaAs n-i-n with InGaAs quantum well at zero bias, as calculated for zero scattering (ballistic device). The full line shows the self-consistent potential. (b): Same as (a), but with scattering included fully self-consistently.

In Fig. 1(a), we show a ballistic NEGF calculation for the n-i-n structure *in the absence of any scattering* and for zero applied bias. Only the Hartree Coulomb interaction is taken into account. The figure displays a contour plot of $\rho(E,z) = -2\,\mathrm{Im}\int d^2kG^<(z,z,k,E)/(2\pi)^3$, i.e. the local, energy-resolved density, as a function of energy and position within the device. The self-consistent total potential is indicated by a full line. When $\rho(E,z)$ is integrated over the energy, we obtain the density. The zero of energy is always put at the Fermi level of the left contact. Due to the absence of inelastic scattering, the carriers cannot fill the quantum well but occupy a resonance that is derived from the third quantum well state. This explains the interference pattern in the well region at room temperature.

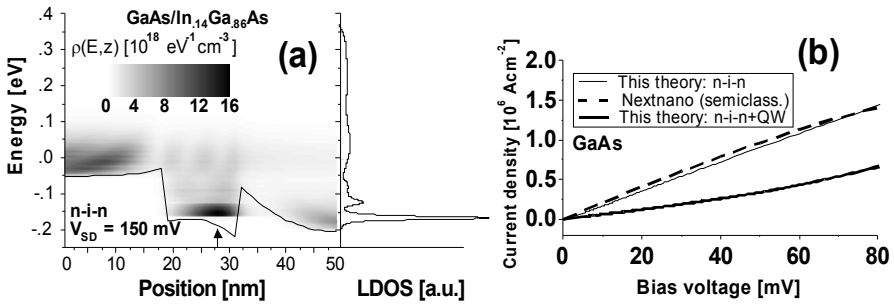

Fig. 2. (a) Same as Fig. 1(b), but with a bias of effectively 150 mV applied. **(b)** Current-voltage characteristics of the GaAs n-i-n structure. The thin line is calculated without a quantum well and compared to a semiclassical calculation carried out with the simulator nextnano3 [7]. The thick line is a full NEGF calculation for the n-i-n structure with a GaInAs quantum well.

The effect of scattering can be seen from the contour graph in Fig. 1(b) where all phonon scattering mechanisms are fully included. To the right of the figure, we display the local density of states near the center of the well region (marked by an arrow). The lowest well state is a true bound state whereas the second one is a resonance state an electron can tunnel out from into the leads. The bottom of the second state lies 59.4 meV below the top edge of the well which is significantly larger than an optical phonon energy. The lowest bound state lies 37.6 meV below the second level which is also a bit larger than $\hbar\omega$. Because we treat scattering within the self-consistent Born approximation, the combination of elastic and inelastic scattering can fill both states in the stationary state.

In Fig. 2(a), we show the same device under an applied bias of effectively 150 mV. At the start of the self-consistent calculation, we apply a bias of 200 mV and allow the Fermi levels to adjust to obey charge neu-

trality within the device and obtain flat band conditions at the contacts. This requires to include the self energies Σ^R near the contacts also within the leads so that the transitions from lead to device are smooth. As one can clearly see, the resonance corresponding to the second well state has been largely emptied by tunneling towards the right lead so that only the lowest well state remains significantly occupied.

Fig. 2(b) displays the I-V characteristics of this diode for small bias. The NEGF calculation agrees very well with a standard semiclassical calculation [7] for a n-i-n structure without a quantum well. The mobility is smaller in the case with the quantum well due to the additional electron charge accumulation within the well that builds up due to the inelastic scattering.

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