Monte Carlo Simulation of Electron-electron Interactions in Bulk Silicon

Guillermo Indalecio and Hans Kosina

Abstract We have developed a novel Monte Carlo (MC) algorithm to study carrier transport in semiconductors in the presence of electron-electron scattering (EES). It is well known that the Boltzmann scattering operator for EES is nonlinear in the single-particle distribution function. Numerical solution methods of the resulting nonlinear Boltzmann 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

Guillermo Indalecio
CITIUS, University of Santiago de Compostela, 15782, Spain e-mail: guillermo.indalecio@usc.es,

Hans Kosina
Institute for Microelectronics, TU Wien, 1060, Vienna, Austria e-mail: kosina@iue.tuwien.ac.at

degradation rely on accurate distribution functions as an input it is important to model EES carefully [5]. In this work we present results of a novel treatment of EES that avoids several of the commonly made approximations.

2 Theory

We study the position-independent case ($\nabla_{\mathbf{r}} f \equiv 0$). Setting $\mathbf{F} = e\mathbf{E}/\hbar$, the Boltzmann equation takes the form

$$\left(\frac{\partial}{\partial t} + \mathbf{F}\cdot\nabla_{\mathbf{k}_1}\right) f(\mathbf{k}_1,t) = Q_{\mathrm{ph}}[f](\mathbf{k}_1,t) + Q_{\mathrm{ee}}[f](\mathbf{k}_1,t) \tag{1}$$

Here, f is the single-particle distribution function, and Q_{ph} denotes the electron-phonon scattering operator. EES is described by the following, nonlinear integral operator.

$$Q_{\mathrm{ee}}[f](\mathbf{k}_1,t) = \int dk_1' \, dk_2' \, dk_2 \, S(\mathbf{k}_1,\mathbf{k}_2;\mathbf{k}_1',\mathbf{k}_2') \times \left[f(\mathbf{k}_1',t) f(\mathbf{k}_2',t) - f(\mathbf{k}_1,t) f(\mathbf{k}_2,t)\right] \tag{2}$$

Integration is over all initial states ($\mathbf{k}_2$) and final states ($\mathbf{k}_2'$) of the partner electron and all final states ($\mathbf{k}_1'$) of the sample electron. We restrict our discussion to the non-degenerate case where in the scattering operator (2) Pauli blocking factors of the form $[1-f(\mathbf{k},t)]$ are not included.

The two-particle transition rate S_{ee} is derived for a screened Coulomb potential using Fermi's Golden rule [6, 8].

$$S_{\mathrm{ee}}(\mathbf{k}_1,\mathbf{k}_2;\mathbf{k}_1',\mathbf{k}_2') = \frac{e^4 n}{\hbar(2\pi\varepsilon_0\varepsilon_s)^2} \frac{\delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_1'-\mathbf{k}_2')}{(\left|\mathbf{k}_1-\mathbf{k}_1'\right|^2+\beta_s^2)^2} \times \delta\left[\varepsilon(\mathbf{k}_1')+\varepsilon(\mathbf{k}_2')-\varepsilon(\mathbf{k}_1)-\varepsilon(\mathbf{k}_2)\right]$$

The two δ-functions state conservation of momentum and conservation of energy, respectively. In accordance with the principle of detailed balance for energy-conserving transitions, the transition rate is symmetric:

$$S_{\mathrm{ee}}(\mathbf{k}_1,\mathbf{k}_2;\mathbf{k}_1',\mathbf{k}_2') = S_{\mathrm{ee}}(\mathbf{k}_1',\mathbf{k}_2';\mathbf{k}_1,\mathbf{k}_2)$$

The total scattering rate is obtained by integration over all final states:

$$\Gamma_{\mathrm{ee}}(\mathbf{k}_1,\mathbf{k}_2) = \int dk_1' \, dk_2' \, S_{\mathrm{ee}}(\mathbf{k}_1,\mathbf{k}_2;\mathbf{k}_1',\mathbf{k}_2')$$

One out of the two integrals can be readily evaluated by means of the momentum-conserving δ-function. Assuming a parabolic and isotropic dispersion relation $\varepsilon(\mathbf{k})$

which is characterized by the effective mass m^*, the remaining integral can be evaluated analytically.

$$\Gamma_{\mathrm{ee}}(\mathbf{k}_1,\mathbf{k}_2) = \frac{ne^4m^*}{4\pi\hbar^3(\varepsilon_0\varepsilon_s)^2\beta_s^2}\,\frac{|\mathbf{k}_2-\mathbf{k}_1|}{|\mathbf{k}_2-\mathbf{k}_1|^2+\beta_s^2}$$

Here, n denotes the electron concentration and β_s the Debye-Hueckel screening parameter. In the presence of EES the Boltzmann equation (1) is nonlinear. Its numerical solution typically requires some iterative method [2] [7].

