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On the influence of band structure and scattering rates on hot electron modeling

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Abstract

The relative importance of band structure and scattering rate modeling for the modeling of hot electrons is evaluated. It turns out that the influence of band structure is dominant, while the details of the scattering models are less significant. Consequently computationally rather efficient models for phonon scattering and impact ionization scattering can be applied without sacrificing accuracy as long as the full band structure is considered.

1. Introduction

For the acceptance of a Monte-Carlo model among the engineering design community a careful trade-off between computational efficiency and physical accuracy is necessary. Unfortunately there is no clear solution to this problem, so that many different Monte-Carlo models exist especially for electron transport [1]. In this paper we focus on the problem of modeling hot electrons efficiently over a broad range of energies (up to 4 eV) with sufficient accuracy. In this context it was demonstrated recently [2] that a good agreement between experimental and simulated results on several key hot electron related quantities like impact ionization coefficient and quantum yield can be achieved simultaneously by using a full band Monte-Carlo model and an impact ionization scattering rate extracted from experimental data. Since so far nothing comparable has been published for models based on a simpler description of band structure, let's assume for the moment that the adoption of the full band structure is a necessary prerequisite for reproducing these desirable results with a Monte-Carlo model. The efficiency of a Monte-Carlo model however depends not only on band structure modeling but quite heavily on the complexity of the scattering models as well and in the original paper [2] a very complex and time consuming model for phonon scattering was used. Therefore we have investigated whether the same results can be reproduced by adopting the much simpler phonon scattering model of Jacoboni et al. [5] in order to enhance the overall simulation efficiency.

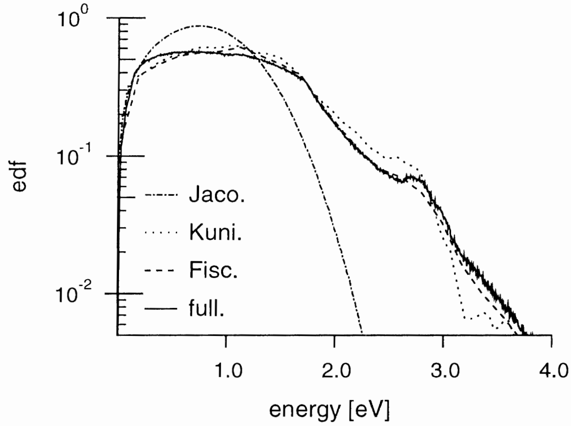

Figure 1: Energy distribution function for the new full band model and from Fischetti et al., Kunikiyo et al. [1] and the original model of Jacoboni et al. [5].

2. Description of the Model

The Monte-Carlo Model used in this paper is based on the full band structure that results from the local pseudo potential method described in [4] and on an extension of Jacoboni's model for phonon scattering to the full band case. The matrix elements of the latter model do not depend on momentum transfer so that this model is computationally very efficient. Only a slight modification of the phonon coupling constants and deformation potentials was necessary (global scaling by a factor of 0.93 was sufficient) in order to reproduce the experimentally observed velocity/field relation with the new full band model. For low energies the band structures of the original Jacoboni model [5] and our new model are in good agreement. Therefore it is a direct consequence of the nearly identical treatment of phonons in both models that all the favorable properties which Jacoboni's model has for low field mobility like the good agreement of the lattice temperature dependence with experiment are valid for our new model as well.

3. Results

In figure 1 the electron energy distribution functions for a homogeneous field of 300 kV/cm of our full band model is compared to the respective results of Fischetti et al. and Kunikiyo et al. [1] which both employed much more complex models for phonon scattering. All three results are remarkable close showing that the distribution function for such fields is insensitive to the complexity of the phonon model (see also [3]). On the other hand the distribution function is very sensitive to the band structure, which is proven by the large differences for energies larger than 2 eV between the distribution functions from Jacoboni's original model and our new model that can be observed in figure 1 as well. Please keep in mind that the two latter Monte-Carlo models employ basicly the same model for phonon scattering.

