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Methods for anisotropic selection of final states in the full band ensemble Monte Carlo simulation framework

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Abstract

In this paper we discuss different algorithms to select final states after scattering within the full band ensemble Monte Carlo (MC) simulation framework. Faster computers have made it possible to use more elaborated microscopic models for simulation of advanced semiconductor devices. Microscopic details like the band structures, the phonon dispersions and k-vector dependent deformation potentials are becoming accessible, which demand good algorithms for the selection of final states after scattering. The algorithm should also be adapted for a numerical representation of the band structure. Such an algorithm based on the rejection method is presented, which has been studied and compared in terms of efficiency and accuracy with two other algorithms for final state selection. The rejection algorithm is considered as suitable for anisotropic scattering mechanisms and when a relatively slow method is used for calculation of the wave-function overlap integral. It is shown that an accurate model of acoustic phonon scattering results in two characters of the process: one short-q process and one long-q process, very similar to a nonpolar optical intervalley process.

Keywords: Carrier transport; Monte Carlo models; Quantum mechanical scattering

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1. Introduction

Simulation and modelling of semiconductor bulk material and devices is very important in order to understand experimental results and the basic physical phenomena regarding charge transport, as well as to predict various device characteristics. The foundation for device modelling is very much dependent on accurate models of the charge transport in the semiconductor material. In silicon, a large effort has been directed towards the investigation of various transport phenomena. This has led to an improved understanding and new models for complex components, which is the basis for computer aided design (CAD). The continuing demand for faster and more power-efficient circuits with increased functionality makes it necessary to reduce the size of the components, and to introduce new materials and combinations of materials, like heterostructures and wide band-gap semiconductors. A large integration of these materials in VLSI systems demand much more knowledge about both bulk material charge transport and device dependent charge transport. In the field of power electronics, the applications are often based on individual devices, which are operated on the limit of what the material can offer. Advanced computer simulations have become a necessity in the development and optimization of these devices. Accurate simulation models demand a thorough understanding of the basic physical phenomena involved in carrier (electron or hole) transport. It should be pointed out that the knowledge of these phenomena cannot always be obtained from measurements. Especially for new materials, the process technology is not sufficiently developed so as to give a solid ground for modelling.

The full band MC method provides a theoretical tool to study the high field properties of a semiconductor [1,2]. The work of Fischetti and Laux [3,4] clearly shows that accurate impact ionization coefficients can be obtained for a wide range of semiconductors. The key idea in MC simulation is to follow the charge carriers in space and time and to calculate their trajectories from the classical equations of motion between the scattering events that are treated quantum mechanically. In this work, we are discussing different algorithms to select final states after a quantum mechanical scattering interaction. The algorithms are evaluated by MC simulation of the electron transport in 4H–SiC. This complex material, with a total of 12 conduction bands and anisotropic shape of the Brillouin zone (BZ), has been selected due to challenges that it provides for a MC model.

2. Problem formulation

In a MC simulation of carrier transport in semiconductors, a random number is used for the determination of free flight time for each carrier. The free flight is interrupted by a scattering event, where a random number is used to select the type of event. In 4H–SiC, which is the material used to test our models, the following scattering mechanisms are considered: acoustic phonon absorption and emission, polar-optical phonon absorption and emission and nonpolar optical phonon absorption and emission, as well as ionized impurity scattering. The probability of scattering