# Monte Carlo Simulation of Electron-electron Interactions in Bulk Silicon

Guillermo Indalecio[1,2] and Hans Kosina[2]

[1] CITIUS, University of Santiago de Compostela, 15782, Spain guillermo.indalecio@usc.es
[2] Institute for Microelectronics, TU Wien, 1060, Vienna, Austria kosina@iue.tuwien.ac.at

**Summary.** We have developed a novel Monte Carlo (MC) algorithm to solve the semiconductor Boltzmann equation in the presence of electron-electron scattering (EES). It is well known that the scattering operator for EES is nonlinear in the single-particle distribution function. Numerical solution methods of the resulting nonlinear equation are usually based on more or less severe approximations. In terms of the pair distribution function, however, the scattering operator is linear. We formulate a kinetic equation for the pair distribution function and related MC algorithms for its numerical solution. Assuming a spatially homogeneous system we derived a two-particle MC algorithm for the stationary problem and an ensemble MC algorithm for the transient problem. Both algorithms were implemented and tested for bulk silicon. As a transient problem we analyzed the mixing of a hot and a cold carrier ensemble. The energy of the hot ensemble relaxes faster with EES switched on. The cold ensemble is temporarily heated by the energy transferred from the hot ensemble. Switching on the electric field rapidly is known to result in an velocity overshoot [1]. We observe that EES enhances the overshoot. The stationary algorithm was used to calculate the energy distribution functions at different field strengths.

## 1 Introduction

It is commonly accepted that EES alters the high-energy tail of the energy distribution function in a semiconductor device [2]. Since physical models of hot carrier degradation rely on accurate distribution functions as an input it is important to model EES carefully [4]. In this work we present results of a novel treatment of EES that avoids several of the commonly made approximations.

## 2 Theory

In the Boltzmann equation (BE), carrier-carrier scattering is described by the following, nonlinear integral operator.

$$Q[f](\boldsymbol{k}_1,t) = \int dk_1'\, dk_2'\, dk_2\, S(\boldsymbol{k}_1,\boldsymbol{k}_2;\boldsymbol{k}_1',\boldsymbol{k}_2') \times \left[f(\boldsymbol{k}_1',t)f(\boldsymbol{k}_2',t) - f(\boldsymbol{k}_1,t)f(\boldsymbol{k}_2,t)\right]$$

Here, $f$ is the single-particle distribution function. Integration is over all initial states ($\boldsymbol{k}_2$) and final states ($\boldsymbol{k}_2'$) of the partner electron and all final states ($\boldsymbol{k}_1'$) of the sample electron. Replacing the product of the distribution functions by the two-particle distribution function $g$

$$f(\boldsymbol{k}_1,t)f(\boldsymbol{k}_2,t) \rightarrow g(\boldsymbol{k}_1,\boldsymbol{k}_2,t),$$

gives a linear scattering operator.

$$Q[g](\boldsymbol{k}_1,\boldsymbol{k}_2,t) = \int dk_1'\, dk_2'\, S(\boldsymbol{k}_1,\boldsymbol{k}_2;\boldsymbol{k}_1',\boldsymbol{k}_2') \times \left[g(\boldsymbol{k}_1',\boldsymbol{k}_2',t) - g(\boldsymbol{k}_1,\boldsymbol{k}_2,t)\right]$$

A Boltzmann-like kinetic equation is derived for the two-particle distribution function $g$, which is posed in the six-dimensional momentum space $(\boldsymbol{k}_1,\boldsymbol{k}_2)$. This equation is linear and can be transformed into an integral equation of the form

$$g(x) = \int g(x')\, K(x',x)\, \mathrm{d}x' + g_0(x)$$
$$x \equiv (\boldsymbol{k}_1,\boldsymbol{k}_2,t)$$

In this work, we solve this integral equation by a Monte Carlo method [3].

## 3 Results and Discussion

In the following simulations we are assuming an electron concentration of $10^{19}$ cm$^{-3}$, and a lattice temperature of 300 K.

