Efficient Modeling of Spatially Varying Degeneracy in Monte Carlo Particle Simulation of Highly Doped Submicron HEMT

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Abstract

An efficient technique has been developed and applied to incorporate the spatially dependent influence of the Pauli exclusion principle in modeling the scattering processes in a two-dimensional Monte Carlo Device Simulator. The degeneracy effects on the performance of highly doped InP-based High Electron Mobility Transistors are investigated. It is found that degeneracy significantly affects the behavior of carriers not only in the channel but also in the contact regions what strongly influences device characteristics like I-V curves and transconductance.

1. Introduction

Modern high electron mobility transistors (HEMT) for high frequency signal generation or amplification exhibit complex material compositions and very high doping levels with large spatial variations in free carrier density. The transport physics is influenced by the so-called Pauli exclusion principle what in turn leads to spatially dependent degeneracy effects in the different regions of the inner and outer transistor. In the last years, the Monte Carlo (MC) simulation has gained much importance for the design of new device structures as it allows to reduce costs and time of the experimental development due to its high simulation accuracy. In the MC method, the scattering of carriers is modeled from first principles so that direct incorporation of the Pauli exclusion principle is possible and has already been worked out for the homogeneous bulk situation by Lugli and Ferry [1]. Due to the large computer memory consumption to store the particle distribution in the three-dimensional wave vector space with high accuracy which is involved in [1], a far too high consumption of computer memory is required if additional high resolution of the spatial dependencies in device simulation has to be modeled. In the following, we present an accurate and very efficient technique to overcome these difficulties.

2. The method

As proposed in [1], the limited number of electron states per volume of wave vector space according to the Pauli exclusion principle is accounted for by the rejection of scattering events using the occupation probability of final states which is given by the distribution function in wave vector space. Tabulating the number of electrons $n(\boldsymbol{k})$ in a volume element $\Delta k_x \Delta k_y \Delta k_z$ of wave vector space gives the distribution function $f(\boldsymbol{k})$ via $n(\boldsymbol{k}) = 2\,V/(2\pi)^3\, f(\boldsymbol{k})\,\Delta k_x \Delta k_y \Delta k_z$.

Instead of discretising the three-dimensional wave vector space directly, it is useful to incorporate possible symmetries of the distribution function and to align the numerical description to the center of the physical distribution function. As shown in Fig. 1 the center in wave vector space is given by k_{drift}. Further the physical distribution function is approximately constant in wave vector space for fixed values of $|k - k_{drift}|$ as already pointed out in [2]. Therefore we tabulate the number of electrons $n(|k - k_{drift}|)$ in a spherical shell of volume $4\pi|k - k_{drift}|^2 \Delta|k - k_{drift}|$ and calculate the distribution function according to

$$n(|k - k_{drift}|) = 2\frac{V}{(2\pi)^3} f^*(|k - k_{drift}|)\, 4\pi|k - k_{drift}|^2 \Delta|k - k_{drift}|.$$

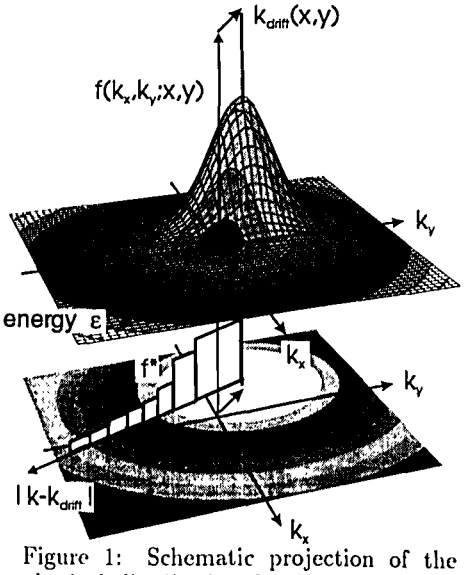

Figure 1: Schematic projection of the physical distribution function f in wave vector space (with equi-energy lines, top) to f^* (see text) (with equi-occupation lines, bottom).

