A Universal Low-Field Electron Mobility Model for Semiconductor Device Simulation

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ABSTRACT

We present analytical electron mobility formulae for Si which treat the dependence on all common dopants, such as P, As, Sb, and B in a unified manner. The expressions are derived from Monte Carlo (MC) calculations which are based on a new approach to ionized impurity scattering that inherently distinguishes the dopant species. By calculating the scattering cross section in the Born approximation including momentum-dependent screening and pair-scattering we finally obtain the total impurity scattering rate which depends through the atomic and electron number on the dopant species. Using this impurity scattering model in our MC simulator we finally obtain the electron mobility as a function of temperature and concentration for P-, As-, Sb-, and B-doped Si. From these first principle data we derive analytical expressions for the majority and minority mobility valid in the temperature range (70-500 K) and up to an impurity concentration of 10^{21} cm^{-3}.

Keywords: electron mobility, ionized impurity scattering, doped silicon, device simulation

INTRODUCTION

The electron mobility in silicon is an important parameter for device design and analysis. Accurate mobility models are necessary for predictive simulation due to the direct dependence of the current on mobility, which is often the most desired quantity. It is well known that under low fields the mobility depends on the doping concentration and on temperature. However, the mobility values in n-type Si may differ by more than 30% even at room temperature depending on the donor species [1].

Many published mobility formulae (e.g [2][3]) are based on the approach by Caughey and Thomas [4] who used a function of the form

$$\mu_n^{LI} = \mu_n^{\min} + \frac{\mu_n^L - \mu_n^{\min}}{1 + \left(\frac{CI}{C_n^{ref}}\right)^{\alpha}} \tag{1}$$

(1) fits the majority mobility data up to 10^{20} cm^{-3} at 300 K. Numerical values for the parameters in (1) for P-doped Si at 300 K are summarized in [5]. For even higher doped Si an additional term has been added to (1)[1].

To simulate bipolar transistors it becomes necessary to distinguish between majority and minority mobility values. Experiments have shown that the minority electron mobility may exceed the majority electron mobility by a factor of 16 at an acceptor concentration of about $6 \cdot 10^{19}$ cm^{-3} [6]. A review of minority carrier transport in Si can be found in [7]. Klaassen [8][9] proposed an analytical model which distinguishes between majority and minority electrons. He assumed, besides the concentration dependence, a temperature-dependent lifetime for the excess carriers. However, his final model proposes a different temperature behavior than experiments [6][10][11][12] do. The reason lies in the different assumptions for the temperature-dependent lifetime.

There is still no universal electron mobility model for Si which is useful for all dopant species. We have derived formulae for the electron mobility in Si both for the most common donors, i.e. P, As, and Sb and for the commonly used acceptor B. These expressions are based on a recently published ionized impurity scattering model which goes beyond the frequently used Brooks-Herring (BH) model based on the linear Thomas-Fermi approximation (TF) [13]. Using this impurity scattering model from first principles in a Monte Carlo simulator we calculated the electron mobility for all dopants in the interesting concentration and temperature range. From these data we derived analytical expressions of the mobility values for all dopants. Hence, this is to date the first physics-based electron mobility model accounting for all possible dopants.

IMPURITY SCATTERING MODEL

Charge Density of Ionized Impurities

The total charge density (in units of the electron charge e_0) of an impurity atom with atomic number Z and electron number N in a solid is given by

$$\rho_{ion}(r) = Z\delta(r) - \rho_e(r) \tag{2}$$

$$N = \int \rho_e(\vec{r}) d^3r \tag{3}$$

The first term in (2) describes the nuclear charge density distribution concentrated in the origin, and $\rho_e(r)$ is the electron charge density of the impurity ion. The

atomic form factor $F(q)$, which represents the electron charge distribution of the impurity in momentum space, is defined as the Fourier transform of the electron charge density [14]

