A Monte Carlo Method for the Study of Non-equilibrium Phenomena in Low Dimensional Semiconductor Structures

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Abstract

We present a numerical study of the non-equilibrium properties of quasi-one dimensional systems with different confining geometries. Carrier cooling following a laser photoexcitation is analyzed by means of a Monte Carlo simulation which includes all relevant scattering mechanisms. Our results indicate that, for wire made available by todays technology, the carrier dynamical properties of these systems are not so different with respect to bulk GaAs.

I. Introduction

The recent advances in compound semiconductor technology have allowed the fabrication of wire-like regions where quasi 1D confinement is achieved in a narrow-band-gap semiconductor material surrounded by another large-band-gap semiconductor [1]. In particular, such wire-like structures have been fabricated with rectangular and V shaped cross sections whose dimensions are comparable to the carrier coherence length [2,3]. In such structures, carrier transport characteristics are expected to differ from the bulk case as the carrier-phonon scattering rate is affected by the changes in the electronic as well as in the vibrational properties induced by layering [4].

Much of the theoretical work dedicated so far to one dimensional structures has covered mainly the so called "extreme quantum limit", i.e. the case in which only one subband is occupied [1,5]. For wire structures available today, such limit can only be reached under extremely low temperature and electric field conditions. Usually, several subbands are present, and their contribution to carrier transport has to be taken into account.

The aim of the present contribution is to extend the analysis of charge transport in quasi one-dimensional systems to nonequilibrium conditions and nonlinear regimes, by studying realistic wire-like structures where many subbands are normally occupied. This is performed by means of an Ensemble Monte Carlo simulation which allows the study of dynamical evolution of photoexcited carriers, a situation often achieved, for instance, in ultrafast optical experiments. By using the electronic levels and wave functions as derived from an exact solution of Schrödinger's equation, we evaluate the electron-phonon and electron-electron scattering rates which are, in turn, used in the simulation to study the carrier relaxation process. In addition, the method allows us to easily include effects like degeneracy and non-equilibrium phonons.

We will investigate two different type of GaAs-based structures, namely rectangular wires obtained from multi quantum well samples by chemical etching [2,6] and V-grooved wires obtained by growing a thin quantum well on an etched V-shaped profile [7].

II.Electronic states and electron-phonon interaction

Chemical etching gives GaAs-based rectangular quantum wire surrounded along one of the confinement directions by AlGaAs layers, and and free-standing along the other confinement direction [6]. In this case, the conduction band electrons can be reasonably described by a factorized envelope function of the type $\psi(x)\psi(y)e^{i\mathbf{k}_z z}$, where $\psi(x)$ and $\psi(y)$ are respectively the solution of the one dimensional Schrödinger equation in a rectangular potential.

The situation is more complicated for the V-grooved structure. There, in order to study the energy levels and associated eigenfunctions of a two-dimensional V-like profile, we consider the following single-particle Schrödinger equation

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V(x,y)\right)\psi(x,y) = \mathcal{E}\psi(x,y) \tag{1}$$

where ∇^2 denotes the two-dimensional Laplace operator and $V(x,y)$ the two-dimensional potential profile. By considering the following set of two-dimensional planewaves over a rectangular domain Ω:

$$\phi(\mathbf{k}_x,\mathbf{k}_y;x,y) = \frac{1}{\sqrt{\Omega}}e^{i(\mathbf{k}_x x+\mathbf{k}_y y)}\ , \tag{2}$$

the Schrödinger equation (1) can be rewritten as

$$\left(\frac{\hbar^2(\mathbf{k}_x^2+\mathbf{k}_y^2)}{2m} + V(\mathbf{k}_x,\mathbf{k}_y;\mathbf{k}'_x,\mathbf{k}'_y)\right)c(\mathbf{k}'_x,\mathbf{k}'_y) = \mathcal{E}(\mathbf{k}_x,\mathbf{k}_y)\ , \tag{3}$$