The obtained distribution function f^* is related to the 'real' distribution function f by a translation with $-k_{drift}$ and an averaging along the angles in wave vector space (thus any radial variations of f are intentionally averaged). The rejection of scattering events uses the stored distribution f^* which is numerically addressed using $|k_{final} - k_{drift}|$ with k_{final} representing the final state of particles after scattering. For two-dimensional device simulation the previously five-dimensional distribution function f (with parameters $k_x, k_y, k_z; x, y$) is replaced by the three-dimensional distribution f^* (with parameters $|k - k_{drift}|; x, y$). For modeling of spatially varying degeneracy f^* as well as k_{drift} are tabulated on an underlying mesh in direct space (see Fig. 4). In total, a reduction of computer memory by approximately three orders of magnitude is achieved compared to the exact method of [1] without any significant loss of simulation accuracy, as will be discussed in detail in the next section.

3. Results

Using the new method, different important transport characteristics have been calculated for a homogeneous GaAs bulk sample and compared with results calculated with the exact method of [1]. As shown in Fig. 2 and 3 the correct drift velocity, energy distribution function as well as the distribution in wave vector space are nicely reproduced by the new method. In Fig. 2 also the calculated drift velocity for the case of using a pure energy distribution (as it is often suggested in the literature and which corresponds to the case of $k_{drift} = 0$ in our method) is presented. Obviously, a too high drift velocity results if the asymmetry of the physical distribution function with respect to the origin in wave vector space is ignored by averaging along equi-energy lines.

In Fig. 3 the energy distribution and the population in wave vector space have been calculated for both cases of including and ignoring the Pauli principle. Due to the

limited number of states per volume of wave vector space the Pauli principle leads to a spread out of the population towards higher energy and wave vectors respectively.

In Fig. 4, an InP-based HEMT structure is shown, which has been investigated as an example for spatially dependent modeling of degeneracy. For each region of the whole simulated device the distribution functions f^* are tabulated and used for the rejection of scattering events. In order to check convergence further calculations have been performed using a higher spatial resolution, but no significant differences to the following results have been found.

The calculated energy distribution functions for the cases of incorporating or ignoring the Pauli exclusion principle are depicted for the source contact regions in Fig. 5. For comparison we also calculated an analytic Fermi-Dirac function, as shown by the dotted line, where the chemical potential has been calculated in the high degeneracy limit by using the electron concentration. As shown in Fig. 5 a very good agreement of the simulated particle distribution with the analytic Fermi-Dirac function (which is a very good approximation for warm electrons in the shown case of low electric field) is obtained.

Fig. 5 shows that the electrons on average are shifted to higher energy due to the Pauli principle, what leads to an increased geometrical diffusion from the contact regions into the channel. The inclusion of the Pauli principle has mainly two influences on the free carrier density in the channel: The Pauli principle in the channel leads to an increased out-diffusion of electrons from the channel to the surrounding regions, whereas the Pauli principle in the contact regions competes to this behavior. In Fig. 6 it is shown that the Pauli principle effectively increases the channel density in the investigated device structure and operation point. This is the reason also for the increased drain-source current as shown in Fig. 7.

4. Conclusions

An efficient technique has been developed which allows to incorporate and resolve the influence of the Pauli exclusion principle in many partial regions of a multi-dimensional MC device simulation by using low memory resources. It is found that spatially varying degeneracy can have an important influence on the transport physics and on the electrical device characteristics and must hence be incorporated in an accurate MC-simulation of highly doped devices.

Acknowledgement

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References

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[2] Y. Yamada, "Modelling Degeneracy for Monte-Carlo Simulation of Electron Transport in GaAs," *Electronics Letters*, vol. 27, pp. 679-680, 1991.

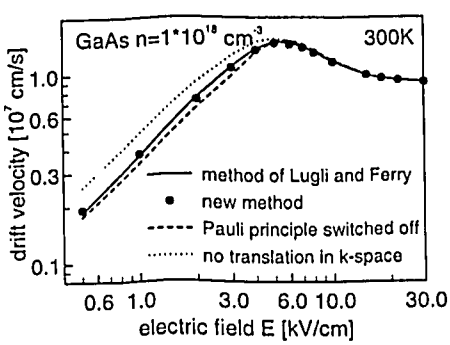

Figure 2: Calculated steady-state drift velocity incorporating the Pauli exclusion principle using different approaches.