For modeling impact ionization related quantities like quantum yield and ionization coefficient we investigated the two scattering rates for impact ionization used by Cartier et al. [2] and Thoma et al. [6]. Both scattering rates include unknown parameters that have to be extracted from experiment. In order to make a consistent comparison of both rates we kept the functional form of both rates but adjusted them

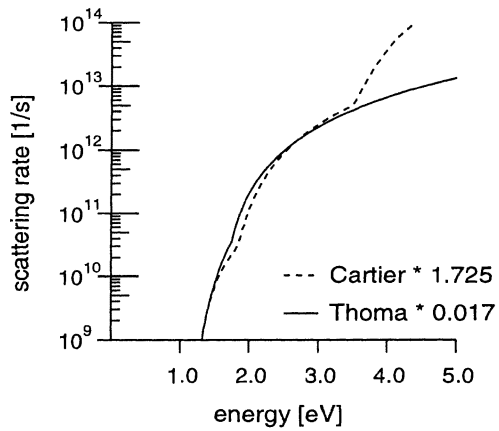

Figure 2: Impact ionization scattering rate of Thoma et al. [6] with a scaling factor of 0.017 and of Cartier et al. [2] with a scaling factor of 1.725.

by global scaling factors such that the quantum yield data of DiMaria et al. [7] at 3 eV was reproduced by our full band model. Doing so the scattering rates as a function of energy became remarkable close below 3.5 eV as can be seen in figure 2. In figures 3 and 4 the results of [7, 8] for quantum yield and impact ionization are compared to the respective results from our new full band model. It can be seen that the agreement of our simulator with the experimental data is just as good as it was reported in [2]. Moreover it becomes clear that this good agreement is insensitive to the exact functional form of the impact ionization scattering rate.

4. Summary

The above results show that even under the assumption that the adoption of the full band structure is necessary to achieve good modeling results for hot electrons over a broad range of electron energies, there are still a lot of possibilities to keep the simulator efficiency at a level that is acceptable for engineering design purposes. For MOS devices the new full band model is only about a factor of two slower than the Monte-Carlo device simulator that we have developed previously [9] and which was based on an analytical band structure description. Thus even on modern high speed workstations full band Monte-Carlo device simulation is feasible.

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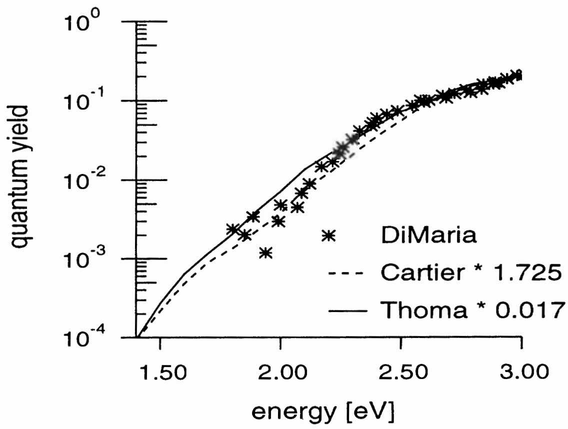

Figure 3: Quantum yield obtained with the full band model with the scaled II scattering rate of Thoma et al. [6] and Cartier et al. [2]. Experimental results: DiMaria et al. [7].

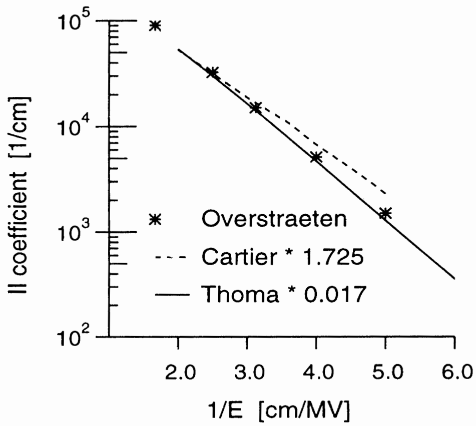

Figure 4: Impact ionization coefficient for the same models as above. Experimental results van Overstraeten et al. [8].