STATE-OF-THE-ART MICRO MATERIALS MODELS IN MINIMOS-NT

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Abstract

Considerable effort was spent on our two-dimensional device simulator MINIMOS-NT to get it ready for simulation of devices with high complexity in respect to materials, geometries, etc. Many of the existing physical models (band gap, mobility, thermal conductivity, energy relaxation times, specific heat, etc.) were refined, some of them were replaced by promising new ones, and many new models were added as well. Being an ancestor of the well-known MOS device simulator MINIMOS [1], its experience with Si devices was inherited. Thereby, MINIMOS-NT became a generic device simulator accounting for a variety of micro-materials, including group IV semiconductors, III-V compound semiconductors and their alloys, and non-ideal dielectrics.

1 Introduction

Several applications of industrial interest employ devices operating in a wide temperature range. Therefore, our models have been designed to meet this challenge in addition to the conventional Silica applications. MINIMOS-NT has been successfully used for simulation of heterostructure devices, e.g. High Electron Mobility Transistors (HEMTs) and Heterojunction Bipolar Transistors (HBTs) [2, 3]. Physics-based DC-simulation, mixed-mode device/circuit simulation, small signal RF-parameter simulation, and device reliability investigations of high practical value were performed.

2 Sets of Partial Differential Equations

In MINIMOS-NT carrier transport can be treated by the drift-diffusion (DD) and the hydrodynamic (HD) transport models. In addition, the lattice temperature can be treated either as a constant or as an unknown governed by the lattice heat flow equation, thus, self-heating (SH) effects are accounted for.

3 Modeling of the Materials Properties

In MINIMOS-NT the properties of III-V ternary materials $A_{1-x}B_xC$ are modeled as a function of the material composition x using the properties of the respective binary materials (AC and BC). In the case of $Si_{1-x}Ge_x$ the properties of the material are modeled based on the properties of both Silicon and Germanium.

3.1 Thermal Modeling for SH

The coefficients of the lattice heat flow equation are the mass density, specific heat, and thermal conductivity of the respective materials. A linear interpolation between the values of the mass density of the basic materials (A and B) is assumed for alloy materials $A_{1-x}B_x$. The temperature dependence of the thermal conductivity is modeled by a simple power law which gives a good agreement with experimental data [4]. A harmonic mean will be taken to model the material composition dependence of the thermal conductivity in the case of alloy materials. The lattice temperature dependence of the specific heat capacity is computed by a new model suggested in [5].

3.2 Carrier Mobility

MINIMOS-NT provides mobility models for various materials which are divided into three main groups according to their particular transport properties: Silicon, Germanium, III-V compound semiconductors, and their alloys. The mobility models have to support both the drift-diffusion (DD) and

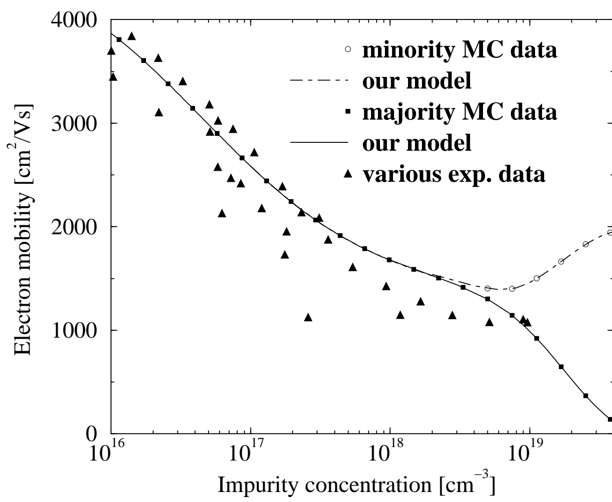

Fig. 1: Electron mobility in InP at 300 K. Our analytical model is compared to MC simulation data and experimental data.

