Genetic Algorithm Applied in Optimising 1D Coupled Quantum Wells Structures

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Abstract:

We present an idea of how a genetic algorithm could be used in design optimisation of nanoelectronic devices. The genetic algorithm evolves new device geometries and parameters from an initial device, searching for better solutions of a specific problem. A model that represent in great detail the dynamics of tunneling events for electrons in coupled quantum wells, making use of fundamental physical principles is used to evaluate the fitness function of these evolved devices.

1. Introduction

The development of the next generations of integrated circuits will require new working devices with extremely small physical dimensions. These new working devices need not to mimic CMOS Field Effect Transistors, where current is controlled by gate voltage. Single electron devices such as SET's (Single-electron Transistors), CQW's (Coupled Quantum Wells), and CQD's (Coupled Quantum Dots) are being considered. To understand single electron transport in such devices, we are developing a consistent model and a robust simulation strategy [1].

These new devices are understood to work in a non-intuitive way, making them hard to design. As a result it makes sense to investigate the use of intelligent automatic design techniques, such as genetic algorithms [2], which have proven to exhibit many desirable properties such as requiring no auxiliary information about the search space, except a fitness function, and are considered to be very robust.

2. Simulation

The simulation model used [1], attempts to represent in greater detail the dynamics of tunneling events for electrons in CQW's, making use of fundamental physical principles. Among those principles we highlight the charge and energy conservation. Our model tries to overcome some of the limitations of the orthodox approach [3], in a physically intuitive manner.

The simulation scheme is presented in Figure 1, where two quantum wells, coupled through a tunneling junction are under the influence of an externally applied electric field. Let us consider that somewhere in the setup there is an excess electron. We are assuming the absence of any additional charges, free to move under the action of an externally applied electric field, or under the influence of the confined electron and its movement. We also assume the absence of magnetic fields.

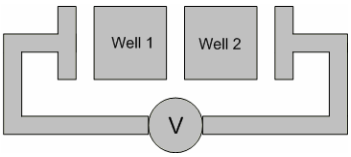

Figure 1: Coupled Wells with Externally Applied Bias.

Simulation starts with an externally applied voltage forcing electron confinement in one of the wells. In first 5 ps (picoseconds) of simulated time the voltage is removed linearly. The electron confinement is then verified evaluating the difference of charge fraction inside each well. Then, a second voltage, in the opposite way is applied, increasing from 10 to 15 ps and decreasing from 15 to 20 ps, linearly. Final results are collected after 25 ps of simulated time.

Figure 2 presents the charge time evolution in each well. Initially the electron is scattered, but a little time later, forced by the voltage ramp, the electron is confined in well 2. Then, the second ramp is applied and forces electron tunneling to well 1. One can see from Figure 2 that no other significant charge exchange is observed until the end of simulation.

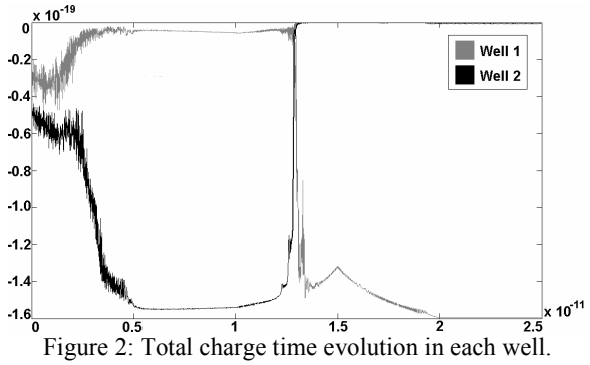

Figure 2: Total charge time evolution in each well.

Figure 3 presents the electronic current, evaluated in the middle of barrier between wells. Comparing Figures 2 and 3 it can be observed that the simulation correctly predicts the charge transfer processes in the system. Tunneling time definition used here is the time while significant current (i.e. greater than 10^{-7}) is present after 10 ps. This criterion is a magnitude order higher than device simulator noise due precision errors.

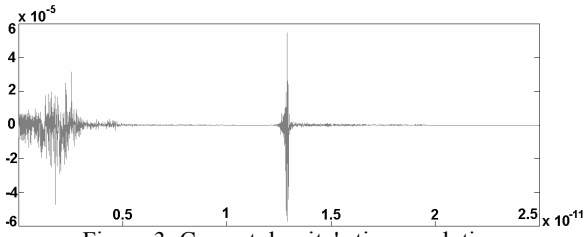

Figure 3: Current density's time evolution.

3. Evolutionary Framework

The idealized evolutionary framework is presented in Figure 4, were the genetic algorithm has been developed in MATLAB [4] and the device simulator in ANSI C. The parameters that will be used are presented in genetic code form in Figure 5.

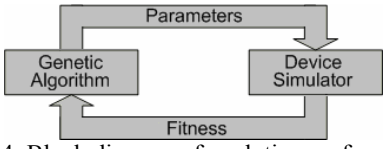

Figure 4: Block diagram of evolutionary framework.

Cell Width	Wells Width	Barrier Width	Potencial Heigth

Figure 5: Genetic code parameters representation.

The block diagram of the genetic algorithm is presented in Figure 6. As a whole, the scheme proceeds in the following fashion:

1 - It starts with a set of initial devices, which are randomly created. These devices are genetically represented in an array of values (code), were each position represents a device parameter.

2 – Solutions are simulated and simulator evaluates fitness of each device.

3 – A selection criterion determines which parent devices will be used to create new offspring devices.

4 – Some genetic operators like recombination and mutation are used to generate a new set of devices.

5 – Repeat steps 2, 3 and 4 until either a specified number of generations have been run, or some threshold for fitness has been achieved.

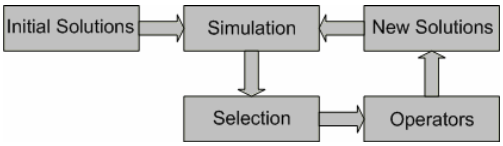

Figure 6: Block diagram of the genetic algorithm.

During the process of evolution some limitations have to be imposed to genetic algorithm search of the solution space to guarantee a final result with feasible devices. Materials properties like barrier insulator breakdown voltage, conductivity, ohmic resistance, in addiction of fabrication technologies limitations are considered.

4. Fitness Function and Operators

The adaptation goal is determine solely from the fitness function. That is a major characteristic of genetic algorithms, which require no prior knowledge of the specific optimization task. So it plays a very important role in any genetic algorithm based system.

Our study does not have yet a final fitness function specified. A relation between charges inside wells associated with the tunneling time, that is determined through current density time evolution, is now being used. Others fitness functions could be specified, allowing design with different characteristics.

The genetic operators that will generate new solutions also play an important role. The traditional operators are recombination and mutation [5]. Recombination operator were offspring parameters are the parents parameters average is now being used, but others operators are been studied and will be implemented soon.

5. Conclusion and Future Work

We are presenting an idea of how genetic algorithms could be applied in the optimisation of nanostructures. New non-conventional device geometries and non-intuitive characteristics could be found.

We also have plans to extend the simulation model for 2D and 3D cases and adapt the evolutionary framework for these cases.

6. Acknowledgements

The authors gratefully acknowledge CAPES-Brasil, CNPq-Brasil and PADCT-Brasil for financial support.

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