"Genetically Engineered" Nanoelectronics

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Abstract

The quantum mechanical functionality of nanoelectronic devices such as resonant tunneling diodes (RTDs), quantum well infrared photodetectors (QWIPs), quantum well lasers, and heterostructure field effect transistors (HFETs) is enabled by material variations on an atomic scale. The design and optimization of such devices requires a fundamental understanding of electron transport in such dimensions. The Nanoelectronic Modeling Tool (NEMO) is a general-purpose quantum device design and analysis tool based on a fundamental non-equilibrium electron transport theory. NEMO was combined with a parallelized genetic algorithm package (PGAPACK) to evolve structural and material parameters to match a desired set of experimental data. A numerical experiment that evolves structural variations such as layer widths and doping concentrations is performed to analyze an experimental current voltage characteristic. The genetic algorithm is found to drive the NEMO simulation parameters close to the experimentally prescribed layer thicknesses and doping profiles. With such a quantitative agreement between theory and experiment design synthesis can be performed.

1 Introduction

Miniaturization of measurement, analytical and communication systems is required to meet the NASA/JPL goal to reduce payload in future space missions. Typical system requirements include the detection of particular spectral lines, associated data processing, and communication of the acquired data to other subsystems. Silicon device technology dominates the commercial microprocessor and memory market, however, semiconductor heterostructure devices maintain their niche for light detection, light emission, and high-speed data transmission. The production of these heterostructure devices is enabled by the advancement of material growth techniques, which opened a vast design space. The full experimental exploration of this design space is unfeasible and a reliable design tool is needed.

The Nanoelectronic Modeling tool (NEMO) was developed as a general-purpose quantum mechanics-based 1-D device design and analysis tool from 1993-97. The tool is available to US researchers by request on the NEMO web site [1]. NEMO is based on the non-equilibrium Green function approach, which allows a fundamentally sound inclusion of the required physics: bandstructure, scattering, and charge self-consistency. The theoretical approach is documented in reference [2] while some of the major simulation results are documented in references [3,4]. This paper highlights the recent work on genetic algorithm based device analysis.

2 Genetic Algorithm-Based Quantum Device Analysis

RTD designs involve the choice of material compositions, layer thicknesses, and doping profiles. The full exploration of the design space using purely experimental techniques is unfeasible due to time and financial constraints. For example, it takes a well-equipped research laboratory approximately five working days [5] for the growth, processing and testing of a particular resonant tunneling diode design. NEMO can provide current voltage characteristics (I-V's) that are in quantitative agreement with experimental data [3,4] within minutes to hours[1] of CPU time for a single set of device and material parameters. With this quantitative simulation capability the design parameter space can be explored expediently once an automated system for the design parameter variation is implemented. This paper summarizes the combination of NEMO with a massively parallel genetic algorithm package (PGAPACK) [6]. For a detailed description of genetic algorithms we refer the reader to reference [7]. In this work the RTD is used as a vehicle to study the effects of structural and doping variations on the electron transport. Several I-V of different devices that are part of a well-behaved test matrix of experimental data published in reference [3] are used as a design target. Details of the

[1] The actual CPU time needed for a single I-V simulation depends strongly on the choice of material systems, bandstructure models, temperature scattering models, and bias points. The individual I-V characteristics presented here take about 30 minutes to compute on a single 200MHz R10000 CPU of an SGI Origin.

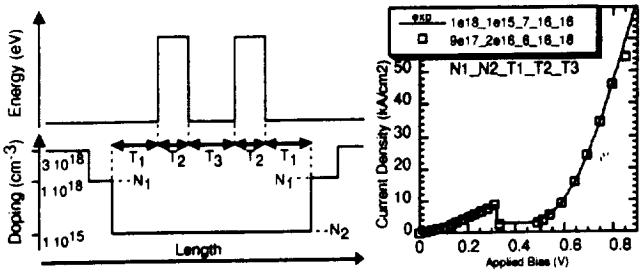

Figure 1: (a) Conduction band edge without charging effects and doping profile along the growth axis of the RTD. (b) Experimental and optimal fit simulated current voltage characteristic. Layer thicknesses are within the experimental uncertainty. The unintentional doping in the central device region is one order of magnitude larger than typically assumed.

preparation of the simulation.target, the fitness function and the physical electron transport model can be found in reference [8].

3 The Numerical Experiment

In the numerical experiment described in Figure 1, five parameters (2 doping concentrations, N_1, N_2, and 3 thicknesses, T_1, T_2, T_3) are varied within the genetic algorithm in order to achieve the best fit to an experimental I-V curve. The simulation is started from a random population of 200 parameter sets. The doping population is logarithmically distributed around the nominal values by factors of 10 ($N_1 \in [1x10^{17},1x10^{19}]$, $N_2 \in [1x10^{14},1x10^{16}]$). The layer thickness population is uniformly distributed around the nominal value by 10 monolayers ($T_1 \in [1,17]$ and $T_2,T_3 \in [6,26]$). In each generation 63 of the worst genes[2] are dropped out of the population and new genes are generated from the rest by mutation and crossover. The mutation and the crossover probablities are set to 50%. Mutation allows the parameters to leave the original parameter range.

4 Simulation Results

One example of our simulation results involving an I-V is shown in Figure 1b. The physical structure was specified to the grower to have 16 monolayers (ml) of barriers (T_2) and well (T_3), no intentional doping in the central device (N_2=1x10^{15} cm^{-3}), N_1=1x10^{18} cm^{-3} doping in the low doping spacers, and 3x10^{18} cm^{-3} in the high doping contacts (see Figure 1a). The simulation is started from the random populations as described in the previous section. The genetic algorithm converges for to the nominal structure values, well within the experimental uncertainty as shown in Figure 1b.

[2] LAPACK is implemented with MPI where N-1 of N processors are slaves to one master processor. In a cluster of 64 CPU's we therefore renew 63 genes in every generation.

It has been found in previous work [3] (by empirical adjustments) that for these experimental samples the well widths must be increased in the simulation by a few monolayers versus the nominal values to achieve the best agreement with experimental current voltage characteristics. The genetic algorithm drives the best fit to the same conclusion.

The the reduced doping in the central device region is intended to reduce ionized dopant scattering in the resonant tunneling diode. The low doping level is typically referred to as "no-intentional doping" and it is typically assumed to be 1x10^{15} cm^{-3}. The simulations indicate that this doping level is about one order of magnitude higher than assumed.

5 Summary

A physics-based resonant tunneling device analysis driven by a genetic algorithm with quantitative agreement between experiment and theory has been achieved. With such quantitative agreement within this material system device synthesis is expected to be possible, where a desired performance characteristic is prescribed to the simulator and a new arrangement of layer thicknesses and doping profiles is generated.

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References

[1] The Nanoelectronic Modeling homepage is moving. See http://www-hpc.jpl.nasa.gov/PEP/gekco/nemo.html.

[2] R. Lake et al., J. Appl. Phys., **81**(12), 7845 (1997).

[3] G. Klimeck et al., IEEE DRC, 1997: p. 92.

[4] R. C. Bowen et al., J. Appl. Phys., **81**, 3207 (1997).

[5] A. C. Seabaugh, Texas Instruments Inc., private communication, 1997.

[6] D. Levine, Parallel Genetic Algorithm Library http://www-unix.mcs.anl.gov/~levine/PGAPACK/index.html.

[7] D. Goldberg, Genetic Algorithms in Search, Optimization and Machine Learning, New York, Addison-Wesley (1989).

[8] G. Klimeck, C. H. Salazar-Lazaro, A. Stoica, and T. Cwik, accepted for publ. in J. of Materials Research Society (1999).