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A Semi-Lagrangian Deterministic Solver for the Semiconductor Boltzmann-Poisson System

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Abstract. In this paper we develop a deterministic numerical method for solving the Boltzmann transport equation for semiconductors based on a transport-collision time-splitting method. Transport phases are solved by means of accurate flux-balance methods while collision steps are computed in the original k-grid. Numerical experiments are shown allowing for a discussion of this method with respect to other present in the literature.

AMS subject classifications: 65M99, 82D37, 82-08

Key words: Kinetic equations for semiconductors, semi-Lagrangian schemes, splitting schemes.

1 Introduction

The semi-classical Boltzmann transport equation (BTE) is a mesoscopic description of the transport/collision of charged particles in an electronic device and is given by

$$\frac{\partial f}{\partial t}+\frac{1}{\hbar}\nabla_k\varepsilon\cdot\nabla_x f-\frac{q}{\hbar}E\cdot\nabla_k f=\mathcal{Q}[f], \tag{1.1}$$

where $f(t,x,k)$ measures the probability density of finding an electron at time t in position x with wave vector k. The parameter $\hbar$ is the Planck constant divided by 2π and q is the positive elementary charge.

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The band structure of the semiconductor crystal is described by the energy-band function which can be approximated by a parabolic function given by

$$\varepsilon(k)=\frac{1}{2}\frac{\hbar^2}{m^*}|k|^2, \tag{1.2}$$

where m^* is the effective electron mass. In a first step, we shall consider the most important scattering mechanisms in Si: acoustic phonon scattering, in its elastic approximation, and optical phonon scattering with a single frequency ω. Therefore, the structure of the collision operator [20,24] is

$$\begin{aligned}\mathcal{Q}[f](t,x,k)&=\int_{\mathbb{R}^3}\left[S(k',k)f(t,x,k')-S(k,k')f(t,x,k)\right]dk'\\&=\int_{\mathbb{R}^3}S(k',k)f(t,x,k')dk'-f(t,x,k)\int_{\mathbb{R}^3}S(k,k')dk'\\&=\mathcal{Q}^+[f]-\mathcal{Q}^-[f]\end{aligned} \tag{1.3}$$

with

$$S(k,k')=K\left[(n_q+1)\delta(\varepsilon(k')-\varepsilon(k)+\hbar\omega)+n_q\delta(\varepsilon(k')-\varepsilon(k)-\hbar\omega)\right]+K_0\delta(\varepsilon(k')-\varepsilon(k)), \tag{1.4}$$

where n_q is the occupation number of phonons

$$n_q=\frac{1}{\exp\left(\frac{\hbar\omega}{k_BT_L}\right)-1}, \tag{1.5}$$

k_B is the Boltzmann constant and T_L the lattice temperature. The kernel K_0 is

$$K_0=\frac{k_BT_LE_{ac}^2}{4\pi^2\hbar{u_l}^2\rho_0}, \tag{1.6}$$

where E_{ac} is the deformation potential, u_l is the sound velocity and ρ_0 is the crystal density. The kernel K is

$$K=\frac{D_tk^2}{8\pi^2\hbar\rho_0\omega}, \tag{1.7}$$

where ω is the frequency and D_tk is the optical coupling constant. The self-consistent electrostatic field is computed through Poisson's equation

$$\Delta\Phi=\frac{q}{\epsilon}[\rho(t,x)-N_D(x)], \tag{1.8}$$

where ρ is the electron density

$$\rho(t,x)=\int_{\mathbb{R}^3}f(t,x,k)dk, \tag{1.9}$$