IONIZED-IMPURITY SCATTERING OF MAJORITY ELECTRONS IN SILICON

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Abstract—The Brooks–Herring approach to ionized-impurity scattering overestimates the low-field mobility of electrons in doped semiconductors. It relies on a static single-site description of the carrier-impurity interaction and on the first Born approximation. We present a consistent ionized-impurity scattering model which accounts for degenerate statistics, dispersive screening and two-ion scattering. The dielectric function is accurately approximated by a rational function. From the Schwinger scattering amplitude a correction to the first Born amplitude is derived. Plasmon scattering as another concentration dependent mechanism is included. Despite the various physical effects taken into consideration the scattering model can be used in Monte Carlo transport calculations without any significant increase in computation time. Monte Carlo calculations of majority electron mobility in silicon are discussed, and good agreement with experimental data is found in the doping range $[10^{14}, 10^{20}]\,\mathrm{cm}^{-3}$. © 1998 Published by Elsevier Science Ltd. All rights reserved

1. INTRODUCTION

In modern semiconductor devices the carrier mobilities are often reduced considerably because of high doping concentrations. To predict the electrical characteristics of such devices by means of Monte Carlo simulation accurate models for scattering from charged impurities are needed.

Comprehensive theoretical investigations on the low-field mobility in heavily doped silicon were published by Kay and Tang[1], Bennett and Lowney[2], and Sanborn and Allen[3]. These authors resort to accurate scattering cross sections derived from phase-shift analysis. Fischetti[4] developed a scattering model showing good agreement with experimental data. He stressed the importance of electron scattering by plasmons at high doping concentrations.

In this work we aim at the development of an ionized-impurity scattering model of a complexity which balances physical rigor and computational efficiency when being employed in a Monte Carlo procedure. As a result of this requirement we pursue a model based on the Born approximation, instead of one based on the more demanding phase-shift method. The simplest model is that of Brooks and Herring[5] which, however, predicts too high mobilities compared to empirical data. The review of Chattopadhyay and Queisser[6] reports various causes for the failure of the Brooks–Herring theory, for example, that screening is overestimated and that multiple scattering is ignored completely. We present a model which attempts to overcome some of the shortcomings of the Brooks–Herring model. The new model includes a pair-scattering correction,

an accurate approximation of the dielectric function, and a second Born correction. A detailed discussion on the validity of these extensions will be given.

2. SCATTERING POTENTIAL

We consider a semiconductor with randomly located impurity centers of concentration N_{I}. As N_{I} increases, the average distance between two impurities decreases such that scattering processes become important in which two or more ions are involved simultaneously. To include multi-potential scattering to the first order, we let pairs of impurities act as scattering centers. The applied potential is given by:

$$V_0(\mathbf{r}) = \frac{Ze}{4\pi\epsilon_0\epsilon_r}\left(\frac{1}{|\mathbf{r}|} + \frac{1}{|\mathbf{r}-\mathbf{R}|}\right). \qquad (1)$$

The charge state of the impurity center is denoted by Z, the distance between the centers by $\mathbf{R}$, and ϵ_r is the relative dielectric permittivity of the semiconductor. As the free electrons will respond to the applied potential a self-consistent potential will form. In the linear response regime it is convenient to work with the Fourier components of (1)

$$V_0(\mathbf{q}) = \frac{Ze}{\epsilon_0\epsilon_r q^2}(1 + \exp(-i\mathbf{q}\mathbf{R})) \qquad (2)$$

Then the total potential can be expressed by means of the dielectric function $\epsilon(\mathbf{q}, \omega)$.

$$V_t(\mathbf{q}) = \frac{V_0(\mathbf{q})}{\epsilon(\mathbf{q}, 0)} \qquad (3)$$

The frequency equals zero since the applied potential (1) is time-independent. Considering only low order screening effects one can resort to the Lindhard dielectric function.