$$F(q) = \int d\vec{r}\, e^{-i\vec{q}\cdot\vec{r}} \rho_e(\vec{r}) \tag{4}$$

The momentum-dependent form factor strongly influences the scattering strength of the ionized impurity. Only for small scattering angles ($q = 0$) $F(q)$ becomes a constant equal to the number of electrons (BH limit). However, with increasing doping concentration and carrier energy the angle-dependence of the atomic form factor becomes important, as scattering events with larger q are more pronounced [13]. Since the impurity ion in a solid is screened by free carriers, the effective potential in momentum space in the random phase approximation for a spatially extented impurity can be expressed by [15]

$$\begin{aligned} \mathcal{U}(q) &= V_0 \frac{Z - F(q)}{q^2 + \beta^2 G(q)} \\ V_0 &= \frac{2m^*}{\hbar^2}\frac{e_o^2}{\epsilon_{Sc}} \end{aligned} \tag{5}$$

where ϵ_{Sc} is the dielectric constant of the semiconductor and e_0 the elementary charge. The inverse Thomas-Fermi screening length β is given by [15]

$$\beta^2 = \frac{n\, e_o^2}{\epsilon_{Sc}\, k_B T} \frac{\mathcal{F}_{-1/2}(\eta)}{\mathcal{F}_{1/2}(\eta)}, \tag{6}$$

where η is the reduced Fermi energy, k_BT the thermal energy, and n the free carrier concentration (no compensation is assumed). The screening function $G(q) \leq 1$ represents the dielectric response of the conduction electrons to an external charge [15]. In the BH approach $G(q) = 1$ is assumed (momentum-independent screening). This assumption becomes questionable in highly doped semiconductors, such as silicon at a doping concentration of 10^{18} cm^{-3}. Note, that $|Z - F(q)|$ is smaller than unity in case of acceptor ions in contrast to donor ions where this factor is larger than one [13].

Thomas-Fermi Atomic Model

To this end the only unknown quantity is the exact charge density distribution of the impurity ion in a solid. There are numerous rather sophisticated methods to calculate the electron charge density distribution. As we are interested in analytical solutions, we use the semi-classical TF model. Its basic idea is to treat the valence electrons as a degenerate Fermi gas of nonuniform, spherically symmetric electron density in a positive charged background [16] at zero temperature. Under this assumption we get a local relation between the electron charge density and the Fermi energy. The total energy consists of the classical Coloumb potential energy of electron-electron E_{e-e} and electron-nucleus interactions E_{e-n}, and the kinetic energy E_k. Thus the total energy functional E is (in atomic units)

$$E = E_k + E_{e-n} + \lambda\,(E_{e-e}) \tag{7}$$

$$E_k = c_k \int \rho_e(r)^{5/3} d^3r\,, \qquad c_k = \frac{3}{10}\left(3\pi^2\right)^{2/3} \tag{8}$$

$$E_{e-n} = -\frac{Z}{\epsilon_{Sc}} \int \frac{\rho_e(r)}{r} d^3r \tag{9}$$

$$E_{e-e} = \frac{1}{2\,\epsilon_{Sc}} \int\int \frac{\rho_e(r)\rho_e(\vec{r'})}{|\,\vec{r} - \vec{r'}\,|} d^3r\, d^3\vec{r'} \tag{10}$$

In (7) λ represents the correlation parameter. Assuming the charge density distribution

$$\rho_e(r) = \frac{N\,\alpha^2}{4\pi}\frac{e^{-\alpha\, r}}{r} \tag{11}$$

we obtain for the energy functional

$$\begin{aligned} E &= c_k^* N^{5/3}\alpha^2 - \frac{NZ\alpha}{\epsilon_{Sc}} + \lambda\,\frac{N^2\alpha}{4\epsilon_{Sc}} \\ c_k^* &= \frac{\Gamma\left(\frac{4}{3}\right)}{2}\left(\frac{3\,\pi}{4}\right)^{2/3}\left(\frac{3}{5}\right)^{7/3} \end{aligned} \tag{12}$$

