

A UNIFIED MOBILITY MODEL FOR DEVICE SIMULATION

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ABSTRACT

The first physics-based *analytical* model is presented that unifies the descriptions of majority and minority carrier mobility and that includes screening of the impurities by charge carriers, electron-hole scattering, clustering of impurities, and the full temperature dependence of both majority and minority carrier mobility. Using this model excellent agreement is obtained with published experimental data on silicon.

INTRODUCTION

The results of device simulations depend critically on the physical models used, e.g. lifetime, recombination and mobility of carriers, and bandgap narrowing. Sometimes experimental information is only available on a combination of mechanisms, e.g. bandgap narrowing in combination with mobility. With respect to the carrier mobility, however, also independent data are available. During the last few years a number of experimental results have been published which show that, starting at a doping concentration of 10^{18} cm^{-3} , the minority carrier mobility in silicon exceeds the majority carrier mobility, even by a factor of three at a concentration of 10^{20} cm^{-3} [1–3]. Several analytical fit functions describing the minority carrier mobility as a function of the impurity concentration have been proposed [1–3]. However, for device simulation programs the mobility should be expressed as a *single* function of donor and acceptor concentrations. Moreover, electron-hole scattering has to be taken accurately into account because for the minority carrier mobility it is as important as impurity scattering.

Here the main features of the model are presented. Further details will be published elsewhere [4].

CONTRIBUTIONS TO THE MOBILITY

There are four contributions to the mobility. In this section they are given for electrons. For holes similar expressions can be derived [4].

Lattice Scattering

Experimental data on the majority electron and hole mobilities as functions of impurity concentration, N , at 300 K are well-described by ([5] and fig. 1)

$$\mu = \mu_{\min} + \frac{\mu_{\max} - \mu_{\min}}{1 + (N/N_{ref,1})^{\alpha_1}} - \frac{\mu_1}{1 + (N_{ref,2}/N)^{\alpha_2}} \quad (1)$$

The coefficients in eq. (1) for electrons and holes are given in [5]. Since we want to retain this good description of the majority mobility in our model, we use eq. (1) as a starting point. The electron mobility due to lattice scattering, $\mu_{e,L}$, is the low-concentration limit of eq. (1):

$$\mu_{e,L} = \mu_{\max} \quad (2)$$

Donor Scattering including Screening

The third term on the right-hand side of eq.(1) is negligible up to doping levels of 10^{20} cm^{-3} (see fig. 1). Effects of ultra-high concentrations on the carrier mobility, described by this third term, will be treated in a separate section. The electron mobility due to donor scattering, $\mu_{e,D}$, is obtained by subtracting the lattice scattering mobility, $\mu_{e,L}$, from eq. (1) using Matthiessen's rule.

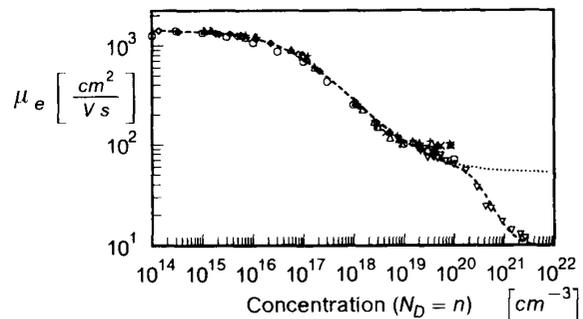


Fig. 1. Majority electron mobility, μ_e , as a function of the impurity concentration. Symbols represent literature data, the dotted line represents the first two terms of eq. (1); the dashed line represents all three terms of eq. (1) and the model calculation ($N_D = n$ with $N_A = p \approx 10^{14} \text{ cm}^{-3}$).

Screening of the impurities by charge carriers is taken into account by modifying the expression for $\mu_{e,D}$ according to the statistical screening theory of Ridley [6], which merges the Conwell-Weisskopf and Brooks-Herring approaches. The resulting expression for $\mu_{e,D}$ reads [4]

$$\mu_{e,D}(N_D, c) = \mu_{e,N} \left(\frac{N_{ref,1}}{N_D} \right)^{\alpha_1} + \mu_{e,c} \left(\frac{c}{N_D} \right), \quad (3a)$$

$$\text{with } \mu_{e,N} = \frac{\mu_{max}^2}{\mu_{max} - \mu_{min}}, \quad (3b)$$

$$\text{and } \mu_{e,c} = \frac{\mu_{min} \mu_{max}}{\mu_{max} - \mu_{min}}, \quad (3c)$$

where c is the total carrier concentration. It should be noted that electron-electron scattering is not accounted for, as it represents only a second order effect [6].

