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Tutorial Title:

Nano-Electronic Devices ï From Semi-Classical to Quantum Modeling

The goal of this Tutorial is to introduce interested scientists from Academia and Industry in advanced simulation methods needed for proper modeling of state-of-the-art nanoscale devices.

Tutorial Content: We will begin with a description of the Monte Carlo device simulation method as a way of solving the Boltzmann Transport Equation for both bulk and confined carriers. Particle-based device simulation scheme will be introduced next. Afterwards we will introduce ways of correcting the classical Monte Carlo scheme to properly account for the short-range Coulomb forces and quantum-mechanical space-quantization effects due to the increased importance of these effects in the operation of nano-scale devices. For the inclusion of the short-range Coulomb interactions within a particle-based device simulation scheme we will introduce the particle-particle-particle-mesh coupling method and the fast multipole method. Regarding the quantum-mechanical corrections within a particle-based device simulation scheme we will discuss the effective potential method due to Ferry and the parameter-free effective potential method proposed by Ringhofer and Vasileska. Example will be given regarding the simulation of short narowire SOI device. We will consider the influence of quasi-two-dimensional confinement on device behavior and discuss fluctuations in device characteristics, such as threshold voltage, due to unintentional dopants. A prototypical 2D Monte Carlo code for modeling MOSFETs will be distributed to the participants.

In the second half of the tutorial we will begin with the description of ballistic transport, calculation of the quantum-mechanical current density when knowing the transmission coefficient. For the calculation of the transmission coefficient, we will give a brief description of the transfer matrix method, scattering matrix approach and the Usuki method. Afterwards, we will introduce the concept of Greenôs functions and their application to modeling of nano-scale devices that either operate on fully quantum-mechanical principles or have pronounced quantum effects so such an approach is needed for proper description of the device operation. In this regard, we will talk about two schemes for solving for the Greenôs functions problem in nano-scale devices. We will first introduce the recursive Greenôs function method that had been the most popular method until recently, since it can be effectively applied to 1D and/or 2D geometries. When discussing the application of the recursive Greenôs function method, that has been promoted by the Purdue Group (Datta, Anantram, Klimeck), we will clearly describe the advantages and deficiencies of this method related to its inability to simultaneously calculate source-drain current and gate leakage (as it is in reality a quasi-1D approach). As a solution to this problem, we will introduce the Contact Block Reduction method due to Mamaluy and co-workers, which is able to simulate devices with arbitrary number of contacts and gives at the same time the current between any two contacts. The other advantage of the CBR method is the fact that this method is easily extendable to three spatial directions which is not the case with either the Usuki method and/or the recursive Green's functions approach. We will finish the tutorial with the example of modeling FinFET devices with the quasi-3D CBR method. Issues that we will present and we consider to be very important for nano-scale FinFETs include: source-drain tunneling and the flattening of the transfer characteristic at low gate voltages, inclusion of interface roughness into the model via real-space treatment and how it affects the device on- and off-current and the device cut-off frequency, the role of temperature and the inclusion of phonon scattering into the theoretical model via the Buttiker's probe method.

A **Table of Contents** of the topics covered in the tutorial is outlined below:

1. Monte Carlo simulation:
    a. Monte Carlo Method for solving the Boltzmann Transport Equation
        i. Bulk carriers
        ii. Confined carriers: quasi-two-dimensional electron gas and quasi-one-dimensional electron gas
    b. Device simulation
    c. Inclusion of short-Range Coulomb interactions in a particle-based device simulation scheme
    d. Inclusion of quantum-mechanical space quantization via an effective potential scheme
    e. Simulation results from modeling narrow-width SOI MOSFET devices

2. Quantum-Mechanical Modeling
    a. Calculation of the current
    b. Transmission coefficient calculation
        i. Transfer Matrix Approach
        ii. Scattering Matrix Approach
        iii. The Usuki Method
    c. Green's functions method
        i. Recursive Green's Functions Approach
        ii. Contact Block Reduction Method
    d. Application example for modeling with CBR method: Modeling of FinFET device