Calculating the first derivative of the total energy with respect to the variational parameter α and the electron number N we get two equations for α and λ:

$$0 = \frac{\partial E}{\partial \alpha} \tag{13}$$

$$0 = \left.\frac{\partial E}{\partial N}\right|_{N=Z} \tag{14}$$

(14) is obtained from the vanishing chemical potential for a neutral atom in the TF model. Solving (13) and (14) with respect to λ and α we finally obtain the variational size parameter α as a function of Z and N:

$$\alpha = \frac{Z^{1/3}}{c_k^*}\,\frac{1 - 2\,\left(\frac{Z}{N}\right)}{\frac{5}{3} - 4\,\left(\frac{Z}{N}\right)^{1/3}} \tag{15}$$

Scattering Rate

The differential cross section in the first BA can be written as [17]

$$\frac{d\sigma_{B1}}{d\Omega} = |\mathcal{U}(q)|^2 \left(1 + \frac{\sin(qR)}{qR}\right) \tag{16}$$

The term in brackets takes into account the scattering of an electron on pairs of ionized impurities. The average separation R between neighboring impurities is defined as [18]

$$R \equiv \langle r \rangle \approx (2\pi\, N_I)^{-\frac{1}{3}} \tag{17}$$

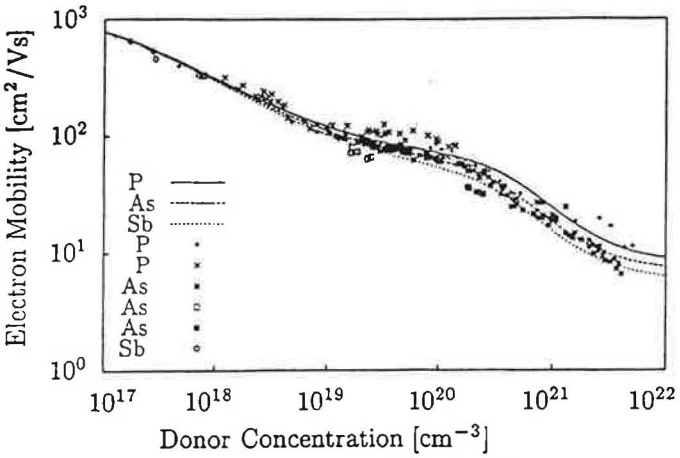

Figure 1: Majority mobility (22) in P-, As-, and Sb-doped silicon at room temperature.

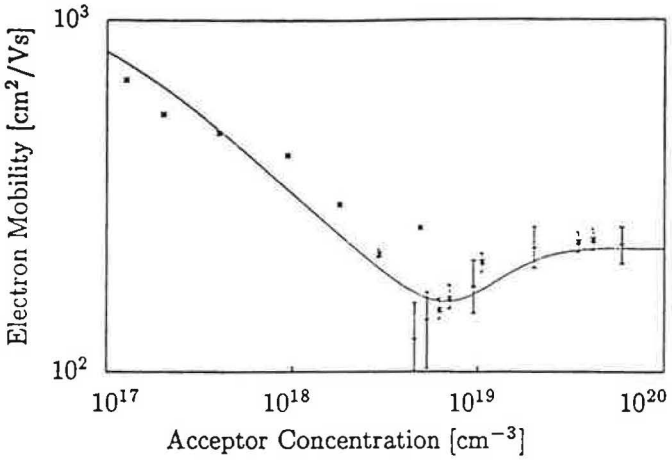

Figure 2: Minority mobility (33) in B-doped silicon at room temperature.

