Implications of dopant-dependent low-field mobility and band gap narrowing on the bipolar device performance

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Abstract. Band gap narrowing is one of the crucial heavy-doping effects to be considered for bipolar devices. We present a new band gap narrowing model which considers the semiconductor material and the dopant species for arbitrary finite temperatures. As the minority carrier mobility is of considerable importance for modeling advanced n-p-n bipolar transistors, we implemented the new universal low field mobility model [1] in MINIMOS-NT [2]. This model distinguishes between majority and minority electron mobilities on one hand, and between different dopant species on the other hand, both as a function of temperature and dopant concentration. This unified treatment is especially useful for accurate device simulation. As a particular example we present the results for SiGe HBT.

1. INTRODUCTION

Many papers were dedicated on the mobility and band gap narrowing in semiconductors in the last 20 years (e.g. [3]). Recently, the scientific community seemed to be more or less satisfied with the models for Si proposed by Klaasen et al. [4] and the research on this topic shifts towards investigating the mobility and the band gap narrowing in more exotic compound materials (e.g. [5]).

The aim of this work is not to oppose to any previous work, also not to contribute in the "best fit competition". Our aim is to give a physically sound explanation of some existing effects and to obtain tractable models suitable for device simulation purposes.

2. PHYSICAL BASIS OF THE NEW MODELS

One of the basic assumptions in the models for ionized-impurity scattering is that the charge of an impurity center is treated as a point charge. In the approach from [1] it was shown that considering the spatial extent of the charge density one can explain various doping effects due to the chemical nature of the dopant at high doping concentrations.

3. LOW-FIELD ELECTRON MOBILITY

In [1] Monte-Carlo (MC) simulation results for the low-field mobility in silicon for arbitrary concentration, temperature and dopant were presented. Based on the MC results analytical formulae, suitable for device simulation, were derived (Fig. 1, 2), e.g. in case of silicon we have

$$\mu_{\mathrm{n,maj}}(N_{\mathrm{D}},T,Z) = \frac{\mu_0 - g - h}{1+\left(\frac{N_{\mathrm{D}}}{C_1}\right)^{\alpha_1}} + \frac{g}{1+\left(\frac{N_{\mathrm{D}}}{C_2}\right)^{\alpha_2}} + h \qquad (1)$$

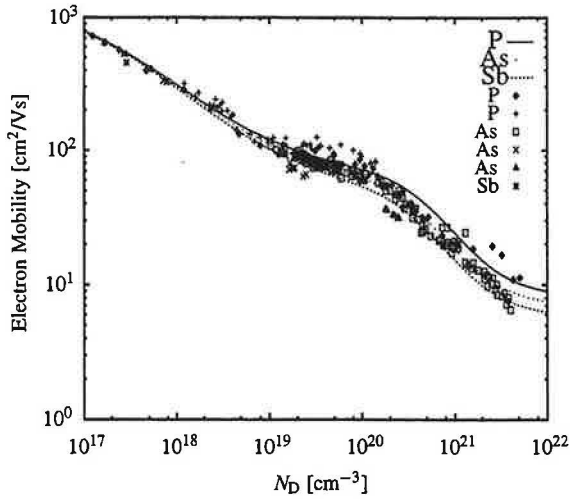

Figure 1: Majority mobility in P-, As- and Sb-doped silicon at 300 K compared with experimental data

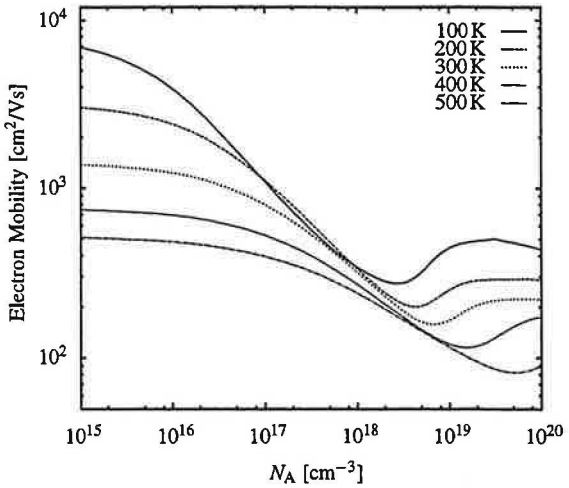

Figure 2: Minority mobility in B-doped silicon as a function of concentration at different temperatures

$$\mu_{n,min}(N_A,T,Z) = \frac{\mu_0+m-k-h}{1+\left(\frac{N_A}{C_1}\right)^{\alpha_1}} + \frac{k}{1+\left(\frac{|N_A-C_a|}{C_2}\right)^{\alpha_2}} - \frac{m}{1+\left(\frac{|N_A-C_b|}{C_3}\right)^{\alpha_3}} + h \quad (2)$$

where $\mu_0, \alpha_1, \alpha_2, \alpha_3, C_1, C_3, C_a, k$, and m are temperature dependent parameters, and g, h, C_2, and C_b are also dopant dependent. After implementation in MINIMOS-NT we studied the cases, in which the difference in the obtained mobility values cannot be neglected anymore, as it is frequently assumed. For example, the minority mobility at heavy doping levels (above 10^{19} cm^{-3}) exceeds the majority mobility more than three times. The difference gets even stronger at low temperatures (sixteen times).