$$\epsilon(\mathbf{q}, 0) \equiv \epsilon(q, 0) = 1 + \frac{\beta_s^2}{q^2} G(\xi, \eta) \qquad (4)$$

$$\beta_s^2 = \frac{e^2 n}{\epsilon_0 \epsilon_r k_B T} \cdot \frac{\mathcal{F}_{-1/2}(\eta)}{\mathcal{F}_{1/2}(\eta)}, \qquad \xi^2 = \frac{\hbar^2 q^2}{8 m^* k_B T},$$

$$\eta = \frac{E_F - E_C}{k_b T} \qquad (5)$$

Here, β_s represents the inverse Thomas-Fermi screening length, $\mathcal{F}_j$ denotes the Fermi integral of order j, and η is the reduced Fermi energy. For the screening function G an integral representation exists which cannot be evaluated analytically[7].

$$G(\xi, \eta) = \frac{1}{\mathcal{F}_{-1/2}(\eta)} \frac{1}{\xi \sqrt{\pi}} \int_0^\infty \frac{x}{1 + \exp(x^2 - \eta)}$$

$$\times \ln \left| \frac{x + \xi}{x - \xi} \right| dx \qquad (6)$$

To normalize the screening function to unity for vanishing ξ ($G(0, \eta) = 1$) we chose a prefactor of $1/\mathcal{F}_{-1/2}(\eta)$ in (6) instead of $1/\mathcal{F}_{1/2}(\eta)$ as, for instance, in[7]. Figure 1 shows the screening function for the non-degenerate case and for $\eta = 5$.

In the following the absolute value of $V_t(\mathbf{q})^2$ will be needed. After taking an average of the term $|1 + \exp(-iqR)|^2$ over the solid angle one obtains:

$$|V_t(q)|^2 = 2 \left(\frac{Ze}{\epsilon_0 \epsilon_r q^2 \epsilon(q, 0)} \right)^2 \left(1 + \frac{\sin(qR)}{qR} \right). \qquad (7)$$

Further, an average value for the distance between the ions has to be chosen. Following Ridley[8] we set $R = (2\pi N_I)^{-1/3}$.

Pair-scattering models were used widely to describe dipole scattering in compensated semiconductors[9–12]. In this work we deal with un-compensated silicon in which no pair formation process caused by Coulombic attraction will occur. It can be argued that if in the presence of only one dopant type pair-scattering plays a role, i.e. if the dopant atoms are not diluted, then also multi-impurity scattering will matter. Meyer and Bartoli[13] critically remarked that in such a case the two-ion approximation will be unsuitable for obtaining quantitative mobility corrections. As a result of a lack of reliable results from a more general theory against which this argument can be verified we think it is worth attempting to use a pair-correction to include some of the effects of coherent multi-ion scattering, which would be ignored fully otherwise.

3. SCATTERING RATE

In silicon the lowest conduction-band valleys are strongly anisotropic giving rise to an anisotropicity of the total scattering rate, $\lambda = \lambda(\mathbf{k})$. When dealing with carrier transport in silicon and other indirect semiconductors one commonly applies the Herring–Vogt transformation (see e.g.[14]) which transforms ellipsoidal energy surfaces in k-space to spheres in the transformed k*-space. One can easily show that this transformation will not remove the anisotropicity of the scattering rate, and it holds $\lambda = \lambda(\mathbf{k}^*)$. Even if the mass is anisotropic one usually resorts to an ionized-impurity scattering rate which was derived under the assumption of an isotropic mass, the value of which is given by the density-of-states mass of the anisotropic valley. This procedure yields an isotropic scattering rate, $\lambda(k)$, which represents some average over the solid angle of $\mathbf{k}$ of the anisotropic rate, $\lambda(k)$. It is believed that the error introduced by this approximation is not significant. Therefore, and for the sake of conciseness, the following formalism for ionized-impurity scattering is derived as if the bands were isotropic.

With a given scattering amplitude $f(q)$ the differential scattering cross section σ is defined as[15]:

$$\sigma(q) = \frac{(2\pi\hbar)^3}{m^{*2} v_g(k)} |f(q)|^2 \rho(E). \qquad (8)$$

This expression is valid for general density of states, $\rho(E)$, and electron group velocity, $v_g(k)$. Using the total scattering cross section, σ_{tot}, and the transport cross section, σ_m, which are defined as:

$$\sigma_{tot}(k) = \frac{2\pi}{k^2} \int_0^{2k} \sigma(q) q \, dq, \qquad (9)$$

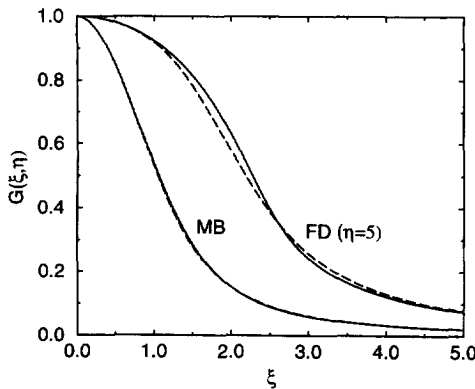$$\sigma_m(k) = \frac{\pi}{k^4} \int_0^{2k} \sigma(q) q^3 \, dq, \qquad (10)$$

Fig. 1. Screening function for the non-degenerate case (MB) and the degenerate case for $E_F = 5kT$. Solid lines: exact, dashed lines: rational approximation.

the total scattering rate λ and the momentum relaxation time τ_m can be obtained.

$$\lambda(k) = N_{\mathrm{p}} v_{\mathrm{g}}(k) \sigma_{\mathrm{tot}}(k) \tag{11}$$

$$\tau_{\mathrm{m}}^{-1}(k) = N_{\mathrm{p}} v_{\mathrm{g}}(k) \sigma_{\mathrm{m}}(k) \tag{12}$$

It is to note that the density of the pair scattering potentials (1) is half the density of the impurity centers, $N_{\mathrm{p}} = N_{\mathrm{I}}/2$.

A crucial assumption is now to use the first Born approximation of the scattering amplitude

$$f(q) \approx f_1(q) = -\frac{1}{4\pi} U(q), \tag{13}$$

where $U(q) = -eV_{\mathrm{t}}(q) 2\, m^*/\hbar^2$. A discussion of this assumption follows in Section 3.2.

Combining the equations presented so far the scattering rate (11) can be expressed as:

$$\lambda(k) = C(k) \int_0^{2k} \frac{1}{(q^2 + \beta_{\mathrm{s}}^2 G(\xi, \eta))^2} \left(1 + \frac{\sin(qR)}{qR}\right) q \, dq, \tag{14}$$

with

$$C(k) = \frac{N_{\mathrm{I}} Z^2 \mathrm{e}^4}{2\pi \hbar^2 (\epsilon_0 \epsilon_{\mathrm{r}})^2 v_{\mathrm{g}}(k)}. \tag{15}$$

Note that in the limit $R \rightarrow 0$ equally charged pairs of impurities scatter up to twice as effectively as independent monopoles[13].

The two-ion case can be considered as the highest order of multi-ion scattering that can be treated by analytical methods. For the sake of computational efficiency of our model higher order terms of the coherent multi-potential interference are neglected.

The Brooks–Herring model can be recovered from (14) firstly by neglecting the two-ion term $(R \rightarrow \infty)$, and secondly by assuming momentum-independent screening by including only $G(0, \eta) = 1$ instead of the full screening function.

3.1. Screening Function

In practical applications the direct use of the screening function (6) in a Monte Carlo procedure will take too much computation time because of the required numerical integration.

In this work we construct a rational approximation of G, which, on the one hand, is sufficiently accurate for the considered transport problem, and, on the other hand, is efficiently to compute. Taylor series expansions of (6) at zero and infinity yield:

$$G(\xi, \eta) = \begin{cases} 1 + f_1 \xi^2 + f_2 \xi^2 + f_3 \xi^6 + \mathcal{O}(\xi^8) & \xi \rightarrow 0 \\ g_1 \xi^{-2} + g_2 \xi^{-4} + g_3 \xi^{-6} + \mathcal{O}(\xi^{-8}) & \xi \rightarrow \infty \end{cases} \tag{16}$$

The expansion coefficients are:

$$f_1 = -\frac{2\mathcal{F}_{-3/2}}{3\mathcal{F}_{-1/2}}, f_2 = \frac{4\mathcal{F}_{-5/2}}{15\mathcal{F}_{-1/2}}, f_3 = -\frac{8\mathcal{F}_{-1/2}}{105\mathcal{F}_{-1/2}}, \tag{17}$$

$$g_1 = \frac{\mathcal{F}_{1/2}}{2\mathcal{F}_{-1/2}}, g_2 = \frac{\mathcal{F}_{3/2}}{4\mathcal{F}_{-1/2}}, g_3 = \frac{3\mathcal{F}_{5/2}}{8\mathcal{F}_{-1/2}}. \tag{18}$$

