A Simple Technique for the Monte Carlo Simulation of Transport in Quantum Wells

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Abstract

A simple technique that can be implemented in the Monte Carlo (MC) simulation of transport in a quantum well is reported. The main difference between the proposed technique and existing methods is the use of three dimension momentum (3Dk) particles in the simulation of a quantum region. The use of 3Dk particles within a quantum well structure facilitates the MC simulation of transport in nanoscale devices which contain both the classical and quantum regions.

1 Introduction

As quantum effects are observed in quantum well structures of nanoscale devices, it is necesary to consider quantum transport within those well structures in MC device simulation; however, today's quantum transport model in MC device simulation requires additional scattering rates and density of states to traditional MC simulation. Therefore, a simple method to consider both semi classical and quantum transport is required.

2 Method

The proposed algorithm assumes that MC particles have three dimension momentum (3Dk) everywhere in a simulated device. Therefore, a particle experiences 3Dk scattering, even within a quantum region such as a quantum well, and the energy along the quantized direction is expressed by the sum of its potential and kinetic energy.

The proposed technique is based on the 3Dk to two dimension momentum (2Dk) particle matching method used in DAMOCLES [1]. The proposed algorithm can be composed of three steps: first, assign each particle its nearest eigenenergy along the quantized direction; second, obtain the statistical quantities of the MC ensemble; third step, replace each MC particle's eigenenergy along the quantized direction by its original energy component. The third step is optional. However, inclusion of the third step provides more stable statistics because the energy of a MC particle is not affected by the simulation process.

In both methods, if a particle's energy along the quantized direction is closer to the conduction band edge than the ground state, the particle's existence is ignored. This process is similar to the quantum effective potential approach [2] in that it maintains the minimum energy of a particle to almost the ground state energy.

As the proposed algorithm does not require 2Dk scattering rates, the algorithm can be promptly implemented to 3Dk MC simulators. In 2Dk quantum transport model the number of scattering matrix elements between subbands increases as the number of the subbands considered increases. However, the proposed technique can consider sufficiently many subbands without the increase of scattering matrix elements.

3 Simulation Results

For verification of the technique, MC simulations of rectangular and triangular silicon quantum well structures have been performed. The purpose of these simulations is to verify the proposed technique. Thus, it is assumed that the conduction band is spherical and parabolic. The scattering processes taken into account are those due to the non-polar optical and acoustic phonons.
Using the proposed technique, the carrier energy distribution and ensemble energy can be obtained. Those results are compared with the 2Dk simulation results. The energy distribution in Figure 1 and Figure 3 show that the technique does not have any artefacts. However, the energy distributions show slight differences between the 3Dk and 2Dk results, which are reflected in the average energy in Figure 2 and Figure 4. The difference between 2Dk and 3Dk statistics is due to the absence of a scattering rate to higher subband levels than the third level.

4 Conclusion

A simple technique for consideration of the quantum transport in quantum well device is presented. The statistical quantities obtained from the technique show slight differences between the 2Dk and 3Dk results. However, the method can be easily implemented in existing MC simulators since the technique uses 3Dk particles. The technique can consider a sufficient number of subbands within a quantum well, without the calculation of scattering rates between the subbands.

Acknowledgements

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References

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[2] D. Ferry, R. Akis and D. Vasileska, "Quantum Effects in MOSFETs: Use of an Effective Potential in 3D Monte Carlo Simulation of Ultra-short Channel Devices", IEDM Tech. Dig., pp. 287-290, 2000.

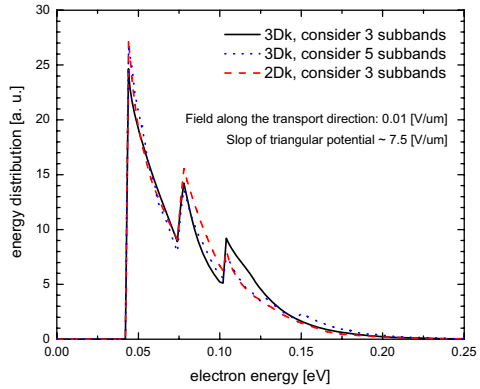

Figure 1: Electron energy distribution in a silicon triangular potential well. 3Dk(2Dk) means 3Dk(2Dk) MC simulation, and 3Dk includes the proposed technique.

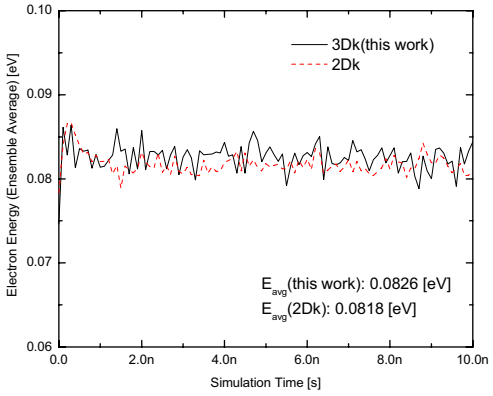

Figure 2: Comparison between the ensemble average energy of 3Dk and 2Dk electrons in a silicon triangular potential.

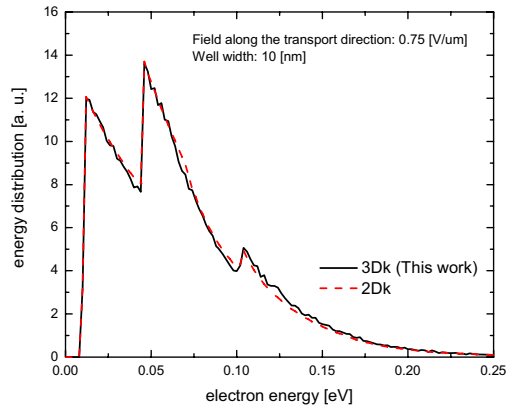

Figure 3: Electron energy distribution in a silicon rectangular well. 3Dk(2Dk) means the result of 3Dk(2Dk) MC simulation, and 3Dk includes the proposed technique.

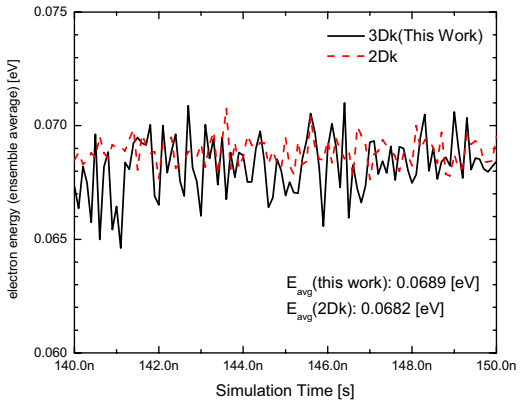

Figure 4: Comparison between the ensemble average energy of 3Dk and 2Dk electrons in a rectangular potential. The fluctuation of 3Dk distribution is due to the small number of carriers over the ground level.