Modeling of transport through semiconductor quantum dots: An approach based on the direct solution of the coupled Poisson-Boltzmann equations

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We report on a computational approach based on the self-consistent solution of the steady-state Boltzmann transport equation (BTE) coupled with the Poisson equation for the study of inhomogeneous transport in semiconductor quantum dots (QDs). The nonlinear, coupled Poisson-Boltzmann (PB) system is solved numerically using finite difference methods. Preliminary studies of high-field and high-temperature transport characteristics of sample QDs show a build-up of strong fields in the QD region, charge redistribution due to the applied and built-in field and interesting fine structure in the high-energy tail of the electron distribution function in the QD region.

The BTE is a complicated integro-differential equation for the electron distribution function which in principle needs to be solved in seven dimensions, corresponding to time, position and momentum space. Most attempts to date to solve the BTE have been primarily based on Monte Carlo methods for the solution of the BTE or hydrodynamic device models based on moments of the BTE. Recently, however, there have been a few attempts to solve the BTE using direct methods.

In our treatment we discretize the rescaled BTE in the two-dimensional phase space (one dimension corresponding to position and one to velocity), using a first-order upwind method. The corresponding system of equations is then solved using a successive overrelaxation method (SOR), which updates the solution iteratively in the 2-dimensional phase space until convergence is reached. From the calculated electron distribution function, the electron density is calculated and used as an input to the Poisson equation which in turn is solved using finite differencing and SOR. The calculated inhomogeneous electric field is then finally used as input in the BTE and the whole process is repeated until convergence is reached. The boundary conditions for the coupled PB system of equations are: *i)* For the Poisson solver, fixed potential at the boundaries. *ii)* For the BTE solver, displaced Maxwell-Boltzmann distributions, using the calculated value of the electric field at the boundaries, in space.

A sample result of the solution of the PB system of equations, using the relaxation-time approximation, is shown in figure 1, where, the potential energy profile, electric field, electron density and electron distribution function at selected points in position are shown for an $N^+N^-N^+N^-N^+$ structure, calculated at the temperature T=300 K and applied bias voltage V_b=0.5 V (see figure caption for the rest of the parameters used in the calculation). Several immediate observations can be made from the presented results: As expected, the potential drop occurs mainly over the active portion of the device, giving rise to large and sharp variations in the electric field, as seen in Fig. 1(a). From the electron density shown in Fig. 1(b) it is further seen that charge redistribution occurs due to the applied and built-in field, giving rise to an accumulation of charge near the injecting contact. Most importantly, the electron distribution function [Fig. 1(c)], shown for the points in space depicted in Fig. 1(a), deviates significantly from a drifted-Maxwellian distribution, displaying a complex structure in the high-energy tail of the distribution function. These features accentuate the inhomogeneous and non-equilibrium nature of the transport through these type of systems.

A full journal publication of this work will be published in the Journal of Computational Electronics.

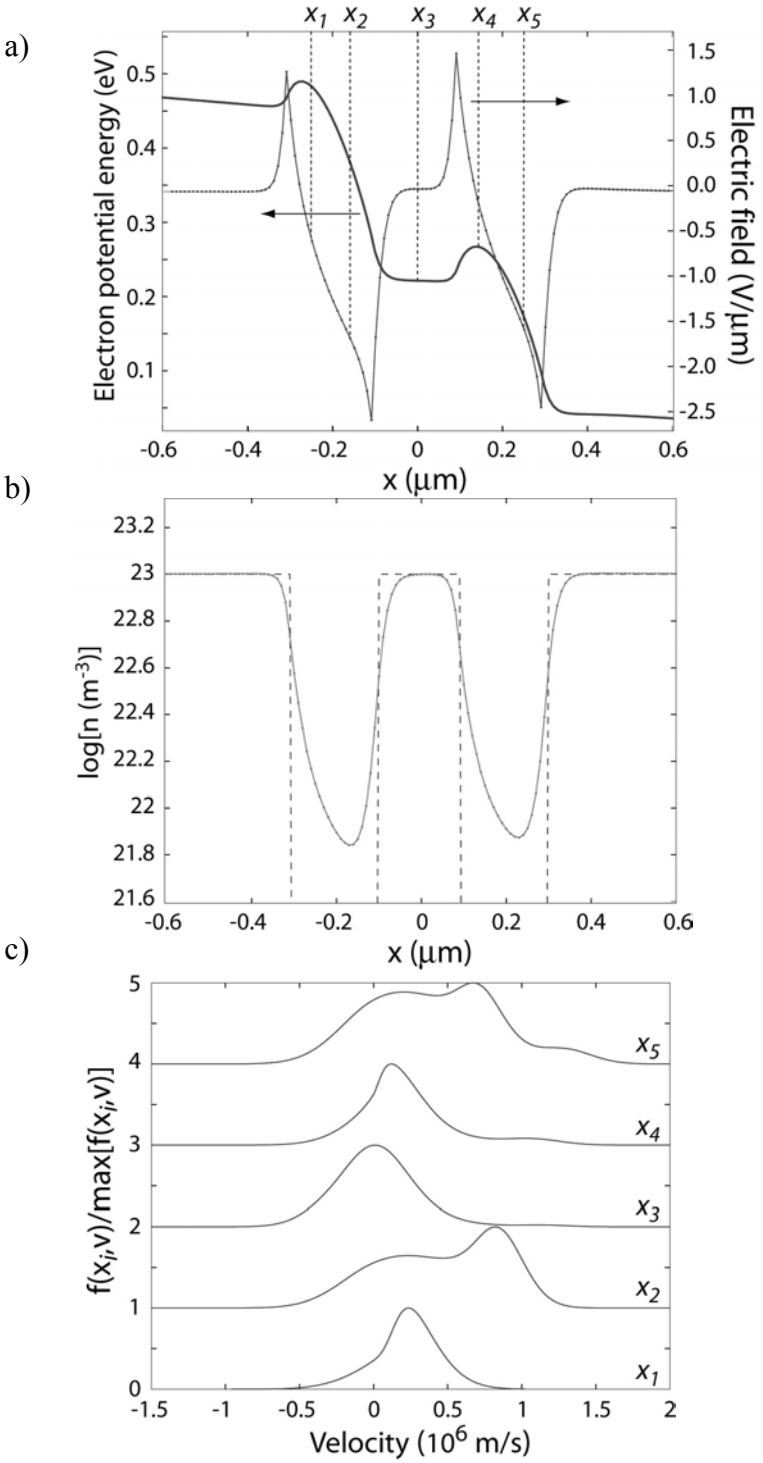

Fig. 1: (a) Electron potential energy and electric field. The labels x_i mark the points in space for which the electron distribution functions in Fig. 1(c) are plotted. (b) Electron density (solid line) and doping density (dashed line, whole range not shown). (c) Normalized electron distribution function. The parameters in the calculation are: The doping densities $N^+=10^{23}$ m^{-3}, $N^-=10^{19}$ m^{-3}, the effective mass $m^*=0.067m_0$, the scattering time $\tau=2.5\cdot10^{-13}$ s. The central $N^-N^+N^-$ region has the dimensions 200/200/200 nm, the contact N^+ regions are 1 μm long.

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