Acceptor Scattering

Already in a paper published in 1957 Blatt [7] showed that at low temperatures the Born approximation breaks down and that from the superior partial-wave method it can be concluded that "in that energy range majority impurities scatter much more effectively than minority impurities." A similar breakdown of the Born approximation occurs at high carrier concentrations. Using the partial-wave method we calculated [4] the ratio, $G(P)$, between the collision cross-sections for repulsive ($\sigma_{\tau,rep}$) and attractive ($\sigma_{\tau,attr}$) screened Coulomb potentials

$$G(P) = \frac{\sigma_{\tau,rep}}{\sigma_{\tau,attr}} = \frac{\sigma_{min}}{\sigma_{maj}} = \frac{\mu_{maj}}{\mu_{min}} = \frac{\mu_{e,D}}{\mu_{e,A}}, \quad (4)$$

$$\text{as a function of } P = 4k^2 r_o^2 \propto \frac{1}{c}, \quad (5)$$

where k is the wavevector and r_o is the Debye screening length [6] (see fig. 2). The contribution to the electron

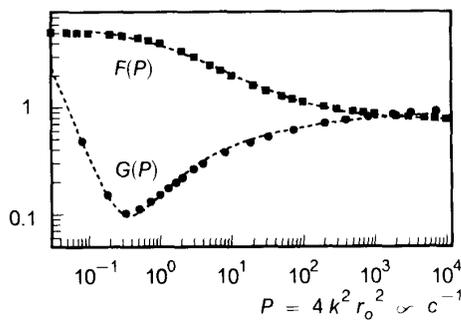


Fig. 2. The function $G(P) = \mu_{e,D} / \mu_{e,A}$ for a temperature of 300 K (solid circles) and the function $F(P) = \mu_{e,h} / \mu_{e,D}$ for a mass ratio equal to unity (solid squares). The dashed lines represent analytical functions describing the results of the calculations [4].

mobility due to acceptor scattering, $\mu_{e,A}$, is now obtained from

$$\mu_{e,A}(N_A, c) = \frac{\mu_{e,D}(N_D = N_A, c)}{G(P)} \quad (6)$$

Hole Scattering

As far as the interaction potential is concerned, holes can be regarded as moving donors. The mobility ratio, $F(P)$, between stationary secondary scatterers with infinite mass and moving secondary scatterers with finite mass can be calculated accurately using the Born approximation (see fig. 2 and [4]), which yields for attractive potentials almost the same collision cross-sections as the partial-wave method. The contribution to the electron mobility due to hole scattering, $\mu_{e,h}$, is now obtained using

$$\mu_{e,h}(p, c) = F(P) \mu_{e,D}(N_D = p, c), \quad (7)$$

where p is the hole concentration. It should be noted that as $F(P) \leq 1 / G(P)$, carrier scattering is more important for the minority carrier mobility than impurity scattering.

ULTRA-HIGH CONCENTRATION EFFECTS

The effects of ultra-high concentrations on the mobility represented by the third term on the right-hand side of eq. (1), can be accounted for by assuming that above an impurity concentration of 10^{20} cm^{-3} the carriers are no longer scattered by impurities possessing one electronic charge and a concentration N , but by impurities with Z electronic charges and a "cluster" concentration $N' = N/Z$. The concentration of charge carriers, c , is not affected. This implies that these ultra-high concentration effects on the carrier mobility can effectively be modelled by replacing N by $Z(N)N$, where $Z(N)$ is the "clustering" function. The donor scattering mobility given by eq. (3a) is modified according to this assumption and added to the lattice scattering mobility using Matthiessen's rule. The

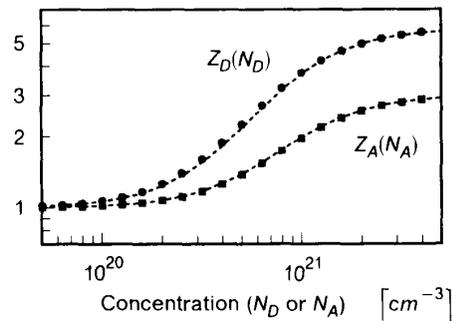


Fig. 3. The clustering functions Z_D (solid circles) and Z_A (solid squares) as a function of N_D and N_A , respectively. The dashed lines represent analytical functions describing the results of the calculations [4].

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resulting mobility is equated to the full eq. (1). Solving for Z at each impurity concentration N yields the "clustering" function $Z(N)$ (see fig. 3 and [4]).