The total cross section $\sigma_t(k)$ is the integral of (16) over the solid angle. The total impurity scattering rate is defined as [19]

$$\begin{aligned} \lambda(k) &= \frac{N_I \hbar k}{m^*} \sigma_t(k) \\ \sigma_t(k) &= \sigma_{B1}(k) + \sigma_c(k) \end{aligned} \tag{18}$$

σ_c is a correction to the first Born approximation based on the scattering amplitude of Schwinger [20]. It can be shown that to first order σ_c can be written as

$$\sigma_c(k) = a_1(k)\,\sigma_{B1}(k) \tag{19}$$

$$a_1(k) = \frac{c}{1 + \frac{4k^2}{\beta^2} - c} \tag{20}$$

$$c = \frac{V_0(Z-N)}{\beta}\left(1 - \frac{V_0(Z-N)}{4\beta}\right) \tag{21}$$

In addition to ionized impurity scattering which is the main scattering process in heavily doped semiconductors, we take into account phonon scattering and electron-plasmon scattering [21]. The latter effect lowers the mobility in p-type Si significantly and is responsible for the dip in the minority mobility (Fig. 2, Fig. 4), which corresponds to the maximum strength of the electron-plasmon interaction. As the plasmons are usually damped an assumption for the damping process and the cutoff wave vector has to be made. As damping effects are of second order we used a damping constant of 10^{-16} s and the inverse screening length (6) as the cutoff vector [22]. Considering the experimental discrepancies in B-doped Si, we found it not worth putting more effort in modeling electron-plasmon scattering. As at higher concentrations degeneracy effects become important, the Pauli exclusion principle (majority electrons only) and the Fermi-Dirac statistics are considered in our calculations. (18) together with the scattering rates of all other possible scattering events is finally used in a Monte Carlo simulator to calculate the electron mobility.

MOBILITY MODEL

Our theoretical model combines the classic atomic model of Thomas-Fermi with a variational principle to obtain a unique charge distribution for each dopant. With a characteristic charge density we have derived scattering rates for each dopant useful for a Monte-Carlo simulator to finally obtain the low field electron mobility.

Majority Electron Mobility

The sheet resistance has to be predicted accurately to estimate the source and drain resistances which are a limiting factor in the performance of MOS devices. It is known that the primary limitation in the accuracy of simulated sheet resistance calculations is the availability of reliable mobility data and models. However, a large spread exists in the early mobility data published in the past. Almost all simulators still use simple mobility models making no distinction between different dopant species.

Masetti *et al.*[1] made extensive measurements of the majority mobility in P- and As-doped Si in the high doping range. To fit the data they used (1) with an additional term. It has been shown that the simplest, but accurate approach to fit our majority mobility data in the doping range $[10^{14}, 10^{22}]$ cm^{-3} is still to use (1) with a second rational term to account for the second local minimum of the mobility in the high doping regime:

$$\mu_{maj}(CI,T,Z) = \frac{\mu_0 - g - h}{1 + \left(\frac{CI}{C_1}\right)^{\alpha}} + \frac{g}{1 + \left(\frac{CI}{C_2}\right)^{\beta}} + h\,. \tag{22}$$

Using the abbreviations $\bar{T} = T/300\text{K}$ and $\bar{Z} = Z/Z_P$ with $Z_P = 15$ the temperature-dependent parameters are defined as follows:

$$\mu_0(T)\left[\frac{\text{cm}^2}{\text{Vs}}\right] = 380 + 20700\,\text{e}^{-3\bar{T}} \tag{23}$$

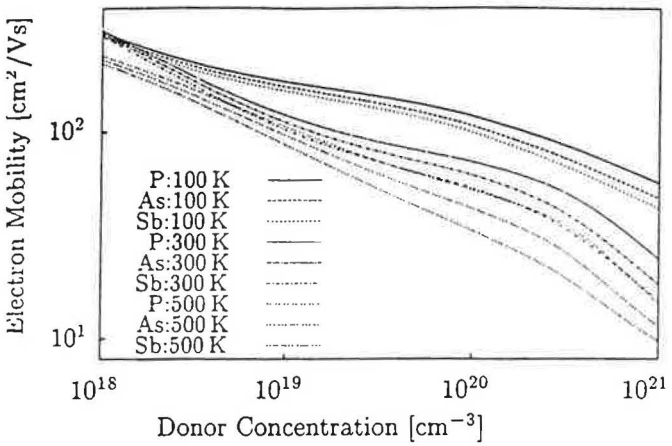

Figure 3: Majority mobility (22) in P-, As-, and Sb-doped Si at 100, 300, and 500 K.

