Efficient quantum-mechanical models in simulation of modern nanoscale devices

A.Fedoseyev [a,*], A. Przekwas [a], M. Turowski [a], M.S. Wartak [b]

[a] *CFD Research Corporation, Huntsville, Alabama 35805, USA.*

[b] *Department of Physics and Computer Science, Wilfrid Laurier University Waterloo, Ontario,N2L 3C5, Canada.*

A family of simple and efficient quantum-mechanical models for simulation of modern nanoscale devices is presented. These models are used for quantitative calculations of quantum currents in nanoscale electronic device. Specifically, we used them to simulate the tunneling current through thin barrier in vertical cavity surface emitting laser (VCSEL), direct and reverse tunnel currents through the tunnel junction, Schottky contact etc.

The models have been successfully implemented within the drift-diffusion approach of our Semi-Device solver. We provided a series of simulation and compared these simple models with published data, experimental measurements and other complicated models including Wigner function method, quantum Boltzmann transport models and others [1,2].

Our main conclusions are: the proposed models are quite accurate, and computationally efficient. The results for single barrier device show a good comparison with Wigner function method results. Schottky contact model compared well with experimental measurements. Tunnel junction model has correctly demonstrated negative differential resistance for forward bias and exponentially growing current for the reverse bias. The implementation is self-consistent, has no tune up parameters, and has not caused slow convergence or numerical instability in the validation test provided.

Experimental data for a single barrier device would be the best test case, but they are not available. Instead, we choose the single tunneling barrier test problem. This problem has been solved by different methods and independently by different authors. The test structure consists of / 2.5 nm 0.22V AlGaAs / barrier in / 40 nm GaAs / AlGaAs / device. This problem was solved by (i) Wigner function method [9], and (ii) using the Quantum Boltzmann transport equation [1,2], (iii) Boltzmann transport equation [1,2], (iv) the DD model [1]. More details on this can be found in [1,2].

[1] A. Fedoseyev, V. Kolobov, R. Arslanbekov and A. Przekwas, Kinetic simulation tools for nanoscale semiconductor devices, /Microelecronic Engineering/, v. 69 (2003) p. 577-586.

[2]. Tsuchiya, H. and T. Miyoshi, (1999) Quantum Transport Modeling of Ultrasmall Semiconductor Devices, Invited Paper, Special Issue on TCAD for Semiconductor Industries. IEICE Trans. Electron E82-C, 880.

* Corresponding author. Tel. (256)726-4928. FAX (256)726-4806.
Email addresses: aif@cfdrc.com (A.Fedoseyev), mwartak@wlu.ca (M.S. Wartak).