TEMPERATURE DEPENDENCE

For the lattice scattering we use the well-known temperature dependence

$$\mu_{e,L} = \left(\frac{300}{T} \right)^{\theta_e} \mu_{\max} \quad (8)$$

The temperature dependence of the electron-donor scattering mobility is taken according to the Conwell-Weisskopf and Brooks-Herring approaches. This implies that no additional parameters for the description of the temperature dependence are introduced. Only the expressions given by eqs. (3b) and (3c) have to be replaced by [4]

$$\mu_{e,N} = \frac{\mu_{\max}^2}{\mu_{\max} - \mu_{\min}} \left(\frac{T}{300} \right)^{3\alpha_1 - 1.5}, \quad \text{and} \quad (9a)$$

$$\mu_{e,c} = \frac{\mu_{\min} \mu_{\max}}{\mu_{\max} - \mu_{\min}} \left(\frac{300}{T} \right)^{0.5} \quad (9b)$$

MODEL EQUATIONS

In order to obtain the electron mobility, μ_e , as a function of N_D , N_A , n , p , and T one proceeds as follows.

Starting with ionized donor and acceptor concentrations, N_D and N_A , respectively, the clustering functions have to be applied to calculate the concentrations to be used in the model

$$N_D \rightarrow Z_D(N_D) N_D \quad \text{and} \quad N_A \rightarrow Z_A(N_A) N_A \quad (10)$$

The problem of weak screening ($P \rightarrow \infty$ if $c \rightarrow 0$) is solved [4] by taking for the parameter P a weighted harmonic mean of the expression given by eq. (5) and its equivalent in the Conwell-Weisskopf approach (cf. the statistical screening theory of Ridley [6]):

$$P_e = \left\{ \frac{n+p}{3.9 \times 10^{20}} + \left(\frac{N_{e,sc}}{1.2 \times 10^{20}} \right)^{2/3} \right\}^{-1} \left(\frac{T}{300} \right)^2, \quad (11)$$

$$\text{where } N_{e,sc} = N_D + N_A + p \quad (12)$$

is the sum of the concentrations of all scattering partners and all concentrations are in cm^{-3} .

Using Matthiessen's rule the electron mobility, μ_e , is now (see eqs. (2), (3a), (6) and (7)):

$$\mu_e^{-1} = \mu_{e,L}^{-1} + \mu_{e,D}^{-1} + \mu_{e,A}^{-1} + \mu_{e,h}^{-1} \quad (13)$$

The last three terms in eq. (13) as given by eqs. (3a), (6)

and (7) are valid only if there is *one* type of scattering partner. In order to ensure that only truly two-body nearest-scatterers are counted among *any* of the possible scattering partners, the collision cross-sections in $\mu_{e,D}$, $\mu_{e,A}$ and $\mu_{e,h}$ have to be modified. Instead of the concentration of the specific scattering partner, the sum of the concentrations of all scattering partners has to be used ($N_{e,sc}$ is used in eq. (11) for the same reason; [4]). Doing so we find for $\mu_{e,D+A+h}$ defined by

$$\mu_{e,D+A+h}^{-1} = \mu_{e,D}^{-1} + \mu_{e,A}^{-1} + \mu_{e,h}^{-1}, \quad (14)$$

the following expression [4]

$$\mu_{e,D+A+h}(N_D, N_A, n, p) = \mu_{e,N} \frac{N_{e,sc}}{N_{e,sc,eff}} \left(\frac{N_{ref,1}}{N_{e,sc}} \right)^{\alpha_1} + \mu_{e,c} \left(\frac{n+p}{N_{e,sc,eff}} \right), \quad (15)$$

$$\text{where } N_{e,sc,eff} = N_D + G(P_e) N_A + \frac{p}{F(P_e)}. \quad (16)$$

An additional advantage of eqs. (14) - (16) is the simplification of the computational procedure.

COMPARISON WITH EXPERIMENTAL DATA

Using our model excellent agreement is obtained with published experimental data on:

- majority mobility vs. impurity concentration (fig. 1);
 - minority mobility vs. impurity concentration (fig. 4);
 - the effect of electron-hole scattering [8] (fig. 5);
 - majority mobility as a function of temperature (fig. 6);
 - minority diffusion length vs. temperature [9, 10] (fig. 7).
- For holes the agreement between model and experimental data is of the same quality [4].

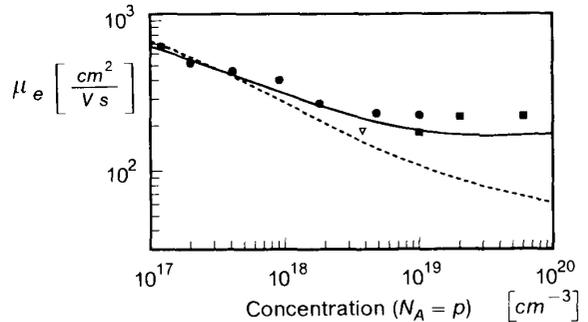


Fig. 4. Minority electron mobility, μ_e , as a function of the impurity concentration: symbols represent literature data (solid squares from [2]) and the solid line represents the model calculation ($N_A = p$ with $N_D = n \approx 10^{14} \text{ cm}^{-3}$). For comparison also the model calculation for the majority electron mobility is shown (dashed line; $N_D = n$ with $N_A = p \approx 10^{14} \text{ cm}^{-3}$).