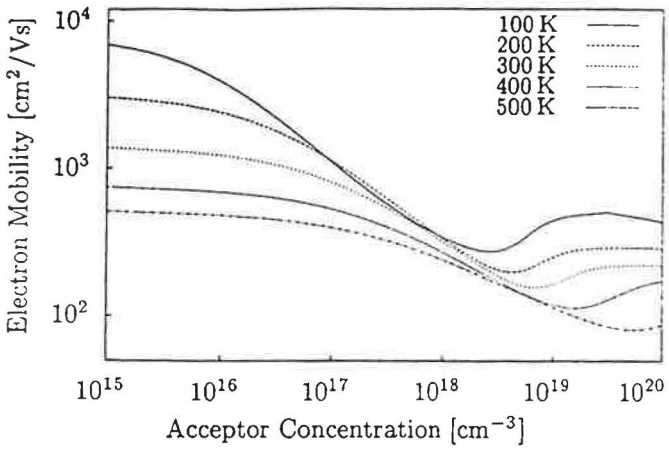

Figure 4: Minority mobility (33) in B-doped silicon at various temperatures.

$$g(T,Z)\left[\frac{\mathrm{cm}^2}{\mathrm{Vs}}\right] = 18 - 8\bar{Z} + (7\bar{Z}+208)\,\mathrm{e}^{-1.5\,\bar{T}} \quad (24)$$

$$h(T,Z)\left[\frac{\mathrm{cm}^2}{\mathrm{Vs}}\right] = \frac{9-\bar{Z}}{\bar{T}} \quad (25)$$

$$\alpha(T) = 0.9 - 0.18\,\bar{T} \quad (26)$$

$$\beta(T) = 0.46 + 1.05\,\bar{T} \quad (27)$$

$$\frac{C_1(T)}{10^{16}}\,[\mathrm{cm}^{-3}] = 11.85\,\bar{T}^3 + 0.45 \quad (28)$$

$$\frac{C_2(T,Z)}{10^{20}}\,[\mathrm{cm}^{-3}] = \left(3+\frac{1}{\bar{Z}^2}\right)\cdot\left(1.2-\bar{T}\mathrm{e}^{(3-7\bar{T})}\right) \quad (29)$$

Note that only three parameters are dopant-dependent through the atomic number Z: g, h, C_2. Using the atomic number of boron $Z_B = 5$ (25) and (29) give also the temperature-dependence of minority electrons (see next section). The dopant-dependence of the parameters is evident from (22) as the second rational term becomes dominant with increasing donor concentration where the dopant-dependence is most pronounced. We found that the temperature-dependence of (23) shows an exponential decrease below 150 K rather than a simple power-law fall off. In fig. 1 we see a comparison of the majority electron mobility for P-, As-, and Sb-doped Si. Note, the decreasing slopes of the mobility curves shifted to higher concentrations with increasing temperatures (cf. Fig. 3). As the effective charge gets smaller with higher doping the effective scattering strength is decreased. Despite the increase of scattering centers at higher doping we have less efficient impurity scattering which results in a smaller decrease in the mobility. As screening is becoming weaker at higher temperatures the decrease in the slope is shifted to higher doping. The agreement with experimental data is excellent for P- and As-doped silicon. Unfortunately, to the knowledge of the authors, there are not sufficient experimental data of Sb-doped Si available to compare our model for Sb over the whole concentration and temperature range (Fig. 1).