For the evaluation of the Fermi integrals see[16]. We choose a rational approximation of the form:

$$\tilde{G}(\xi, \eta) = \frac{1 + a\xi^2 + b\xi^4}{1 + c\xi^2 + d\xi^4 + e\xi^6}. \tag{19}$$

The difference between the degrees of the denominator and the numerator must be 2 to let G and $\tilde{G}$ have the same asymptotic behavior ($G(\xi) \propto \xi^{-2}$, $\xi \rightarrow \infty$).

Comparing both the Taylor series expansions of G and $\tilde{G}$ yields a linear equation system for the unknowns (a, b, c, d, e). As we consider two Taylor series, one at zero and one at infinity, we have some freedom in chosing the powers to match. Let E_n denote the linear equation which has to be solved to match the power ξ^n. Matching the powers ξ^2 and ξ^{-2} give two simple equations, namely $a = c + f_1$ and $b = g_1 e$, respectively. These can be used for substitution to reduce the rank of the final equation system from 5 to 3. For the remaining unknowns the following equations are found.

$$\begin{aligned} E_4 &= f_1 c + d - g_1 e + f_2 = 0 \\ E_6 &= f_2 c + f_1 d + e + f_3 = 0 \\ E_{-4} &= -c + g_1 d + g_2 e - f_1 = 0 \\ E_{-6} &= g_1 c + g_2 d + g_3 e - 1 = 0 \end{aligned} \tag{20}$$

These are four linear equations for three unknowns. A stable approximation was obtained when also the the powers ξ^4 and ξ^{-4} were matched exactly by solving $E_4 = 0$ and $E_{-4} = 0$. Finally, since not both E_6 and E_{-6} can be solved simultaneously, we solved a linear combination of them.

$$uE_6 + E_{-6} = 0 \tag{21}$$

We varied the parameter u at different Fermi levels η and found some optimum where the maximum relative error of the screening function has a minimum. The η-dependence of the optimum u can roughly be approximated by $u_{\mathrm{opt}} = 7.2 \, (1 + 10^{\eta/5})$.

Figure 1 compares the exact screening function (6) evaluated by numerical integration and the rational approximation. The approximation is fairly good for the non-degenerate case (MB) and for weak degeneracy, and deteriorates slightly for higher degeneracy (FD, $\eta = 5$). It should be noted that the vast majority of scattering events have ξ-values smaller or even much smaller than one. This means that a slightly inaccurate approximation of F for $\xi > 1$ will have virtually no impact on the calculated mobility.

3.2. Second born correction

To discuss the validity of the first Born approximation (BA) we follow the work of Meyer and Bartoli[17] who introduce the dimensionless vari-

ables y and F. With a wave number U_0 defined as:

$$U_0 = \frac{2m^*}{\hbar^2} \cdot \frac{Ze^2}{4\pi\epsilon_0\epsilon_r} \qquad (22)$$

y and F can be written as:

$$F = \frac{|U_0|}{\beta_s}, \qquad y = -\frac{k}{U_0}. \qquad (23)$$

For electrons in silicon ($\epsilon_r = 12$, $m^*_n = 0.32\, m_0$) we obtain $U_0 = 1\, \mathrm{nm}^{-1}$. A sufficient criterion for the first BA to be valid is $|y| > 1$, that is, $k > |U_0|$ or $E > 120$ meV. As this criterion does not give any information on the vast majority of thermally distributed electrons we consider the criterion $|F| \ll 1$ which is also applicable at small energies. $|F| \ll 1$ implies $\beta_s > |U_0|$. In silicon at room temperature β_s exceeds a value of $|U_0| = 1\, \mathrm{nm}^{-1}$ at doping concentrations higher than $2.2 \times 10^{19}\, \mathrm{cm}^{-3}$, i.e. the first BA performs better at doping concentrations above this value than below. At such high doping concentrations the strength of the scattering potential, characterized by F, is effectively reduced due to screening. Note, that the discrepancy between the Brooks-Herring model and the measured mobility is large especially in the upper concentration range (Fig. 2) where the first BA should start to become valid. Therefore, we suppose that the discrepancy observed for $N_I > 10^{19}\, \mathrm{cm}^{-3}$ cannot be eliminated only by removing the first BA, e.g. by doing phase shift analysis for a screened Coulomb potential. Instead, other physical effects being dominant in this region need to be identified.