where the coefficients $c(\mathbf{k}'_x,\mathbf{k}'_y)$ are the Fourier component of the total wavefunction $\psi(x,y)$ and $V(\mathbf{k}_x,\mathbf{k}_y;\mathbf{k}'_x,\mathbf{k}'_y)$ are the matrix elements of the potential profile in the plane-wave basis given in Eq. (2). By means of a standard numerical procedure, we derive the eigenvalues $\mathcal{E}$ corresponding to the energy levels and the Fourier coefficients $c(\mathbf{k}'_x,\mathbf{k}'_y)$ of the corresponding eigenfunction. Once such coefficients are known, we obtain for each energy level $\mathcal{E}$ the corresponding eigenfunction according to $\psi(x,y) = \sum_{\mathbf{k}'_x,\mathbf{k}'_y} c(\mathbf{k}'_x,\mathbf{k}'_y)\phi(x,y)$. Our numerical results have been obtained for the case of a V-like potential profile shown in Fig. 1. The V-like region is caracterized by a potential V_1 and all the surrounding region by a potential V_2. Fig. 2 shows a plot of the carrier density corresponding to the first four electronic levels. As expected, the ground state exibits a single maximum in the center of the V-like region, while the excited states extend over the whole V-groove exhibit an increasing number of maxima as the order of the level increases.

Starting from the electronic wave functions and energy levels just described, we have computed the electron-phonon scattering rate for the two structures, assuming in both cases bulk LO phonon modes. This approximation should be quite acceptable in these

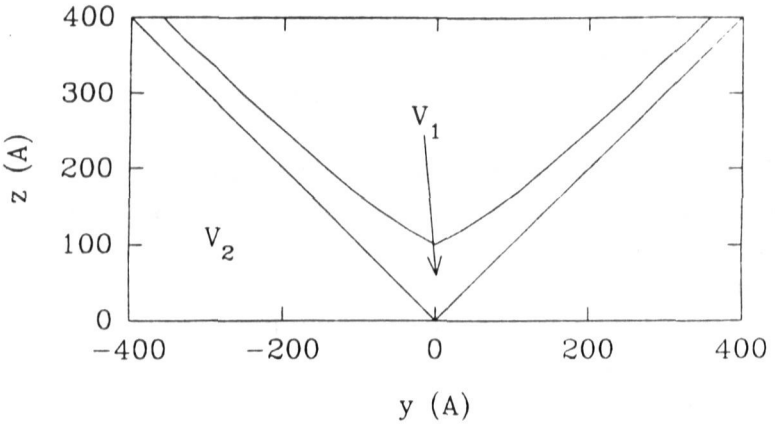

Fig. 1. Section of the V-grooved quantum wire.

