error as a function of time step and error as a function of computational time are presented.

# Transport in Nanostructures: A Comparative Analysis Using Monte Carlo Simulation, the Spherical Harmonic Method, and Higher Moments Models

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With the modern transistor size shrinking below 45nm the traditionally used classical drift-diffusion model to describe transport in the conducting channel is gradually loosing its validity. Several effects are responsible. With the channel length decreasing the electric field gradient is rapidly increasing. Carriers get accelerated by the driving field and, because of the reduced length of the channel, they do not thermalize before they reach the drain contact. In this case the assumption underlying the classical transport model, that the driving electric field produces only a weak perturbation of the local equilibrium distribution function is violated, and the exact Boltzmann transport equation with all scattering mechanisms included must be solved in order to determine the carrier distribution function and the current.

The Boltzmann equation in silicon can be solved by Monte Carlo techniques, where barrier scattering with phonons and impurities is included. As a result the distribution function along the nanostructure from source to drain is obtained which allows to calculate the current. Although most accurate, the solution of the Boltzmann equation is extremely time consuming and is not useful for practical design applications, when timely results are needed.

Several generalizations of the classical drift-diffusion model are possible. An obvious approach is to introduce higher moments of the distribution function. In this way carrier heating is taken into account resulting in the hydrodynamic transport model or the energy transport model, depending on additional assumptions. If one additionally accounts for deviations of the distribution function from the Maxwellian shape, one obtains the six-moments transport model. All transport models contain parameters which relate the corresponding moment densities to their fluxes. The solution of the Boltzmann equation obtained using the Monte Carlo technique can be employed to calibrate these parameters.

Another way of generalizing the classical drift-diffusion model is to use a spherical harmonic expansion of the distribution function. We demonstrate that a transport model based on the first two terms in the spherical harmonic expansion exactly corresponds to the drift-diffusion model with low-field mobility. We perform a comprehensive analysis of the validity of the higher-moments transport models with the model based on spherical harmonics expansion by rigorously comparing their results with results of the Monte Carlo solution of the Boltzmann transport equation.