4. BAND GAP NARROWING

Band gap narrowing is an important heavy-doping effect for bipolar devices. The correct modeling of the conduction and valence band-edge energies has basic importance for the simulation results. Though band gap narrowing is very difficult to be modeled rigorously due to the multiple carrier interactions [6] one can approximate the energy shift to first order by the classical self-energy of the electron in the field of an ionized impurity. Thus we obtain

$$\Delta E_g = e \cdot \lim_{r\to 0}[V_s(r) - V(r)] \quad (3)$$

$$V(r) = \frac{1}{(2\cdot\pi)^3}\int V(q) e^{i\cdot\mathbf{q}\cdot\mathbf{r}}\mathbf{dq} \quad (4)$$

where $V(r)$ is the Coulomb potential of a point charge and $V_s(r)$ is the screened Coulomb potential of an electron in an electron gas. Eq. 3 represents the change in the electrostatic energy of an electron before and after the electron gas redistribution. After [1] we have

$$V(q) = \frac{e^2}{\varepsilon_0\cdot\varepsilon_r}\cdot\left(\frac{Z-F(q,\alpha)}{q^2+\beta^2}\right) \quad (5)$$

$$F(q,\alpha) = \frac{N\cdot\alpha^2}{q^2+\alpha^2} \quad (6)$$

Solving Eq. 4 and replacing V(r) in Eq. 3 leads to final expression for the band gap narrowing effect

$$\Delta E_g = -\frac{e^2}{4\cdot\pi\cdot\varepsilon}\cdot[\beta\cdot N^* + \alpha_I\cdot N_I^* + \alpha_{SC}\cdot N_{SC}^*] \quad (7)$$

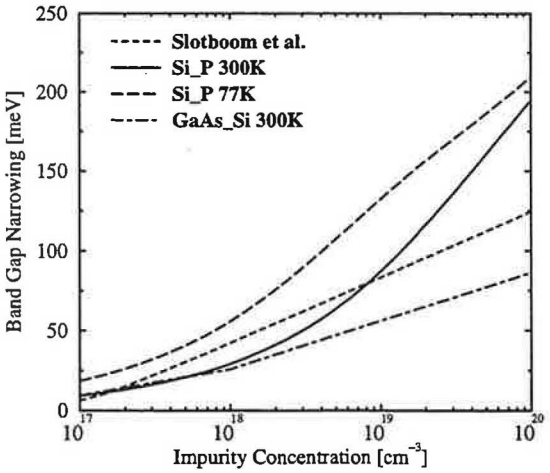

Figure 3: Band gap narrowing versus impurity concentration

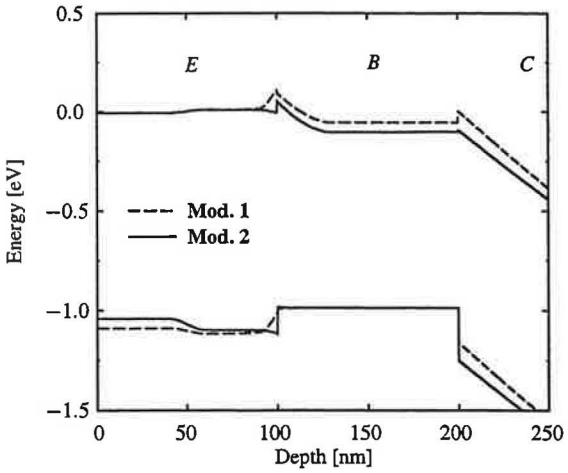

Figure 4: Effective band edge energies for Mod.1 and Mod.2 at 77K

$$N^* = Z_I - \frac{N_I}{1-\beta^2/\alpha_I^2} + Z_{SC}\cdot\left(\frac{1}{1-\beta^2/\alpha_{SC}^2}-1\right) \tag{8}$$

$$N_I^* = N_I\cdot\left(\frac{1}{1-\beta^2/\alpha_I^2}-1\right) \tag{9}$$

$$N_{SC}^* = N_{SC}\cdot\left(1-\frac{1}{1-\beta^2/\alpha_{SC}^2}\right) \tag{10}$$