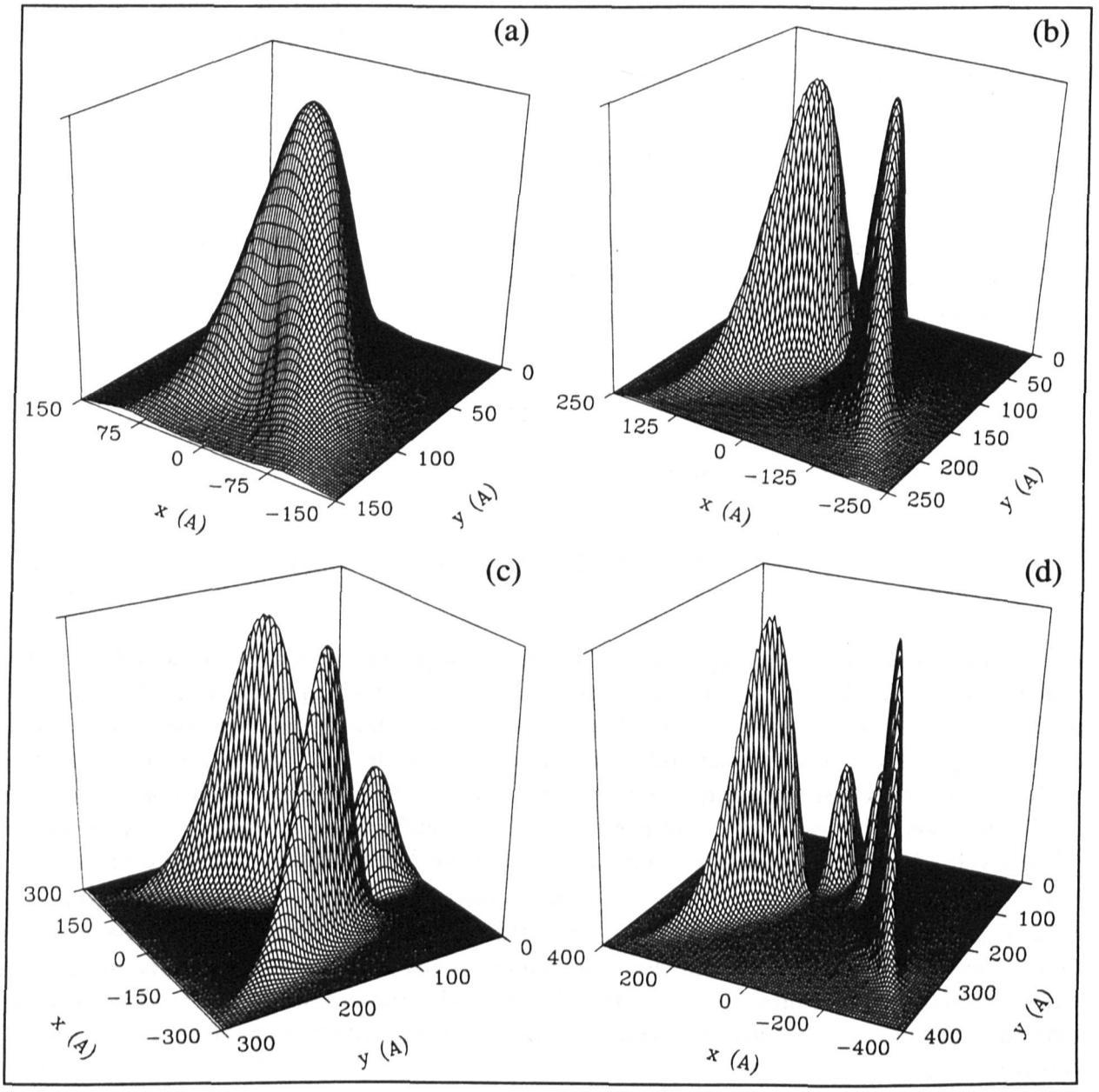

Fig. 2. Electron charge density in the V-grooved quantum wires for the first four energy levels.

systems, which have a large spatial extension, due to the recent findings that the overall electron-LO phonon scattering rate in quantum wells does not differ significantly from the bulk one once the contribution of confined and interface phonon modes is properly accounted for [8]. Figures 3 (a) and (b) show respectively the scattering rate for the rectangular quantum wire and the V-grooved wire (solid lines) [9], compared with bulk GaAs rate (dashed line). In the V-grooved structure, only the first five energy levels are accounted for. Apart from the different position of the energy levels in the two quantum wires, the behavior is very similar and the overall scattering rates in both wires is similar to that of the bulk.

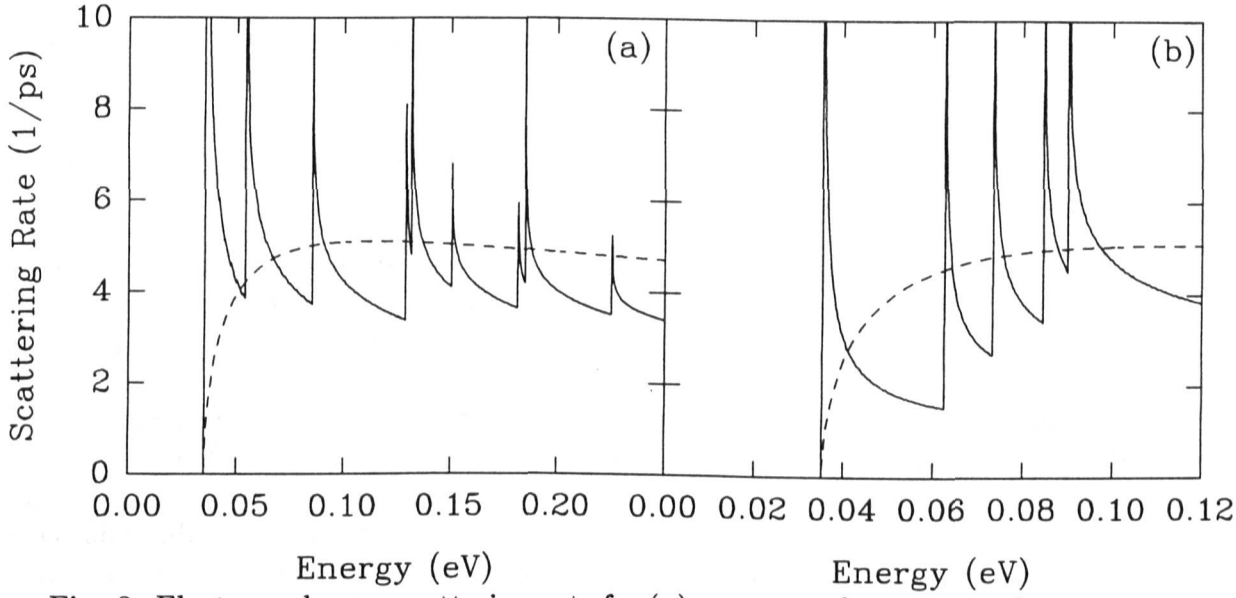

Fig. 3. Electron-phonon scattering rate for (a) a rectangular cross section quantum wires and (b) a V-grooved quantum wires (solid lines), compared with the bulk scattering rate (dashed line).