In this work we used the Schwinger scattering amplitude[18] to derive a correction to the first Born scattering amplitude. Ebden and Darewych[19] have shown that cross sections calculated in the plane-wave Schwinger approximation are always in closer agreement with the exact cross section than the second BA. The considered potentials were of Yukawa and Gaussian type. They also identified a particular strength of the potential ($F = 3$ in our nomenclature, or $N_I = 2 \times 10^{18}\, \mathrm{cm}^{-3}$) for which one bound state exists, and for which the first BA is closer to the exact cross section than the Schwinger or the second BA.

We performed a Taylor series expansion of the differential cross section with respect to the variable $z = kq(\beta_s^4 + 4\beta_s^2 k^2 + k^2 q^2)^{-1/2}$ and retained only the zero order term which is independent of z and hence of q. If σ_{B1} denotes the differential scattering cross section in the first BA, the lowest order correction can be written as:

$$\Delta\sigma(q) = s_0(k)\sigma_{B1}(q). \qquad (24)$$

To be consistent with the derivation of $s_0(k)$ the cross section σ_{B1} should include single-potential scattering only and momentum-independent screening. In 24 $s_0(k)$ is defined by:

$$s_0 = \frac{a}{1 + \dfrac{4k^2}{\beta_s^2} - a}, \qquad a = \frac{U_0}{\beta_s}\left(1 - \frac{U_0}{4\beta_s}\right). \qquad (25)$$

Resulting from the q-independence of s_0 the correction of the scattering rate can be written simply as:

$$\Delta\lambda(k) = s_0(k)C(k) \cdot \int_0^{2k} \frac{q\,dq}{(q^2 + \beta_s^2)^2}. \qquad (26)$$

One problem encountered when using the second Born scattering amplitude is that its imaginary part diverges on $\beta_s \rightarrow 0$. This divergence problem is also reflected in (25) since we have $\lim_{\beta_s \rightarrow 0} s_0(k) = -1$ such that the correction would fully compensate the first Born term. For the unscreened Coulomb potential it can be shown that the first BA gives the exact scattering cross section[20]. For semiconductors this means that for very small carrier concentrations, that is when $\beta_s \rightarrow 0$ or $F \rightarrow \infty$, scattering rates calculated from the first BA will suffice.

In this work we consider majority electrons which are attracted by the positivley charged donors ($U_0 > 0$). Meyer and Bartoli [17] computed a correction factor H_0 for the first Born cross section (BCS) and found that $H_0 \geq 1$ for attractive potentials. This inequality holds for all relevant carrier energies and potential strengths. Further, for $U_0 > 0$ all higher order terms of the Born series are positive and thus can only lead to an increase of the cross section compared to the first BCS. Since the complete Born series is a formally correct solution to the scattering problem we can draw conclusions about the Schwinger approximation by comparing it with the Born series. As can be seen from (25) the correction will become negative if $F > 4$. From the previous discussion we infer that in case of majorities a negative correction will be unphysical. We hence trust the correction only for sufficiently weak scattering potentials ($F < 4$ or $N_I > 10^{18}\, \mathrm{cm}^{-3}$) and
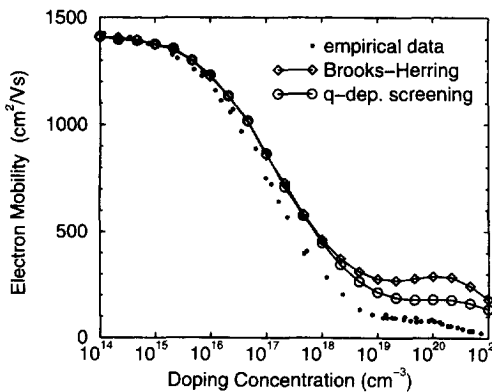

Fig. 2. Electron mobility including momentum-dependent screening in comparison with the Brooks-Herring model ($G(\xi, \eta) \equiv 1$) and empirical mobility data after Masetti *et.al.* (Si, 300 K).

neglect the second Born correction for stronger potentials ($F > 4$). In this way we also enforce the correct limit, $\sigma \rightarrow \sigma_{B1}$, for vanishing screening, $F \rightarrow \infty$.

