

Low temperature electrostatic simulations of realistic large-scale structures

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ABSTRACT

We present a tool in the NEMO5[1] nano-electronics simulation software, targeting large scale quantum confined structures such as quantum dots, Quantum Point Contacts (QPCs) and quantum Hall interferometers. This tool can either do a semi-classical electrostatic or a quantum mechanical Schrödinger-Poisson simulation of the substrate and hetero-structure with top-gates. It can be used to obtain potential and charge-density (along with the wave-functions). This information can be used for insights into device design, or as an input to the NEMO5 tight-binding and transport solvers to do a multi-scale multi-physics simulation of the device.

INTRODUCTION

Advances in Scanning Tunneling Microscopy (STM) and Molecular Beam Epitaxy (MBE) techniques are allowing fabrication of high quality confined structures[2][3]. Some applications of these techniques are in the fabrication of quantum dots for quantum computing, QPCs for read-out of quantum state, Fabry-Pérot interferometers for measuring quantum Hall effect etc. Design of these devices is not a straightforward task.

Simulation tools are helpful in determining the optimal gate configuration and voltages for getting specific electronic configurations. Tools such as QCAD[4] and nextnano³[5] already exist for simulating electrostatics in Si and GaAs based devices. This tool targets similar simulations in the NEMO5 framework, which gives it potential to be a powerful bridge between realistic devices and detailed physics simulations including non-equilibrium quantum transport capabilities. This tool is also targeted for the nanoHUB users making it accessible to everyone.

METHODOLOGY

We first solve for the semi-classical density and potential using the Thomas-Fermi approximation to get a good initial guess. This potential is then used to solve the effective mass Schrödinger and Poisson equations self-consistently. The predictor-corrector method is used for faster convergence of the Schrödinger-Poisson system.

We employ Dirichlet boundary conditions for top gates in GaAs and Si-SiO₂ hetero-structures. Top gates in Si-SiO₂ structures are treated as Schottky or Ohmic contacts. For Schottky contacts, we set the Dirichlet boundary condition as

$$\phi_{dirichlet} = V_g + \frac{\Phi_S - \Phi_M + E_C - E_F}{q}$$

where Φ_S and Φ_M are semiconductor and metal work functions respectively, and V_g is the gate voltage. The electrons are assumed to be confined in 3D by the gates.

We use Finite Element Method (FEM) to discretize Schrödinger and Poisson equations in 3D. The libraries LibMesh[6], PETSc[7] and SLEPc[8] are used for discretizing and solving the equations. The library VTK is to be used for reading in 3D gate structures, which are converted from SEM images. For now, we create gate structures using simple shapes.

RESULTS

We can currently solve semi-classical density using our tool. Fig. 1 shows potential in a Si Double Quantum Dot[9] (DQD) device from a self-consistent semi-classical simulation. Fig. 2 shows potential for the same device simulated using Sentauros[10]. The potentials in Fig. 1 and Fig. 2 differ a bit because of different boundary conditions, Fig. 3 shows converged potential for a GaAs DQD device.

Our next goal is to perform self-consistent Schrödinger-Poisson simulations of these devices

and calibrate capacitances with experimental measurements.

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REFERENCES

- [1] S. Steiger, M. Povolotskyi, H. H. Park, T. Kubis, and G. Klimeck, "NEMO5: A parallel multiscale nanoelectronics modeling tool," *IEEE Trans. Nanotechnol.*, vol. 10, no. 6, pp. 1464–1474, 2011.
- [2] M. Manfra, "Molecular Beam Epitaxy of Ultra-High Quality AlGaAs/GaAs Heterostructures: Enabling Physics in Low-Dimensional Electronic Systems," *arXiv Prepr. arXiv1309.2717*, pp. 347–376, 2013.
- [3] F. J. Rueß, W. Pok, T. C. G. Reusch, M. J. Butcher, K. E. J. Goh, L. Oberbeck, G. Scappucci, A. R. Hamilton, and M. Y. Simmons, "Realization of atomically controlled dopant devices in silicon," *Small*, vol. 3, no. 4, pp. 563–567, 2007.
- [4] X. Gao, E. Nielsen, R. P. Muller, R. W. Young, A. G. Salinger, N. C. Bishop, M. P. Lilly, and M. S. Carroll, "QCAD Simulation and Optimization of Semiconductor Quantum Dots," no. April, pp. 1–20, Mar. 2014.
- [5] S. Birner, S. Hackenbuchner, M. Sabathil, G. Zandler, J. a. Majewski, T. Andlauer, T. Zibold, R. Morschl, a. Trellakis, and P. Vogl, "Modeling of semiconductor nanostructures with nextnano3," *Acta Phys. Pol. A*, vol. 110, no. 2, pp. 111–124, 2006.
- [6] B. S. Kirk, J. W. Peterson, R. H. Stogner, and G. F. Carey, "libMesh: a C++ library for parallel adaptive mesh refinement/coarsening simulations," *Eng. Comput.*, vol. 22, no. 3–4, pp. 237–254, Nov. 2006.
- [7] S. Balay, W. D. Gropp, L. C. McInnes, and B. F. Smith, *Efficient Management of Parallelism in Object Oriented Numerical Software Libraries*. Birkhäuser press, 1997.
- [8] V. Hernandez, J. E. Roman, and V. Vidal, "SLEPc," *ACM Trans. Math. Softw.*, vol. 31, no. 3, pp. 351–362, 2005.
- [9] M. Veldhorst, C. H. Yang, J. C. C. Hwang, W. Huang, J. P. Dehollain, J. T. Muhonen, S. Simmons, A. Laucht, F. E. Hudson, K. M. Itoh, A. Morello, and A. S. Dzurak, "A Two Qubit Logic Gate in Silicon," pp. 1–6, 2014.
- [10] "Synopsys Sentaurus Semiconductor TCAD Software." East Middle eld Road, Mountain View, CA 94043 USA.