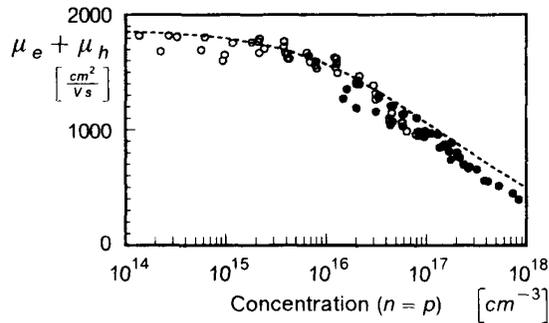


Fig. 5. Sum of electron and hole mobility, $\mu_e + \mu_h$, as a function of carrier concentration. Symbols represent literature data [8] and the dashed line represents the model calculation ($n = p$ with $N_D = N_A \cong 10^{14} \text{ cm}^{-3}$).

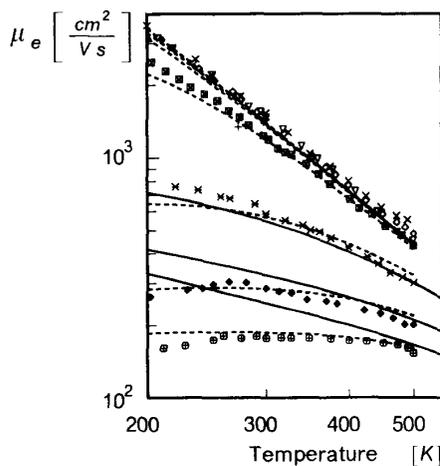


Fig. 6. Majority electron mobility, μ_e , as a function of temperature for various impurity concentrations. Symbols represent literature data and dashed lines represent the model calculations ($N_D = n$ with $N_A = p \cong 10^{14} \text{ cm}^{-3}$). For the highest concentrations (from bottom to top: 2.5×10^{18} , 10^{18} and $2 \times 10^{17} \text{ cm}^{-3}$) the minority electron mobility is also indicated (solid lines).

CONCLUSIONS

The first physics-based analytical model is presented that unifies the descriptions of majority and minority carrier mobility and that includes screening of the impurities by charge carriers, electron-hole scattering, clustering of impurities, and the full temperature dependence of both majority and minority carrier mobility. The electron (and hole) mobility (μ_e and μ_h) are given as analytical functions of local variables: ionized donor, ionized acceptor,

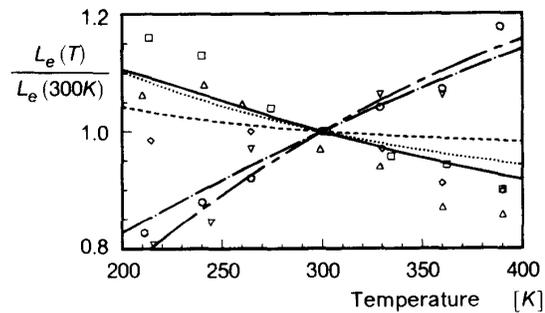


Fig. 7. Minority electron diffusion length, $L_e(T)$, as a function of temperature, normalized to its value at 300 K, for various impurity concentrations. Symbols represent literature data from [9] and lines represent the model calculations ($N_A = p$ with $N_D = n \cong 10^{14} \text{ cm}^{-3}$, [10]):

○ ○ ○	— — — — —	$2.4 \times 10^{17} \text{ cm}^{-3}$,
▽ ▽ ▽	— — — — —	$2.5 \times 10^{18} \text{ cm}^{-3}$,
◇ ◇ ◇	- - - - -	$9.5 \times 10^{18} \text{ cm}^{-3}$,
△ △ △	⋯ ⋯ ⋯	$2.0 \times 10^{19} \text{ cm}^{-3}$,
□ □ □	— — — — —	$5.9 \times 10^{19} \text{ cm}^{-3}$.

electron and hole concentrations and the temperature (N_A , N_D , n , p and T). The excellent agreement between our model and all published experimental data on the carrier mobility in silicon reinforces the model predictions on less investigated aspects of the mobility, e.g. the temperature dependence of the minority carrier mobility, which is distinctly different from that of the majority carrier mobility (see fig. 6). Furthermore this agreement ensures that our model is a sound basis for a revised determination of the bandgap narrowing.

Part of this work was funded by ESPRIT Project 2016.

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