3.3. The Friedel Sum Rule

The Friedel sum rule implies charge neutrality stating that the screening charge must exactly cancel the impurity charge. Using the first BA for the phase shifts the Friedel sum rule can be rewritten as a condition on the potential[21]

$$Z = \frac{4\pi e}{k_B T} N_C \mathcal{F}_{-1/2}(\eta) \int_0^\infty V_t(r) r^2 \, dr, \qquad (27)$$

where N_C denotes the effective density of states of the conduction band. The Friedel sum rule is valid as long as the scattering centers do not interact and the average value of the electron wavelength is smaller than the mean distance between the centers[3,22]. In the following, therefore, we shall restrict our discussion to the single-ion scatting potential given by:

$$V_t(q) = \frac{Ze}{\epsilon_0 \epsilon_r} \cdot \frac{1}{q^2 + \beta_s^2 G(\xi, \eta)} \qquad (28)$$

Having G represented as a rational function the scattering potential (28) will be a rational function as well. This function can be decomposed into partial fractions with respect to the variable q^2.

$$V_t(q) = \frac{Ze}{\epsilon_0 \epsilon_r} \sum_i \frac{c_i}{q^2 + \beta_i^2} \qquad (29)$$

The β_i^2 are obtained as roots of the denominator polynomial of V_t and will in general be complex valued. Evaluating (28) and (29) at $q = 0$ we find that the coefficients c_i and the β_i^2 obey the following equation.

$$\frac{1}{\beta_s^2} = \sum_i \frac{c_i}{\beta_i^2} \qquad (30)$$

The inverse Fourier transform now yields a real-space potential which is the sum of several screened Coulomb potentials.

$$V_t(r) = \frac{Ze}{\pi \epsilon_0 \epsilon_r} \sum_i \frac{C_i \exp(-\beta_i r)}{r} \qquad (31)$$

Inserting this equation into (27) and performing the integration gives:

$$\frac{e^2 N_C \mathcal{F}_{-1/2}(\eta)}{\epsilon_0 \epsilon_r k_B T} \sum_i \frac{c_i}{\beta_i^2} = 1. \qquad (32)$$

Obviously, with β_s defined by (5) and the condition (30) this equation is satisfied. It is interesting to note that the sum rule imposes a condition on the screening parameter β_s but not on the q-dependence of the screening function. Only the fact that $G(0, \eta) = 1$ appears to be relevant in this regard.

Within the second BA the sum rule cannot be simplified to (27), and an exact analysis by analytical methods is no longer possible. Patterson and Lehoczky[23] used phase shifts derived by the Schwinger variational principle. Assuming only s-waves to be relevant they find a correction to the screening length which is applicable at high doping concentrations. For majority electrons a reduced screening length is predicted, which also agrees with a result of Kay and Tang[1] who report a slight increase of the majority mobility in the upper doping range when the screening length is corrected so as to satisfy the sum rule.

In this work we show that multi-potential scattering plays an important role at high doping concentrations implying that in this regime the sum rule is no longer valid. Therefore, a screening length correction based on the sum rule seems to be not justifiable in the considered case, and hence we refrain from using such a correction.

3.4. Plasmon scattering

The electron-electron interaction is usually split into a long-range part, also termed electron-plasmon interaction, and a short-range part interpreted as binary electron–electron scattering (see e.g.[14]). From the overall electron-electron interaction only plasmon scattering is considered in this work. In silicon this mechanism is important at doping concentrations above $10^{18} \, \text{cm}^{-3}$[4].