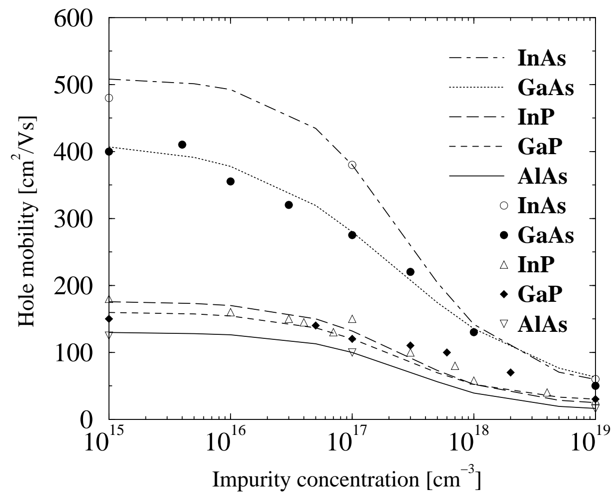

Fig. 2: Hole mobility vs. doping concentration at 300 K. Comparison between the model and experimental data.

the hydrodynamic (HD) transport models. While the high-field mobility is modeled differently, the low-field mobility is independent of the used transport model. This suggests to group the various effects affecting the mobility into low-field and high-field effects.

In MINIMOS-NT the established mobility model for Silicon of MINIMOS 6 [6] is implemented. A model which distinguishes between the majority and minority electrons, as well as between dopant species is described in [7]. The temperature dependence of the lattice mobility preserves the expression from the mobility model of MINIMOS 6. The mobility reduction due to ionized impurity scattering is accounted for by temperature dependent coefficients. The model is applicable to any material of interest (e.g. see Fig. 1). The results delivered by the model for the hole mobility as a function of the doping concentration for various III-V group binary semiconductors compared to measured data are shown in Fig. 2.

Mobility reduction due to a high field is modeled for DD equations. For HD equations the deviation from the ohmic low-field mobility is modeled as a function of the carrier temperature after Hänsch et al. [8]. The energy relaxation times and the saturation velocities are modeled separately.

In the case of III-V semiconductor alloys the model employs the low-field mobilities of the basic materials and combines them by a harmonic mean. The respective interpolations between the basic materials are also done in the models for the saturation velocities and, in the case of HD simulation, of the energy relaxation times. The models are based on experimental or Monte Carlo simulation data and employ analytical functional forms which cover the whole material composition range. The energy relaxation times are used in the HD mobility models, in the energy balance equations of the hydrodynamic transport model, and in the lattice heat flow equation. The energy relaxation times for electrons depend on the lattice temperature and on the carrier temperature [9].

3.3 Bandgap Energy and Bandgap Narrowing

Various models define the temperature dependence of the bandgap energy in the semiconductor (e.g. [10]). Special attention is paid to the band offsets at the heterointerfaces and the thermionic-field emission model which must be used in the case of abrupt heterojunctions. For an alloy $A_{1-x}B_x$, the temperature-dependent bandgaps of the constituents (A and B) are calculated first. The bandgap and the energy offset are then calculated depending on the material composition.

In previous work we emphasized on band gap narrowing as one of the crucial heavy-doping effects to be considered for bipolar devices [11]. We have developed a new physically-based analytical band

gap narrowing model applicable to compound semiconductors, which accounts for the semiconductor material, the dopant species, and the lattice temperature.

3.4 Effective Carrier Masses and Effective Density of States

In MINIMOS-NT the user deals with relative carrier masses, i.e. the effective masses scaled by the free electron mass. A linear temperature and a quadratic temperature dependence are used in the case of electrons and holes, respectively. For an alloy the temperature dependence is introduced first. Then a quadratic interpolation of the masses is used as a function of the material composition.
The model for the density of states represents a theoretical expression which takes into account the number of equivalent energy minima. In case of a transition between a direct and indirect bandgap, the valley degeneracy factor is modeled accordingly.

3.5 Generation and Recombination

Carrier generation in space charge regions and recombination in e.g. high injection regions is modeled using the well known Shockley-Read-Hall (SRH) equation. A trap assisted band-to-band tunneling model (BBT) describes the generation of carriers in high field regions. The model modifies the SRH lifetimes by field enhancement factors. Surface recombination is accounted for by a model which modifies the SRH lifetimes depending on the carrier surface recombination velocities and the surface distance. The Auger-processes are modeled using a triple concentration product. The processes are the inverse processes to the impact ionization process. The direct BBT model describes the carrier generation in high field regions without any influence of local traps. The type of the impact ionization model depends on the used equation set. Using the DD equation set, an electric field dependent model is used to calculate the generation rate. In HD simulations the carrier temperatures are solved together with the carrier concentrations and the potential. The information about the carrier temperatures is used for the hydrodynamic impact ionization model.