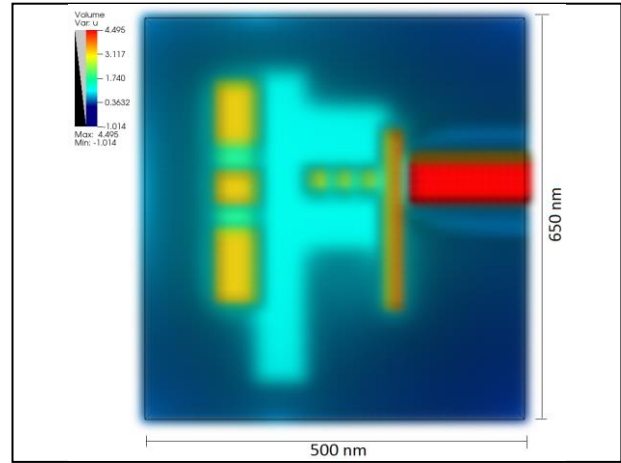


Fig. 1. Potential on top surface from a semi-classical simulation of a Si DQD device with top Al gates using NEMO5.

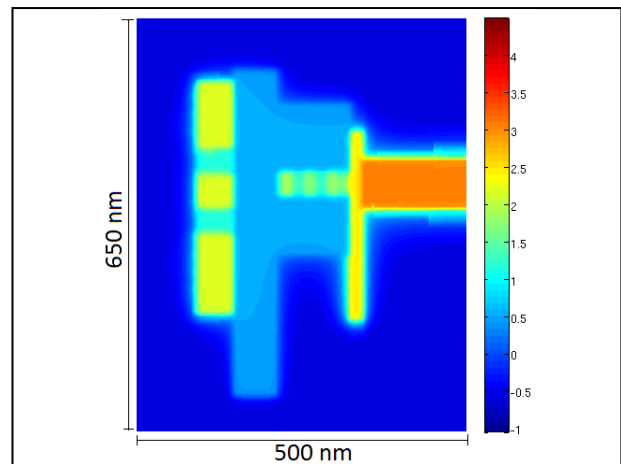


Fig. 2. Potential on top surface from a semi-classical simulation of a Si DQD device with top Al gates using Sentaurus for comparison with Fig. 1.

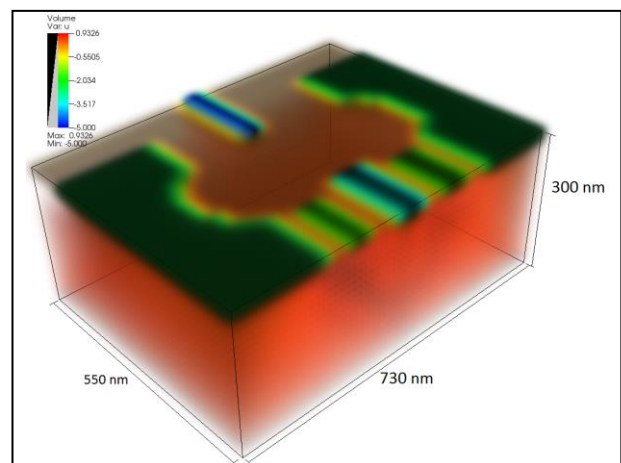


Fig. 4. Potential inside a GaAs spin DQD from a semi-classical simulation using NEMO5 tool.