The plasmon frequency modeled by $\omega_p^2 = e^2 n / \epsilon_0 \epsilon_r m^*$ determines the final energy after scattering: $E_f = E \pm \hbar \omega_p$. Here and in the following the upper sign refers to absorption and the lower sign to emission of a plasmon. The final wave number k_f is defined as solution of the equation $E(k_f) = E_f$. Energy conservation restricts the possible momentum transfer to an interval between q_{min} and q_{max}.

$$q_{min} = |k - k_f|, \qquad q_{max} = k + k_f \qquad (33)$$

The integrated scattering rate is obtained using the interaction Hamiltonian after Pines (see e.g.[14]).

$$\lambda(k) = \frac{e^2 \hbar}{16 \pi \epsilon_0 \epsilon_r m^{*2} \omega_p v_g(k)} \left(N(\omega_p) + \frac{1}{2} \mp \frac{1}{2} \right)$$

$$\times (k^2 - k_f^2)^2 \ln \frac{q_c}{q_{min}} \qquad (34)$$

The maximum momentum that can be transferred by plasmon interaction is β_s. Hence the cut-off wave number in (34) is given by $q_c = \min(q_{max}, \beta_s)$. $N(\omega_p)$ denotes the average number of the plasmon excitations which is estimated by assuming equilibrium Bose statistics.

$$N(\omega_p) = \left(\exp\left(\frac{\hbar \omega_p}{k_B T_n}\right) - 1 \right)^{-1} \qquad (35)$$

The electron temperature T_n in (35) strongly affects the results of Monte Carlo transport calculations.

At high electric fields T_n should be estimated from the average electron energy in a self-consistent manner by means of an iterative procedure. An initial guess for T_n can be obtained by switching off plasmon scattering and employing only the remaining scattering processes included in the particular transport model. In subsequent Monte Carlo calculations plasmon scattering is switched on and better guesses for T_n are obtained. Using simply the lattice temperature in (35) would plasmon scattering make relax the carrier temperature towards the lattice temperature, and the resulting averages would be strongly falsified, especially in the high-field region.

The necessity of a self-consistently determined electron temperature was also discussed by Mansour et al.[24]. They found that in the self-consistent case the resulting plasmon emission and absorption rates are nearly equal.

4. THE MONTE CARLO METHOD

In the following we describe briefly the details how the ionized impurity scattering model can be implemented in a Monte Carlo procedure in a computationally efficient way. In principle it is possible to analytically integrate the differential scattering cross section when a rational approximation is used for the screening function. The two-ion contribution to the scattering rate can be expressed in terms of sine and cosine integral functions with complex argument. Thus, numerical integration can be avoided. However, even the repeated evaluation of the sine- and cosine integral functions turned out to be time consuming. Therefore, we resort to an acceptance/rejection scheme which does not require the scattering rate to be known explicitly.

To the integrand of (14) we construct a supremum:

$$\frac{1}{(q^2 + \beta_s^2 G(\xi, \eta))^2}\left(1 + \frac{\sin(qR)}{qR}\right) \le p_{sup}(q) \qquad (36)$$

which has a Brook-Herring type q-dependence.

$$p_{sup}(q) = \frac{2}{(q^2 + \beta_1^2)^2} \qquad (37)$$

Here, $\beta_1^2 = \beta_s^2 G_{min}$, with G_{min} being the screening function evaluated at $q_{max} = 2k$. The scattering rate employed in the Monte Carlo procedure is calculated from (37), and is thus larger than the physical scattering rate. To find an appropriate q the so-called combined technique[14] can be applied. If a q-value has to be rejected, the scattering event has to be rejected as well, and self-scattering has to be performed instead. Otherwise, the q-value is accepted, and so is the scattering event.

5. RESULTS AND DISCUSSION

The low-field mobility in uncompensated silicon at room temperature (300 K) will be discussed in this section. In addition to the scattering mechanisms presented so far the transport model comprises acoustic intra-valley scattering and six different types of phonon inter-valley scattering[14]. As we restrict our discussion to low-field transport a simple, non-parabolic band model appears sufficient. We adopt an isotropic effective electron mass of $m_n^* = 0.32 \, m_0$ and a non-parabolicity factor of $\alpha = 0.5 \, eV^{-1}$.

Silicon at 300 K will become degenerate for $n \approx 2 \times 10^{19} \, cm^{-3}$. Therefore, the Pauli exclusion principle is included by means of a rejection technique[14] assuming equilibrium Fermi-Dirac statistics for the final states.