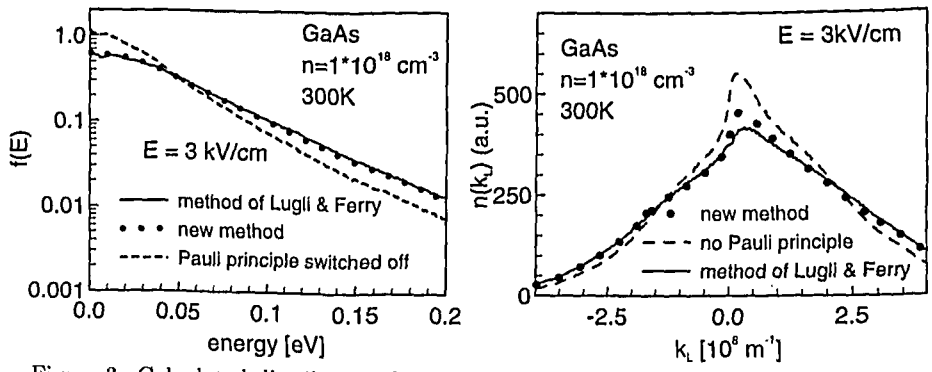

Figure 3: Calculated distribution functions in energy space (a) and in wave vector space in drift-direction (b) for a fixed electric field.

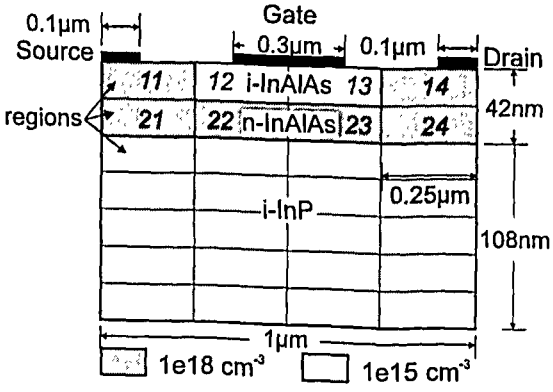

Figure 4: The investigated device structure and geometrical discretization of the spatially resolved distribution functions.

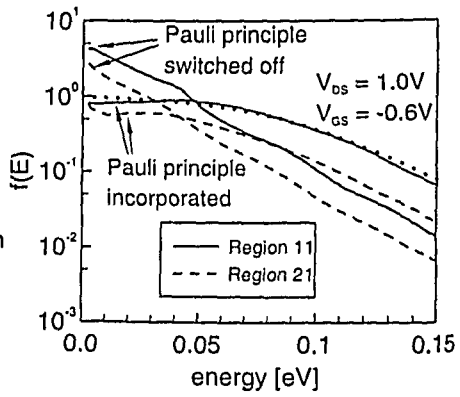

Figure 5: Calculated energy distribution functions in the source contact regions. For comparison, an analytical Fermi-Dirac function is shown by the dotted line.

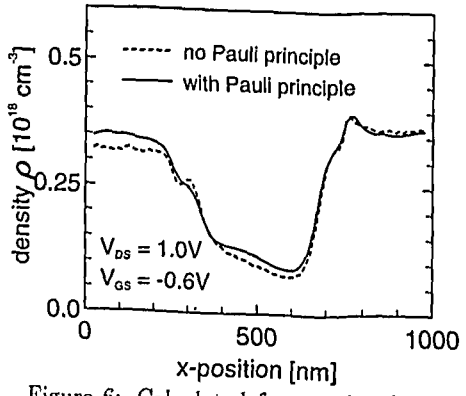

Figure 6: Calculated free carrier density in the channel region.

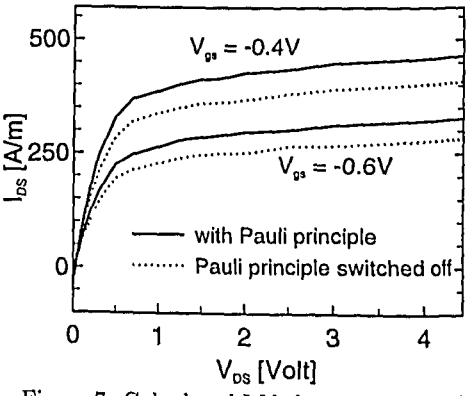

Figure 7: Calculated I-V characteristics of the investigated HEMT.