In this work we chose a different approach. When changing from a single-particle description to a two-particle description the transport equation becomes linear. This step is formally accomplished by replacing the product of two distribution functions by the two-particle distribution function g.

$$f(\mathbf{k}_1,t)f(\mathbf{k}_2,t) \to g(\mathbf{k}_1,\mathbf{k}_2,t)$$

From (1) one can derive a Boltzmann-like kinetic equation for the two-particle distribution function g, which is posed in the six-dimensional momentum space $(\mathbf{k}_1,\mathbf{k}_2)$.

$$\left(\frac{\partial}{\partial t}+\mathbf{F}\cdot\nabla_{\mathbf{k}_1}+\mathbf{F}\cdot\nabla_{\mathbf{k}_2}\right)g(\mathbf{k}_1,\mathbf{k}_2,t) = Q_{\mathrm{ph}}[g](\mathbf{k}_1,\mathbf{k}_2,t)+Q_{\mathrm{ee}}[g](\mathbf{k}_1,\mathbf{k}_2,t) \quad (3)$$

In the two-particle picture, the nonlinear operator (2) turns into a linear integral operator.

$$Q_{\mathrm{ee}}[g](\mathbf{k}_1,\mathbf{k}_2,t) = 2\int dk_1'\,dk_2'\,S_{\mathrm{ee}}(\mathbf{k}_1,\mathbf{k}_2;\mathbf{k}_1',\mathbf{k}_2')\left[g(\mathbf{k}_1',\mathbf{k}_2',t)-g(\mathbf{k}_1,\mathbf{k}_2,t)\right] \quad (4)$$

Details about the derivation of (3) and (4) will be presented in a forthcoming publication.

The linear kinetic equation (3) can be transformed into an integral equation of the following form.

$$g(x) = \int g(x')\,K(x',x)\,dx' + g_0(x), \qquad x \equiv (\mathbf{k}_1,\mathbf{k}_2,t) \quad (5)$$

In this derivation, the very same steps as in the case of the Boltzmann equation are applied [4]. Using the formalism described in [4] we derive a stationary and a transient Monte Carlo algorithm for the solution of the integral equation (5).

In the stationary algorithm, the trajectories of a pair of particles are calculated over a long period of time. Electron-phonon scattering events of the two particles are independent from each other and treated as in the case of the Boltzmann equation. An EES event, however, changes the states of the two particles simultaneously,

whereby total momentum and energy are exactly conserved. Averages can be computed using the before-scattering method [3].

In the transient algorithm, an ensemble of trajectory pairs is simulated, starting from a given two-particle initial distribution. Averages are computed as ensemble averages at given points in time.

3 Results and Discussion

In the following simulations an electron concentration of 10^{19} cm^{-3} and a lattice temperature of 300 K are assumed. First 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. EES has no effect on the equilibrium distribution, see Figures 1 and 2. At 77 K, EES causes a broadening of the non-equilibrium distribution (Fig. 1), whereas as 300 K such a broadening is not observed (Fig. 2). The reason is that at 300 K phonon scattering is much stronger and the relative importance of EES is small.

Fig. 3 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 is applied. During a short period after the field step the carriers experience the high electric field and are accelerated accordingly, whereas the mean energy

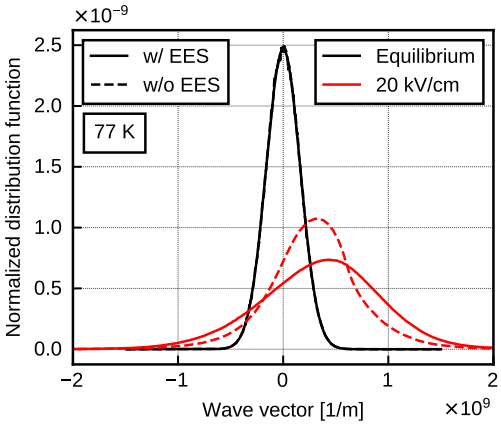

Fig. 1 Momentum distribution functions at equilibrium and at 20 kV/cm, lattice temperature 77 K.

