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A New Approach for the Reliable Simulation of Resonant Tunnelling Diodes

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The simulation of resonant tunnelling diodes based on the coupling between a Monte Carlo algorithm, applied to device regions where potential changes smoothly, and the solution of the Wigner function equation in the quantum region (double barrier), is performed for the first time. The results of this work show the advantages of our proposal over present simulation tools, and point out the potentiality of the technique for the reliable simulation of any vertical transport quantum device.

1. Introduction

Resonant tunnelling diodes (RTD's) have recently received much attention due to their application as microwave signal generators and to high speed electronics. Much effort has been dedicated to the development of reliable simulation tools for these devices with an eye towards an improvement in device design and fabrication. In this regard, the Wigner function formulation of quantum mechanics has been demonstrated to be a powerful basis, since it gives a description in phase-space in analogy to classical systems, and dissipative effects can be included in the formulation by adding a relaxation time term or a Boltzmann collision operator in the quantum Liouville equation. Among other results, the intrinsic bistability and current oscillations experimentally found in the negative conductance region [1] have been qualitatively reproduced within this framework. However, to make accurate predictions of device behaviour, it is necessary to extend the simulation domains far above typical small values (70-80 nm), which have been previously considered to avoid excessive computational burden [2-4]. With this aim, we have developed a simulation tool for RTD's that allows to considerably extend the simulation domains by coupling a classical Monte Carlo to the Wigner function solver, the former being applied to device regions where classical transport is expected. A coupling model between both treatments of current transport has been required.

2. The simulation tool

Our simulator solves the Wigner function transport equation (including dissipative effects by means of a relaxation time term) in the quantum region (double barrier) and the Boltzmann equation in the classical regions. A Monte Carlo code, including phonon and impurity scattering, has been used to solve the latter equation. At each iteration step, charge carriers are injected from the reservoirs (external contacts to the device) according to an ohmic contact model [5]. From the quantum regions, the portion of the Wigner distribution function at the boundaries with momentum pointing towards the classical regions is used to randomly determine the momentum of injected carriers and the number of them. To solve the quantum Liouville equation, the Monte Carlo distributions of carriers in k-space in the adjacent cells to the quantum window are used as boundary conditions. Only a straightforward transformation is required to convert this distribution to the Wigner formalism. Finally, to achieve self-consistency, the Poisson equation is integrated at the end of each time step in the whole device. The process is iterated until steady-state conditions result.

3. Results

Rather than obtaining accurate results, the main aim of this work is to demonstrate that our proposal is promising to develop a new simulator for RTD's, and to point out the advantages of it over present tools. In figure 1, the I-V characteristic that results from the application of successive voltage steps of 0.02V increment is depicted. The evolution of current up to steady-state, that results after the sudden voltage switches, is also represented (averaged over the iteration period to filter noise). Only about 500 iterations are needed to obtain a stable current (except in the negative conductance region). Being the device dimension of 450 nm, the computational time required to obtain the I-V curve is not significantly higher than

those of present simulation tools, which consider only the solution of the quantum Liouville equation in boxes of 70-80 nm width. This is so because, for typical Monte Carlo parameters, it is the Liouville solver which determines the CPU time. Figure 2 shows the steady state electron density and potential profile obtained at resonance. Clearly, the main qualitative features expected are obtained (charge accumulation in the well, charge neutrality at the extremes of the device and a carrier density peak slightly separated from the first barrier). The fact that charge accumulation in the emitter and charge depletion in the collector extend far above the quantum boundaries points out the need to consider the simulation domains of this work. The momentum distribution of carriers under resonance (figure 3) shows that the tunnelling ridge (already found in previous Wigner distribution function simulations) is also reproduced, although it progressively vanishes due to thermalization of carriers in the collector. The absence of spurious at the boundaries between the classical regions and the quantum window indicates that the coupling model presented is useful to extend the integration regions and to perform a more rigorous simulation of RTD's.

4. Conclusions

In summary, we have developed a new simulation tool for RTD's which allows an extension of the simulation domains. This has been achieved by solving the Boltzmann equation in the classical regions by means of a Monte Carlo solver, which has been coupled to a Liouville solver, applied to the quantum regions. The results shown in the work, although preliminary, clearly reproduce the main features expected for this devices, and show the need to increase the spatial simulation domains up to the values considered in this work, which are far above the usual values found in the literature.

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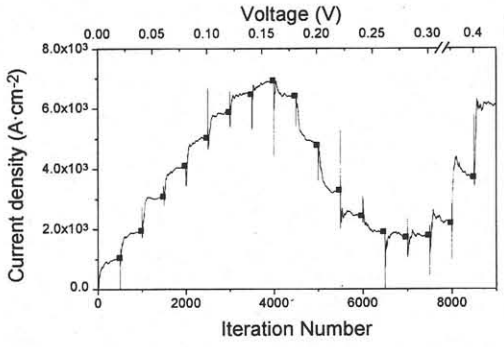

Fig.1: Evolution of current obtained by applying voltage switches of 0.02V to a RTD with barriers of 3 nm width and 0.3 V height, and a well width of 8nm. In the classical region the cell size is 2.5 nm and the simulation is started-up with 100 particles per cell. The considered doping level is $1.8x10^{16}cm^{-3}$ and the time step is 10 fs.

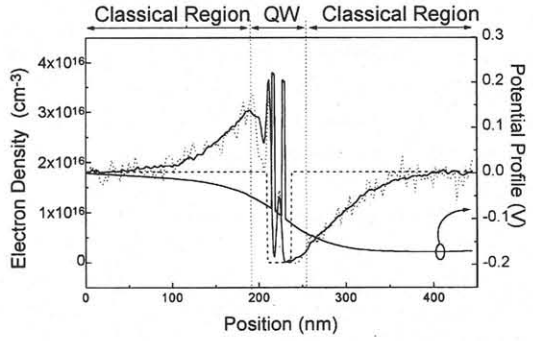

Fig.2: Self consistent potential profile and electron concentration corresponding to the simulation of fig. 1, obtained under resonance. Both the instantaneous (dotted line) and the charge density averaged over the latter iteration steps (solid line) are depicted.

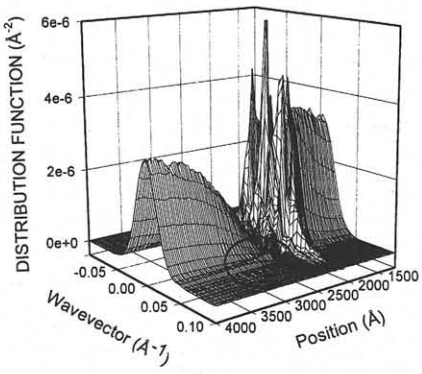

Fig. 3: Phase space distribution function that results at resonance, showing the tunnelling ridge (circle). To perceive the details, only a portion of the device is shown.