The subscripts *SC* and *I* refer to a semiconductor and impurity, respectively. Z and N are the atomic number and the number of electrons of a given material. α can be interpreted as size parameter of the electron charge density, α_0 is the Bohr radius, and β denotes the inverse Thomas-Fermi length. They are expressed as

$$\alpha = \frac{Z^{1/3}}{c_k\cdot\alpha_0\cdot\varepsilon_0\cdot\varepsilon_r}\cdot\frac{1-2\cdot\left(\frac{Z}{N}\right)}{\frac{5}{3}-4\cdot\left(\frac{Z}{N}\right)^{1/3}} \tag{11}$$

$$c_k = \frac{\Gamma(4/3)}{2}\cdot\left(\frac{3\cdot\pi}{4}\right)^{2/3}\cdot\left(\frac{3}{5}\right)^{7/3} \tag{12}$$

$$\beta^2 = \frac{n\cdot e^2}{\varepsilon_0\cdot\varepsilon_r\cdot k_B\cdot T}\cdot\frac{F_{-1/2}(\eta)}{F_{1/2}(\eta)} \tag{13}$$

The Fermi integrals $F_{1/2}(x)$ are defined as in [7]. Using full Fermi-Dirac statistics in Eq. 13 the simulation results are valid for any doping concentration. Thus, our band gap narrowing model is the first theoretically derived model predicting different shifts for various dopant species. Lacking experimental data does not allow to confirm our simulation results at present.

As a particular example we present in Fig. 3 the results for Si doped GaAs and P doped Si. Note the stronger band gap narrowing at 77K, caused by higher degeneracy. Neglecting of this effect results in error of about 50%. In Fig. 4 we illustrate this difference for the effective band edge energies.

5. RESULTS

The respective temperature and mole fraction dependent models of the physical parameters of the alloys were implemented into MINIMOS-NT, our two-dimensional device simulator with approved capabilities of simulating devices with complex structure [2].

As a particular example, after calibration to the the experimental data available, the electrical behavior

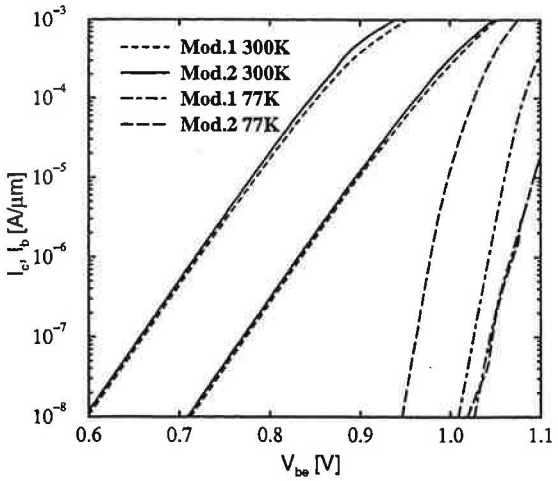

Figure 5: Gummel plots at $V_{ce} = 2V$ for Mod.1 and Mod.2

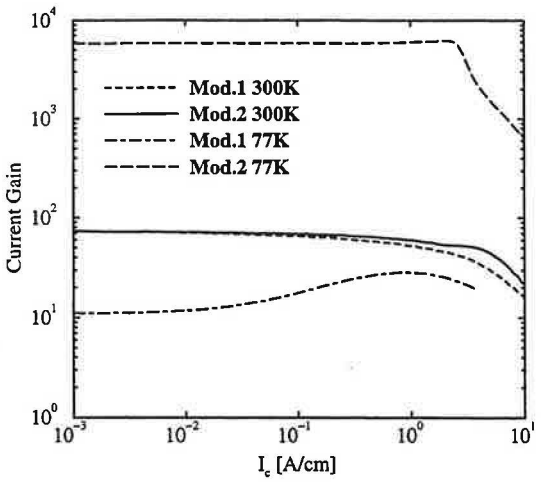

Figure 6: Current gain versus collector current for Mod.1 and Mod.2

of SiGe HBT was studied at different temperatures using a hydrodynamic transport model. Our investigations were performed in a comparative way for different dopant species and concentrations using the new models and the old ones. Fig. 5 we present the Gummel plots for SiGe HBT at 77K and 300K obtained with the model of Slotboom et al. [3] (Mod.1) and with our new model (Mod.2). Note the significant difference in the current density values at 77K, resulting for in higher current gain with the new model (Fig. 6), which is confirmed by experiments.

In summary, new band gap narrowing and mobility models are presented and their impact on the HBT device performance is studied.

Acknowledgment

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