III. Simulation results

As the scattering rate for the V-groove and the rectangular wire are similar we performed the similation only for the rectangular wire. We espect that the results will be qualitatively the same for the V-groove wire. Our Monte Carlo simulation accounts for the electron-polar optical phonon as well as the electron-electron interaction for both intrasubband and intersubband transitions. The model used here is similar to that described in ref. 10 but the effect of non-equilibrium phonons have been accounted for with a rejection technique. The study of the effect played by the hot phonon population is more difficult in this system, compared to the bulk case, due to the lack of isotropy. The phonon population has been collected using a three-dimensional mesh. The cooling of the excited carriers following a laser excitation is shown in Fig. 4 (a), (b) and (c) respectively for the one dimensional densities of 10^5 cm^{-1}, 3×10^5 cm^{-1} and 10^6 cm^{-1}. As already verified [11] the cooling in the quantum wire (solid line) is slower compared to the bulk (dashed line) due to the reduced intersubband scattering rate, but this effect is modified by the presence of the hot phonon population. At very low densities, i.e. when the phonon population is not driven out of equilibrium, there is a big difference in the cooling between the wire and the bulk. Vice versa at the higher density this difference is strongly reduced. This effect can be clearly attributed to the

reduced efficency of hot phonon reabsorption in the quantum wire caused by the spatial anisotropy of the system.

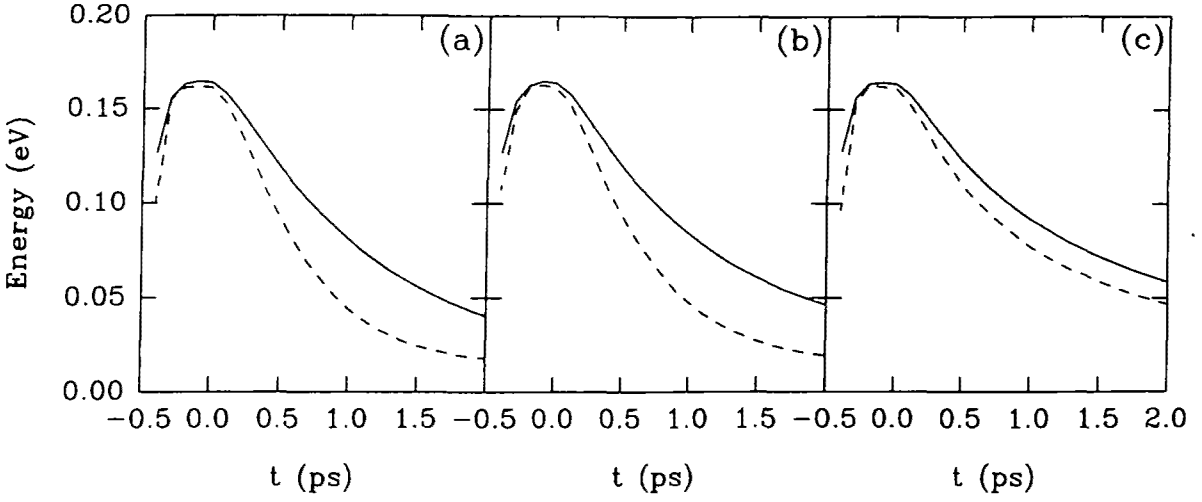

Fig. 4. Electron mean energy after a laser photoexcitation in a quantum wire (solid lines) for three different densities: (a) 10^5 cm^{-1}, (b) 3×10^5 cm^{-1} and (c) 10^6 cm^{-1}, compared with the equivalent results in bulk GaAs (dashed lines).

In conclusion, we have shown that the Monte Carlo method can be easely applied to the study of low dimensional systems described by any type of geometrical potential confinement. The dynamical properties of the carriers can be invesitgated in strongly non-linear and non-equilibrium conditions with any number of occupied subbands. Our results show that, for the relatively large wire made available by the actual technology, the difference between the behaviour of these system and a bulk system is much lower of that predicted and probably only in systems extremely narrow a faster carrier transport will be found.

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