Minority Electron Mobility

There are only few experimental data available in only limited doping ranges for the electron mobility in B-doped Si [6][10][11][12][23]. However, the uncertainties according the experimental error are rather high, and pronounced discrepancies among the reported data are found (Fig. 2). The origin of these sometimes contradicting results lies in the fact that the minority electron mobility is not measured directly, but derived from the diffusivity through the diffusion coefficient D. The only way for direct diffusivity measurement is by measuring the transit time of the minority carriers excited by light [10][11][12]. A different approach allows to derive D from measured diffusion length and lifetime. However, considering the very small quantities L [μm] and τ [ns], the experimental errors can be more than 30 %. This can easily give an error of a factor of two or more in D. The diffusion length L can be written as

$$L = \sqrt{D\,\tau} \quad (30)$$

where τ denotes the lifetime of the minority electrons. The diffusion coefficient D can be expressed through the Einstein relation as

$$D = \mu\,\frac{k_B\,T}{e_0} \quad (31)$$

The minority electron mobility μ is finally

$$\mu = \frac{|e_0|\,L^2}{\tau\,k_B\,T} \quad (32)$$

Different assumptions for the temperature-dependent lifetime of the excess electrons give finally the contradicting minority mobility data in B-doped Si at low temperatures compared to [10]. Swirhun *et al.* [6][23] took the minority carrier lifetime to be independent of temperature, while Wang *et al.* [10][12] used a lifetime

increasing linearly with decreasing temperature down to 30 K.

In addition to the experimental uncertainties, one additional problem arises when dealing with modeling of minority transport in Si. The applicability of an effective mass for the valence band in Si is questionable. Moreover, the value for the heavy hole mass strongly affects the minority mobility. Data for the effective hole mass are found in the literature in the range of 0.59 m_0 [24] to 1.7 m_0 [21]. Lower values let the mobility behave more monotonically decreasing similar to the majority case. Higher values lead to the well-known dip in the mobility due to the decreasing electron-plasmon interaction. The reason is that the effective hole mass enters the plasma frequency and hence the plasmon energy. Analyzing the density of states data for the valence band obtained by full band MC calculations the maximum reasonable effective hole mass is 1.3 m [n addition, damping effects and the questionable c[illegible]f vector at low doping make modeling of electron-plasmon scattering in p-type material even more complicated. Encounting all these problems and uncertainties when dealing with minority transport we found it not worth taking additionally electron-hole scattering into account which may become an important scattering process in highly doped p-material. It is very difficult to treat this process correctly as the distribution functions of the electrons and holes have to be known. On the other side electron-hole scattering resembles ionized impurity scattering. Under the assumption that the scattering potential can be described by a TF potential and the hole mass is much larger than the electron mass the scattering cross section even becomes exactly the same as for impurity scattering. However, considering the experimental data for highly B-doped Si we can see that the minority electron mobility is much higher compared to the majority values, especially at lower temperatures. To include an additionally scattering process would make the agreement with the experiment even worse.

The minima in fig. 4 moving to higher concentrations with increasing temperature reflect the vanishing electron-plasmon interaction. Whereas fig. 5 shows the minority electron mobility as a function of temperature. Note, the strong increase in mobility with decreasing temperature for higher concentrations due to vanishing electron-plasmon interaction.

Hence to model the minimum in the minority electron mobility properly we modify (22), so that we finally obtain for the minority electron mobility μ_{min} the following expression:

$$\mu_{min}(CI,T,Z_B) = \frac{\mu_0 + m - k - h}{1 + \left(\frac{CI}{C_1}\right)^{\alpha}} + \frac{k}{1 + \left(\frac{|CI - C_a|}{C_2}\right)^{\beta}} - \frac{m}{1 + \left(\frac{|CI - C_b|}{C_3}\right)^{\gamma}} + h \qquad (33)$$