3.6 Interface Models

The device geometry is partitioned into independent regions, so-called segments. For these segments different sets of parameters, models and algorithms can be defined independently. The segments are linked together by interface models which account for the interface conditions. The interface models for the carrier concentrations specify the solution for the continuity equations with the unknown concentration quantities on the device segments. To calculate the carrier concentrations and the carrier temperatures at the interface of two semiconductor segments three different models are implemented in MINIMOS-NT. These are a model with continuous quasi Fermi level across the interface (CQFL), the thermionic emission model (TE), and the thermionic field emission model (TFE). The derivation of these models is described in [12].

4 Simulation Results

Several types of HBTs have been analyzed to obtain one concise set of model parameters, used in all simulations. For example, in Fig. 3 we present the simulated forward Gummel plot for an AlGaAs/GaAs HBT compared to experimental data. The simulation results at 373 K demonstrate the ability of MINIMOS-NT to reproduce correctly the thermal device behavior. Furthermore, very good agreement also for the reverse Gummel plots has been achieved, e.g. in Fig. 4 the comparison with measured data for InGaP/GaAs HBT is shown.

5 Summary

Several sophisticated models have been created and employed to get good agreement with experimental results, and also to aid getting an insight and understanding of the real device and thus achieve better device performance.

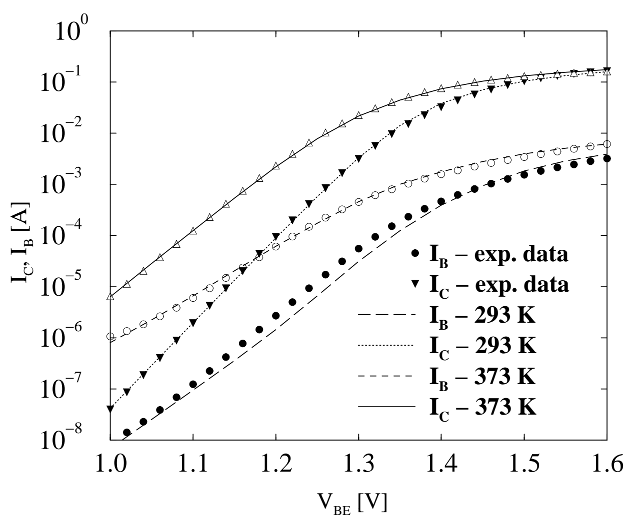

Fig. 3: Forward Gummel plots at $V_{CB} = 0$ V. Comparison with measured data at 293 K and 373 K.

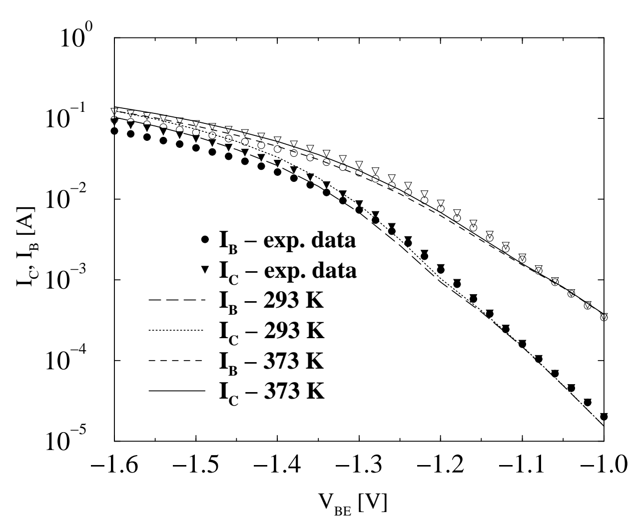

Fig. 4: Reverse Gummel plots at $V_{CB} = 0$ V. Comparison with measured data at 293 K and 373 K.

Acknowledgment

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