Boundary conditions effects on EPM Full Band Boltzmann-Poisson models for Electronic Transport

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INTRODUCTION

The purpose of our work is to develop Discontinuous Galerkin (DG) Finite Element Method (FEM) based numerical solvers for Boltzmann-Poisson (BP) mathematical models of hot electronic transport in semiconductors, which consider a more realistic picture of this physical phenomena. The methodology to accomplish it follows several lines. The first one is by incorporating a full electronic band structure, given by Empirical Pseudopotential Methods (EPM), including then in the model the anisotropy of the band far away from the local conduction band minimum, as it is needed for a correct description of the energy band and related group velocity for the charge carriers in hot electronic transport. The second one is to extend the previously developed scheme for one conduction band for electrons to a multi-band BP system for conduction and valence bands that describes electron and hole transport with their respective collision scattering mechanisms. The third one is to do a numerical study of boundary conditions appearing in semiclassical kinetic models like BP, such as specular reflection, diffusive reflection, or a combination of both reflections, and the effect of these boundary conditions on the behavior of the solution, in analogy with the boundary layer problems generating shock waves in the kinetic theory for gas dynamics described by a Boltzmann Equation [4].

The dynamics of electron transport in modern semiconductor devices can be described by the semiclassical Boltzmann-Poisson (BP) model:

$$\frac{\partial f_i}{\partial t} + \frac{1}{\hbar}\nabla_{\vec{k}}\,\varepsilon_i \cdot \nabla_{\vec{x}} f_i - \frac{q_i}{\hbar}\vec{E}\cdot\nabla_{\vec{k}} f_i = \sum_j Q_{i,j} \quad (1)$$

$$\nabla_{\vec{x}} \cdot (\epsilon\,\nabla_{\vec{x}} V) = \sum_i q_i \rho_i - N(\vec{x}), \vec{E} = -\nabla_{\vec{x}} V \quad (2)$$

$f_i(\vec{x},\vec{k},t)$ is the probability density function (pdf) over phase space $(\vec{x},\vec{k})$ of a carrier in the i-th energy band in position $\vec{x}$, with crystal momentum $\hbar\vec{k}$ at time t. The collision operators $Q_{i,j}(f_i,f_j)$ model i-th and j-th carrier recombinations, collisions with phonons or generation effects. $\vec{E}(\vec{x},t)$ is the electric field, $\varepsilon_i(\vec{k})$ is the i-th energy band surface, the i-th charge density $\rho_i(t,\vec{x})$ is the k-average of f_i, and $N(\vec{x})$ is the doping profile.

Deterministic solvers for the BP system using Discontinuous Galerkin (DG) FEM have been proposed in [1], [2] to model electron transport along the conduction band for 1D diodes and 2D double gate MOSFET devices. In [1], the energy band $\varepsilon(\vec{k})$ model used was the nonparabolic Kane band model. These solvers are shown to be competitive with Direct Simulation Monte Carlo methods [1]. The energy band models used in [2] were the Kane and Brunetti, $\varepsilon(|\vec{k}|)$ analytical models, but implemented numerically for benchmark tests.

Boundary conditions for BP electronic transport model vary according to the considered device and physical situation. Charge neutrality boundary conditions are common in 1D and 2D devices:
$f_{out}(t,\vec{x},\vec{k})|_\Gamma = N_D(\vec{x})\frac{f_{in}(t,\vec{x},\vec{d})|_\Gamma}{\rho(t,\vec{x})}$, Γ subset of $\partial\Omega_{\vec{x}}$.
Specular reflection over the Neumann Inflow Boundary Γ_N^- is applied at insulating boundaries:
$f(\vec{x},\vec{k},t) = f(\vec{x},\vec{k}',t)$ for $(\vec{x},\vec{k}) \in \Gamma_N^-, \quad t > 0.$
$\vec{k}'$ s.t. $\nabla_{\vec{k}}\varepsilon(\vec{k}') = \nabla_{\vec{k}}\varepsilon(\vec{k}) - 2(\nabla_{\vec{k}}\varepsilon(\vec{k})\cdot\eta(\vec{x}))\eta(\vec{x})$.