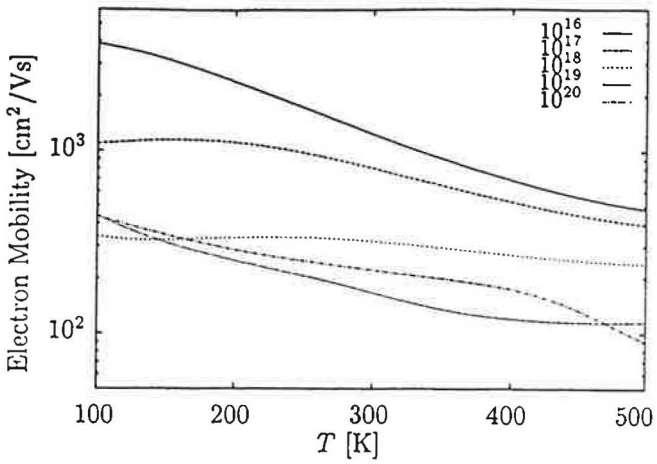

Figure 5: Minority mobility (33) in B-doped silicon for various acceptor concentrations.

with the following set of equations together with (25) and (29) with $Z = Z_B = 5$ for the temperature-dependent parameters:

$$\gamma(T) = \frac{0.6}{\bar{T}} + 1.4 \qquad (34)$$

$$k(T)\left[\frac{\mathrm{cm}^2}{\mathrm{Vs}}\right] = \frac{134}{\bar{T}} + 70 \qquad (35)$$

$$m(T)\left[\frac{\mathrm{cm}^2}{\mathrm{Vs}}\right] = \frac{65}{\bar{T}} + 73 \qquad (36)$$

$$\frac{C_a(T)}{10^{19}}\left[\mathrm{cm}^{-3}\right] = 6\left(2 - 3\,\mathrm{e}^{-2.1\bar{T}}\right) \qquad (37)$$

$$\frac{C_b(T)}{10^{18}}\left[\mathrm{cm}^{-3}\right] = 6.7 - 12.9\,\bar{T}^{0.25}\,\mathrm{e}^{-1.26\,\bar{T}} \qquad (38)$$

$$\frac{C_3(T)}{10^{16}}\left[\mathrm{cm}^{-3}\right] = 2\left[300 + \mathrm{e}^{5.5\,\bar{T}}\right]. \qquad (39)$$

μ_0, α, β, and C_1 in (33) are already defined by (23), (26), (27), and (28), respectively.

CONCLUSION

We have presented a universal electron mobility model for all common dopants in Si. The agreement with experimental data for P- and As-doped Si is remarkably good. For Sb-doped Si further experiments are desired to confirm our results. In case of majorities the mobility formulae are in good agreement with experimental data over the concentration range $(10^{14}, 10^{22})$ cm^{-3} in the temperature range (70-500 K). For minorities we confirm the higher minority mobility compared to the majority values. One reason is the electron-plasmon interaction which is a predominant scattering process in p-Si. Secondly, the negative effective charge is increased with higher concentrations which results in a smaller scattering rate at repulsive scattering centers. Unfortunately, different approaches to measure the minority mobility

lead to strong discrepancies in the published experimental data. Quantitative predictions are therefore almost impossible to make. It might be doubtful, if the strong temperature-dependence, especially at low temperature, claimed by the experimentalists has a physical evidence or is due to wrong assumptions for the temperature-dependence of the excess carrier lifetime. The strong temperature-dependent minority mobility with increasing concentration can only be reproduced by increasing the hole mass to unreasonable high values. However, full band Monte-Carlo data give an upper limit of about 1.3 (in units of the free electron mass m_0) for the hole density mass. Nevertheless, even higher values for the hole mass can be found in the literature [21].

In conclusion, we can say there are still many open questions in minority carrier transport which have to be solved to arrive the stage of a quantitative understanding of the matter. It is hoped that the results outlined here will stimulate more experimental work to confirm definitely the decrease of the majority mobility observed with increasing Z of donor species in n-Si. Additionally, further experiments are necessary to remove the remaining uncertainties and discrepancies concerning the electron lifetime and temperature-dependence of the electron mobility in p-Si.

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