Fig. 1 shows how an ensemble of hot electrons gets cooled down when interacting with the phonons of the crystal lattice and additionally with an electron ensemble at lattice temperature. The mean energy of the hot electrons relaxes faster when EES is present. The mean energy of the cold electrons is temporarily increased by the energy transfer from the hot carriers. Averages are calculated by sampling the two ensembles at equidistant time steps. The number of particle pairs simulated is $2 \cdot 10^4$.

Another application of the transient MC algorithm is the study of the response of the carriers to an abrupt change in the electric field. At 1 ps a field step of 50 kV/cm has been applied. Fig. 2 shows that EES enhances the velocity overshoot and gives a faster rise of

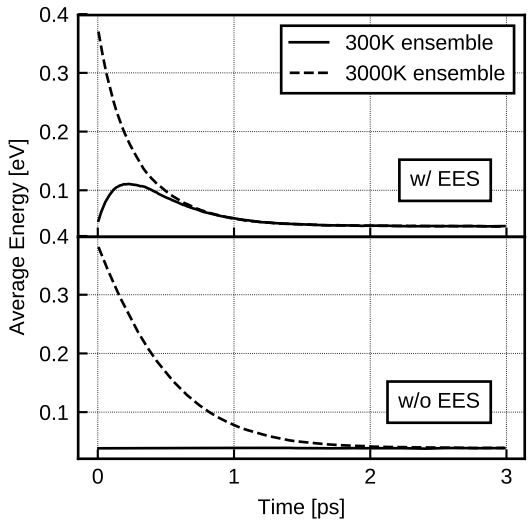


**Fig. 1.** Relaxation of the mean energy is affected by EES. The initial two-particle distribution function assumed consists of a hot ensemble at 3000K and a cold ensemble at 300K.

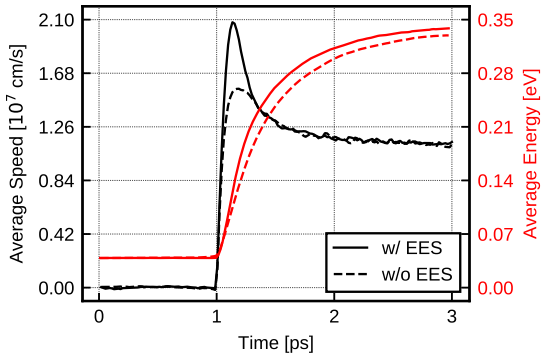


**Fig. 2.** Velocity overshoot (left, black) and energy transient (right, red) after applying an electric field step of 50 kV/cm at 1 ps.

the mean energy towards the stationary value. Again, in the simulation we sampled an ensemble of $2 \cdot 10^4$ particle pairs at equidistant time steps.

Finally, we apply the stationary MC algorithm to calculate the momentum distribution functions at different field strengths. In accordance with thermodynamics, in equilibrium a Maxwellian distribution is obtained in our simulations. EES has no effect on the equilibrium distribution, see Fig. 3. With an electric field applied there is a noticeable difference for a lattice temperature of 77 K. With EES the non-equilibrium distribution is wider.

## 4 Conclusions

We have developed a two-particle Monte Carlo algorithm for the solution of a two-particle kinetic equation that includes electron-electron scattering.
We demonstrate the impact of electron-electron scattering on the transient relaxation of an ensemble of hot carriers, on the veloicty overshoot in the presence of a field step, and on the shape the momentum distribution function.

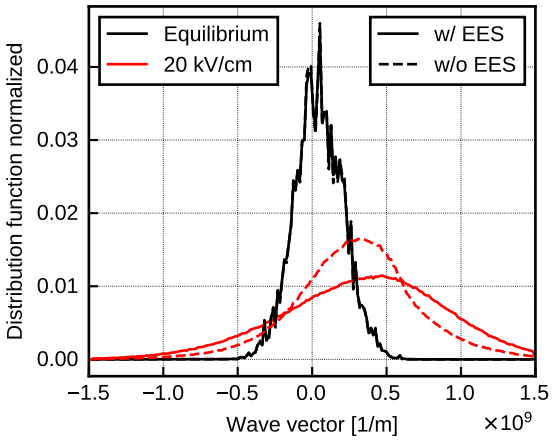


**Fig. 3.** Momentum distribution functions at equilibrium and at 20 kV/cm, lattice temperature 77 K.

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