Electron-Electron Scattering in Monte Carlo-based Device Simulations

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Introduction

Understanding reliability issues and degradation mechanisms is key to improving device quality. Hot carrier degradation (HCD) occurs when electrons of high kinetic energy cause material damage. An important requirement for modeling HCD is good knowledge of the local carrier distribution function. An accurate calculation of the high-energy tail should take into account electron-electron scattering (EES) [1] and a realistic band structure model.

Recently, a Monte Carlo (MC) algorithm for solving a two-particle kinetic equation has been developed, which treats both single-particle scattering and two-particle scattering in a consistent way [2]. In this work, we present a statistical enhancement method for the two-particle MC algorithm and the treatment of EES in a non-parabolic band.

Model

The basic idea is to simulate the time evolution of two electron states simultaneously. Each electron can individually undergo phonon scattering or both electrons can simultaneously experience EES [2].

In an EES event, both energy and momentum are conserved. For a parabolic band, the allowed momentum transfer vectors $\vec{q}$ are located on a sphere, and the EES rate can be obtained by analytical integration. In the case of a non-parabolic band that surface becomes an ellipsoid of rotation (Fig. 1), and analytical integration of the transition rate is no longer feasible. To simplify the integrand, we use an upper bound that allows for an analytic evaluation. The upper bound of the EES rate obtained in this way is used in a rejection technique. A specific transition is accepted with the given acceptance probability; otherwise, self-scattering is selected [3].

The distribution function varies by many orders of magnitude. To resolve the high-energy tail of the distribution in a MC simulation, statistical enhancement is required. Methods successful in the one-particle picture, such as particle splitting and gathering, cannot be used in the two-particle picture. Instead, we exploit the fact that any result of a stationary MC simulation represents a time average:

$$\langle A \rangle = \frac{1}{T} \int_0^T A(\vec{k}(t), \vec{r}(t)) \, \mathrm{d}t \, . \qquad (1)$$

We split the simulation period T into time frames. If a rare event of interest occurs in a certain time frame, simulation of that frame is repeated, and its statistical weight is reduced accordingly.

Results and Conclusion

Figure 2 shows the energy distribution function (EDF) on the surface of a planar MOSFET. In the transition region between channel and drain, electrons reach energies higher than those that ballistic trajectories passing the potential maximum would allow. This effect is described in [1]. Figure 3 illustrates the influence of carrier concentration and the dispersion relation on the EDF at the channel/drain junction. The slope of the high-energy tail increases with the carrier density. The parabolic transport model predicts a larger enhancement of the tail than the nonparabolic model does.

Figure 4 shows the distribution of the sampling points in the energy domain. The repeated time frame approach has been applied in a cascade of three steps. Figure 5 demonstrates that the statistical enhancement algorithm allows us to calculate three more orders of magnitude of the EDF. At lower energies, the EDFs calculated with standard and statistically enhanced MC are virtually identical.

Acknowledgment

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REFERENCES

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[3] J. Gull, L. Filipovic and H. Kosina, *Electron-electron scattering in non-parabolic transport models*, SISPAD, (2024), doi: 10.1109/SISPAD62626.2024.10733120.

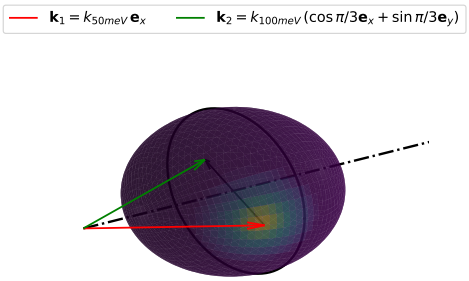

Fig. 1. For a non-parabolic dispersion the final states are located on an ellipsoid. The colour maps the transition rate $T(\vec{q})$ as a function of the momentum transfer vector $\vec{q} = \vec{k}_1' - \vec{k}_1 = \vec{k}_2 - \vec{k}_2'$. The transition rate is not symmetric with respect to the principal axes of the ellipsoid, complicating analytical integration.

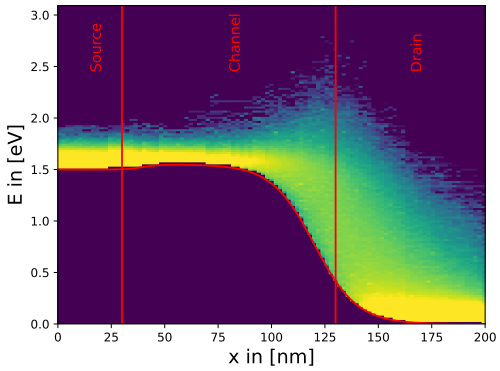

Fig. 2. EDF along a MOSFET channel, assuming a Kane dispersion and $n = 1 \times 10^{19}\,\mathrm{cm}^{-3}$: The population of electron states with high kinetic energy at the channel/drain junction increases due to EES. Adopting the Kane dispersion accelerates energy relaxation toward the drain.

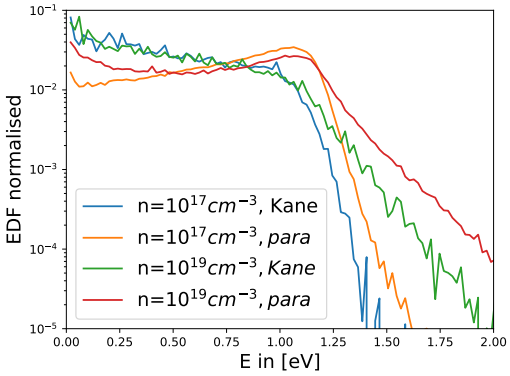

Fig. 3. EDF at the channel/drain junction: Higher carrier densities n lead to an increased population of high-energy states, which can contribute to device degradation.

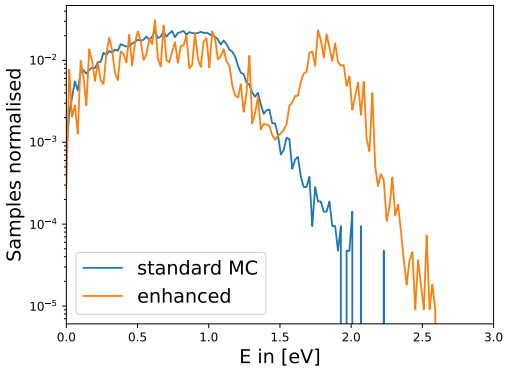

Fig. 4. Statistical enhancement increases the sampling of high-energy states and enables the study of the distribution at even higher energy levels.

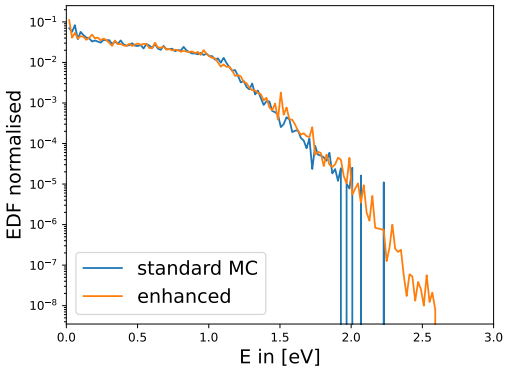

Fig. 5. Enhanced energy resolution: By cascading the statistical enhancement approach, the EDF can be resolved over additional three orders of magnitude.