A Two-Particle Monte Carlo Method for Carrier Transport in the Presence of Electron-Electron Scattering

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The Boltzmann collision operator taking into account electron-electron scattering (EES) is nonlinear in the single-particle distribution function. Numerical solution of the resulting nonlinear Boltzmann equation requires an iterative method. In terms of the two-particle distribution function, however, the scattering operator is linear. We have formulated a kinetic equation for the two-particle distribution function and derived Monte Carlo (MC) algorithms for the numerical solution of that equation [1].

The stationary transport problem for a uniform electric field is solved by a two-particle MC algorithm. A pair of trajectories is traced for a long period of time and quantities of interest can be computed by several methods: time-averaging, sampling at equidistant time steps, and before-scattering sampling. Fig. 1 shows the electron distribution functions in bulk silicon. The nonequlibrium distributions are broadened due to EES especially at low temperatures.

The transient transport problem for a bulk semiconductor is solved by an ensemble MC algorithm. The time evolution of an ensemble of particle pairs is computed, and quantities of interest are obtained as ensemble averages. As a transient problem we analyzed the mixing of a hot and a cold carrier ensemble. The energy of the hot ensemble relaxes faster in the presence of EES (Fig. 2). The effect of EES on the velocity overshoot is shown in Fig. 3.

The stationary algorihtm has been extended to non-uniform electric fields. We calculate the energy distributions for a potential profile proposed in [2]. At room temperature a slight enhancement of the high energy tail is observed (Fig. 4), which, however, is less pronounced than that reported in [2].

The novelty of the proposed method is that the problem to be solved is linear. Storing and iteratively updating the single particle distribution is not required by this method.

[1] G. Indalecio and H. Kosina. Monte Carlo Simulation of Electron-electron Interactions in Bulk Silicon. Book of Abstracts of "The 12th International Conference on Scientific Computing in Electrical Engineering (SCEE)", 97 – 98 (2018)

[2] P. A. Childs and C. C. C. Leung. A one-dimensional solution of the Boltzmann transport equation including electron-electron interactions. Journal of Applied Physics 79, 222 (1996)

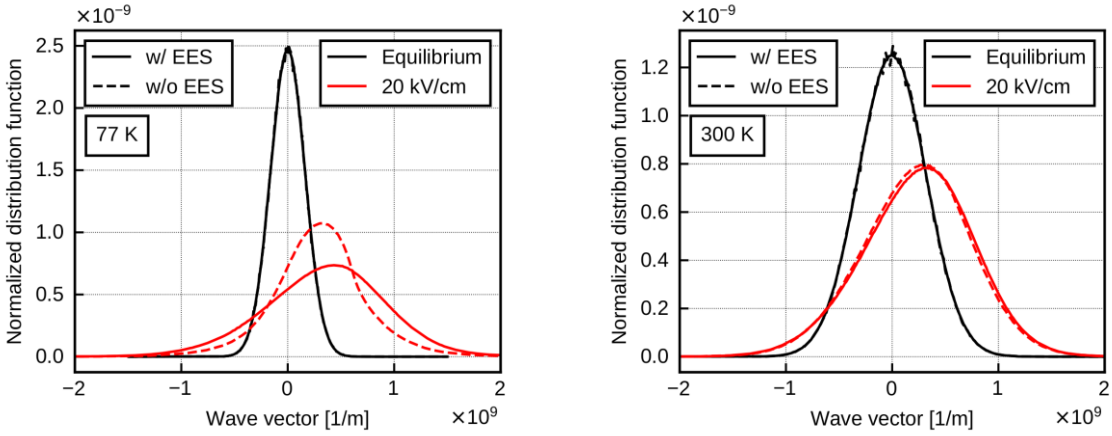

Fig.1: Effect of EES on the bulk distribution function at 77K (left) and 300K (right) in thermal equilibrium and non-equilibrium.

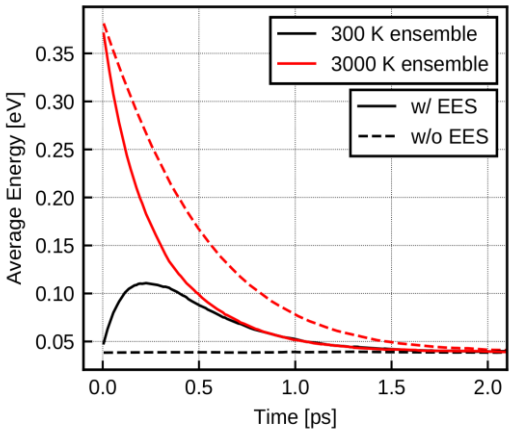

Fig.2: Enhancement of energy relaxation due to EES. The initial two-particle distribution function assumed is a aproduct of a cold Maxwellian at 300K and a heated Maxwellian at 3000K.

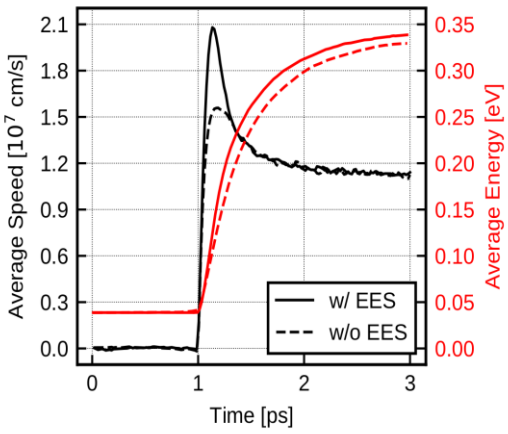

Fig.3 Effect of EES on the velocity overshoot (black line) and the energy transient (red line). An electric field step of 50kV/cm is applied at 1 ps. Lattice temperature is 300K.

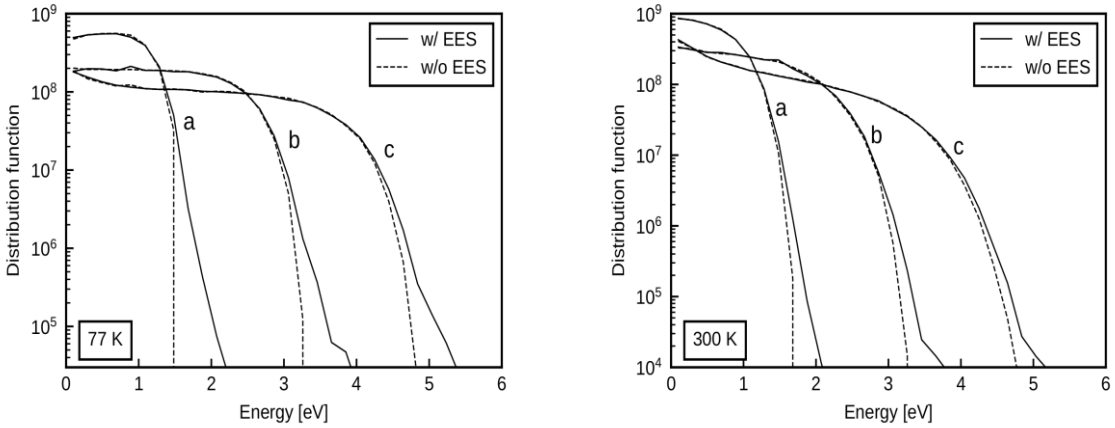

Fig.4: Enhancement of the high energy tail due to EES. The potential profile and three lateral positions reported in [2] have been used.