Kinetic effects on the transport properties of nanostructured devices investigated by deterministic solutions of the Boltzmann-Poisson system.

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In highly integrated semiconductor devices, the scale length of individual components is comparable with the distance between successive scattering events of the carriers. An accurate description of the charge transport in such regimes requires the treatment on a kinetic level. Sophisticated kinetic transport models are based on semiconductor Boltzmann equations (BE) coupled with the Poisson equation determining the phase-space distribution of electrons and the electric field in a self-consistent way. The high-field electron transport in polar semiconductors, such as gallium arsenide or indium phosphide, as well as in graphene is essentially influenced by the non-equilibrium behavior of optical phonons [1,2]. Therefore, we consider a transport model consisting of a coupled set of Boltzmann equations for electrons and optical phonons to take into account the hot-phonon effects dynamically. To solve this set of kinetic equations, we developed efficient deterministic solution methods. The methods are based on a full discretization of the phase space. Conservative finite-difference schemes with shock-capturing reconstructions of the numerical fluxes are applied to approximate the distribution functions accurately even at the junctions of sharp doping profiles [3]. Hence, the developed numerical techniques allow us to perform detailed studies of the transport properties of submicron semiconductor devices in far-from-equilibrium situations. The deterministic approach offers the possibility to directly obtain the distribution functions without statistical noise at computational effort comparable with that of Monte Carlo methods [4]. We present kinetic effects on the electron transport in a silicon npn-structure, which are studied by comparing the solution of the Boltzmann equation with corresponding maximum entropy distributions. An indium phosphide diode is considered to investigate the impact of non-equilibrium polar optical phonons on the electron transport. Further, we demonstrate the applicability of the developed scheme on graphene by fully accounting for the special properties of this novel material. The main distinction to common semiconductor materials lies in the reduced dimensionality, the zero-energy-gap, and the constant velocity dispersion relation, often referred to as Dirac-cone. We present how these characteristics, together with the influence of optical phonons, affects the electronic transport in graphene.

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