Simulation of Schottky barrier diodes with a direct solver for the Boltzmann-Poisson system

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Nowadays device simulation is usually performed by applying macroscopic models. However, with ongoing miniaturization, several assumptions necessary to justify these models lose their validity because the mean free path of the electrons becomes comparable with the device dimensions. In such cases, the electron transport is described by the Boltzmann transport equation (BTE) coupled with the Poisson equation. There were several direct methods presented in the past years. A finite difference approach was proposed in [1]. Later, higher order methods [2] as well as shock capturing algorithms [3] were applied. A finite element formulation with a piecewise constant approximation of the electron distribution with respect to energy and angle was introduced in [4].

We consider the Boltzmann-Poisson system (BP) for one-dimensional devices, which requires the treatment of two dimensions in the velocity space. Therefore, the model is applicable for semiconductors that can be described by spherically symmetric band models. Included scattering mechanisms are elastic first-order scattering of electrons with acoustic phonons and inelastic zeroth-order scattering with optical phonons.

For numerical simulations, we present a direct method to solve the BP system. To this end, we apply a piecewise polynomial approximation [4] to the distribution function in the velocity space, as well as high-order shock capturing algorithms in real space [5]. The latter are especially important to model metal-semiconductor junctions accurately, because the free carrier concentration varies by several magnitudes near such interfaces. The Poisson equation can be solved by direct integration. It can be shown that the gained solutions fulfill the continuity equation for electrons as well as the balance equation for the energy density.

We apply the direct Boltzmann-Poisson solver (DBPS) to simulate silicon based Schottky barrier diodes. In a first test case, we considered a doping of $n_D = 10^{15}\ cm^{-3}$ at the metal semiconductor junction. Resulting particle and energy density profiles, as well as current-voltage characteristics are compared with those obtained by Monte Carlo (MC) simulations [6] in Figures 1, 2 and 3, respectively. Corresponding results for $n_D = 10^{16}\ cm^{-3}$ are shown in Figures 4, 5 and 6. All results show a good agreement with the Monte Carlo results.

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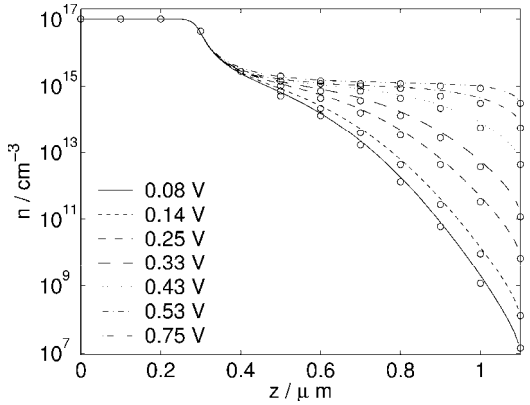

Figure 1: Comparison of carrier density profiles for $n_D = 10^{15}$ of DBPS (lines) with MC (circles).

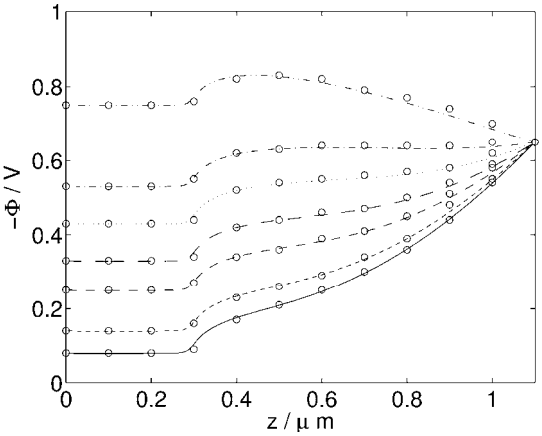

Figure 2: Comparison of electric potential profiles for $n_D = 10^{15}$ of DBPS (lines) with MC (circles).

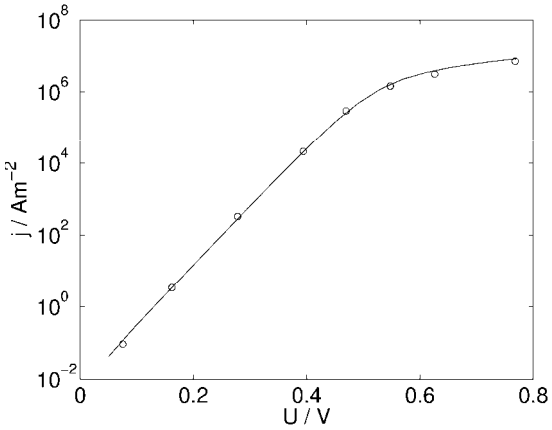

Figure 3: Comparison of current-voltage characteristics for $n_D = 10^{15}$ of DBPS (line) with MC (circles).

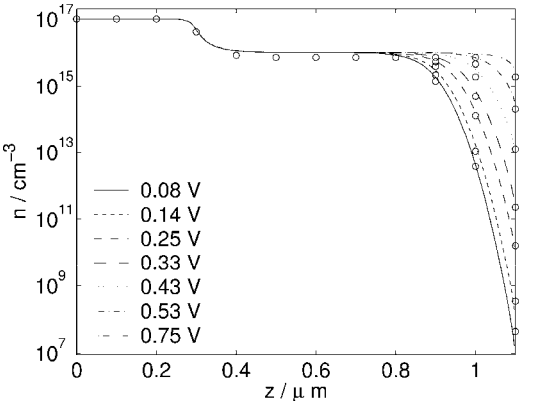

Figure 4: Comparison of carrier density profiles for $n_D = 10^{16}$ of DBPS (lines) with MC (circles).

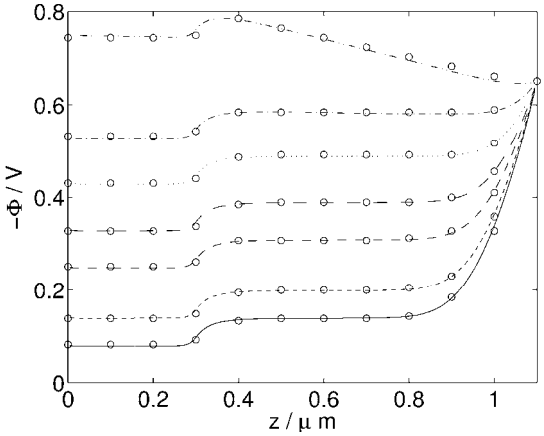

Figure 5: Comparison of electric potential profiles for $n_D = 10^{16}$ of DBPS (lines) with MC (circles).

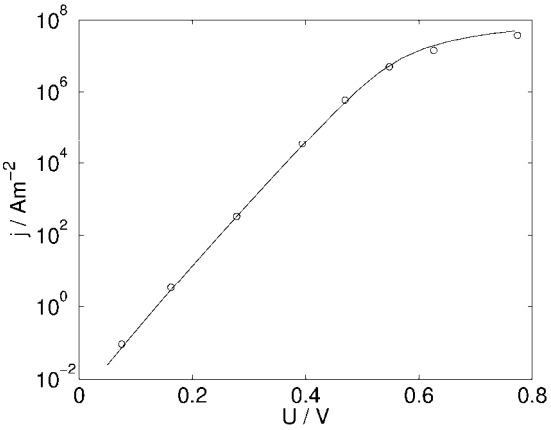

Figure 6: Comparison of current-voltage characteristics for $n_D = 10^{16}$ of DBPS (line) with MC (circles).

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