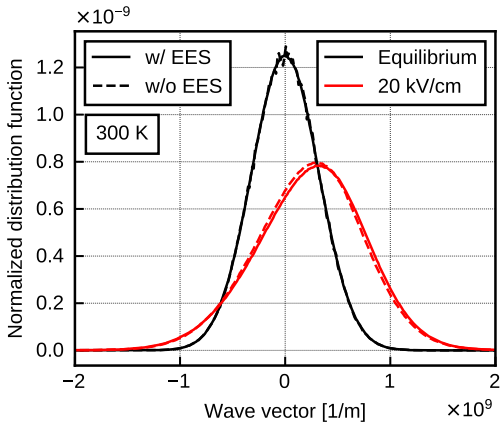

Fig. 2 Momentum distribution functions at equilibrium and at 20 kV/cm, lattice temperature 300 K.

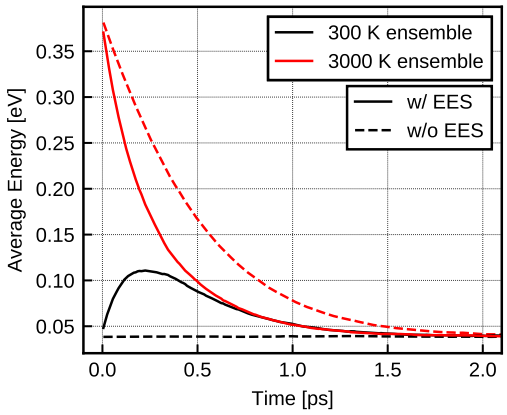

Fig. 3 Relaxation of the mean energy is affected by EES. The initial two-particle distribution function assumed consists of a hot ensemble at 3000K and a cold ensemble at 300K.

and thus momentum relaxation due the electron-phonon scattering is still low. In this situation of a phenomenon known as the velocity overshoot occurs. Our results indicate that the velocity overshoot even gets enhanced by EES as shown in Fig. 4. We believe that the enhancement in the overshoot can be explained as follows. Two particles entering the high field region experience an EES event where momentum is transferred from one particle to the other. If the momentum transfer is largely oriented along the field direction, one electron gains velocity and the other one is slowed down. The low energetic electron, however, experiences a small electron-phonon scattering rate and has a higher probability to stay in the high field without scattering, so that it will also have a large momentum gain from the field. Therefore, both electrons involved in the EES event eventually reach a higher velocity than they would without the EES event. Fig. 4 also shows that EES gives a faster rise of 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.

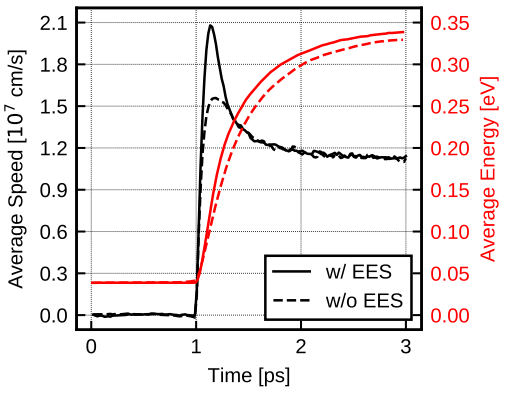

Fig. 4 Velocity overshoot (left, black) and energy transient (right, red) after applying an electric field step of 50 kV/cm at 1 ps.

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 velocity overshoot in the presence of a field step, and on the shape the momentum distribution function.

Acknowledgements G.I. acknowledges support by the Programa de Axudas a Etapa Posdoutoral da Xunta de Galicia under grant number 2017/077, and H.K. support by the Austrian Research Promotion Agency (FFG), project MORAFLASH (contract No. 850660).

References

1. G. Baccarani and M.R. Wordeman. An investigation of steady-state velocity overshoot in silicon. *Solid-State Electronics*, 28(4):407 – 416, 1985.
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.
3. C. Jacoboni and P. Lugli. *The Monte Carlo Method for Semiconductor Device Simulation*. Springer, Wien-New York, 1989.
4. H. Kosina, M. Nedjalkov, and S. Selberherr. Theory of the Monte Carlo method for semiconductor device simulation. *IEEE Transactions on Electron Devices*, 47(10):1898–1908, 2000.
5. S. E. Rauch, G. La Rosa, and F. J. Guarin. Role of e-e scattering in the enhancement of channel hot carrier degradation of deep-submicron NMOSFETs at high V_{GS} conditions. *IEEE Transactions on Device and Materials Reliability*, 1(2):113–119, 2001.
6. B.K. Ridely. *Quantum Processes in Semiconductors*. Oxford University Press, 2013.
7. N. Takenaka, M. Inoue, and Y. Inuishi. Influence of inter-carrier scattering on hot electron distribution function in GaAs. *Journal of the Physical Society of Japan*, 47(3):861–868, 1979.
8. K. Tomizawa. *Numerical Simulation of Submicron Semiconductor Devices*. Artech House, 1993.