Diffusive reflection is a known condition from the kinetic theory for gas dynamics, in which the distribution function at the Inflow boundary is proportional to a Maxwellian [5]: For $(\vec{x},\vec{k}) \in \Gamma_N^-$,
$f(\vec{x},\vec{k},t) = Ce^{-\varepsilon(\vec{k})/K_B T}\int_{\nabla_{\vec{k}}\varepsilon\cdot\eta>0}\nabla_{\vec{k}}\varepsilon\cdot\eta(\vec{x}) f dk.$

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WORK & PRELIMINARY RESULTS

This work studies numerically electron transport along conduction bands and charge transport along both conduction and valence bands for Si, computed by EPM (which gives a full energy band structure spectral approximation in $\vec{k}$-space [3] for a crystal lattice model as the sum of potentials due to individual atoms and associated electrons, with few parameters fitting empirical data such as optical gaps, absorption rates, etc.) comparing it to traditional analytic band models. This work does as well a numerical study of the effect of boundary conditions on the behavior of the pdf related to shock waves generated by a boundary layer.

We present results of a DG numerical scheme applied to deterministic computations of the BP system in spherical coordinates for the momentum $\vec{k}$, to compute the related pdf describing hot electron transport along the conduction energy band for $n^+ - n - n^+$ Silicon diodes, with n channel lengths of 400 nm and 50 nm, using an EPM full band, as well as a symmetrized radially averaged EPM band. We compare them with traditional analytical band models such as the Parabolic or Kane, which give a simple (usually taken isotropic) description of the conduction band, valid just close to a local conduction band minimum and for low electric fields. We present DG simulations for a 2D double gate MOSFET device, applying boundary conditions of specular, diffusive, and mixed linear combination reflections at the top and bottom of the silicon region, and charge neutrality conditions on the source and drain contacts. Preliminary results related to a multiband BP system for electron and hole transport in the conduction and valence bands will be presented.

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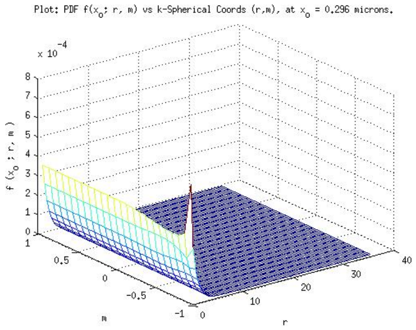

Fig. 1. PDF $f(r, \mu; t_0, x_0)$ vs. $\vec{k}$-spherical coordinates (r, μ) at $x_0 = 0.3\mu m$, $t_0 = 5.0ps$, for a $1\mu m$ diode with a $400nm$ channel, 0.3 V bias, with an EPM average conduction band.

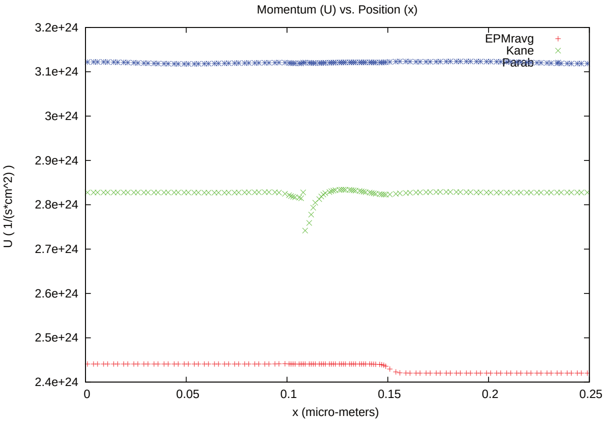

Fig. 2. Current (Momentum U) vs. Position (x) for Parabolic, Kane, EPM Average Conduction Band Models, at $t = 5.0ps$, for a 0.25 μm diode with a 50nm channel and 0.3 V bias.

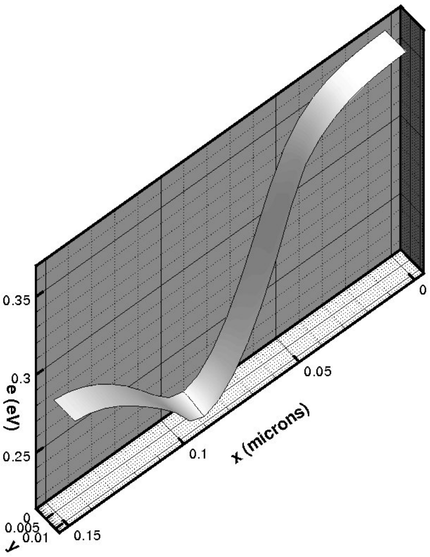

Fig. 3. Average Energy (e) vs. Position (x, y) at $t = 1.0ps$, for a 2D double gate MOSFET using a Kane energy band and a specular reflection boundary condition.