The upper mobility curve in Fig. 2 based on the Brooks-Herring model including the Pauli principle will serve as a reference for the following discussion. The agreement of this model with empirical data[25] is poor. Disagreement can be observed for $N_I > 10^{16} \, cm^{-3}$. For $N_I = 10^{19}$ and $10^{20} \, cm^{-3}$ the predicted mobilities are too high by a factor of 2.8 and 3.8, respectively. Obviously, there must be significant physical effects which are not included in the Brooks-Herring model. One of these effects is momentum-dependent screening which affects mobility for $N_I > 10^{18} \, cm^{-3}$ (Fig. 2). The concentration dependence of this effect can be understood as follows. Screening is primarily a function of the transferred momentum q (Fig. 1). At small electron concentrations the distribution of the scattering angle shows a high probability for small-angle scattering. For the small q-values involved the screening function virtually does not differ from unity, which means that momentum-dependent screening effects are negligible. The situation changes with higher concentrations where the probability of scattering events with higher q-values increases. Chung and Ferry found that momentum-dependent screening in InP and GaAs has only little influence on the mobility[26]. As shown in this work, in silicon the influence is significant (Fig. 2). The reason is that the decay of the screening function over q is largest for non-degenerate statistics (Fig. 1). For strong degeneracy the screening function becomes almost flat. Resulting from the lower Fermi level in silicon at a given carrier concentration a much steeper screening function applies in silicon than in the above mentioned compound semiconductors.

Addition of the two-ion correction results in a small mobility reduction for $N_I > 10^{16} \, cm^{-3}$ and in a more pronounced reduction for $N_I > 10^{19} \, cm^{-3}$ (Fig. 3). In the upper concentration range the contribution of the two-ion correction is not negligible.

The second Born correction affects electron mobility for $N_I > 10^{18} \, cm^{-3}$ (Fig. 4), and its influence decreases for very high doping concentrations. The
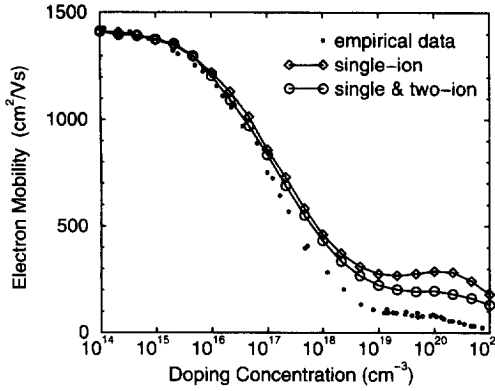
Fig. 3. Electron mobility including the two-ion correction in comparison with the Brooks–Herring model and empirical data.

Fig. 5. Evaluation of the plain Brooks–Herring model with and without plasmon scattering in comparison with empirical data.

latter behavior is anticipated since the correction (25) is proportional to U_0/β_s, a factor vanishing for $\beta_s \rightarrow \infty$. In comparison with the mobility reduction caused by momentum-dependent screening and pair scattering the second Born correction appears as the weakest effect. Although for concentrations below 10^{18} cm^{-3} both criteria $|y| > 1$ and $F \ll 1$ are violated the first BA reproduces the trend of the mobility curve very well, while the second Born correction is ineffective because of the cut-off introduced in Section 3.2.

Plasmon scattering reduces the mobility in an intermediate concentration range of about $[5 \times 10^{17}, 5 \times 10^{19}]$ cm^{-3} (Fig. 5). For lower concentrations plasmon momentum is too small to contribute significantly to the momentum relaxation of the electrons. For higher concentrations the plasmon energy is high compared to the thermal energy of the electrons such that the probability for plasmon emission is low.

Including all effects gives a mobility curve depicted in Fig. 6. The new model can be applied in
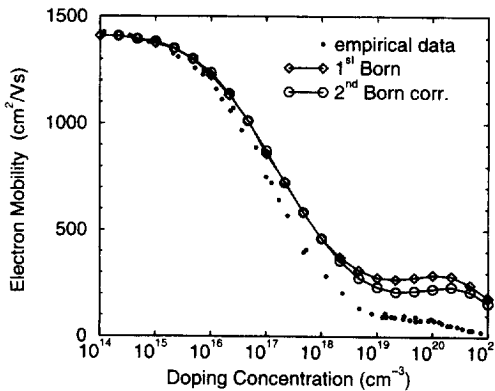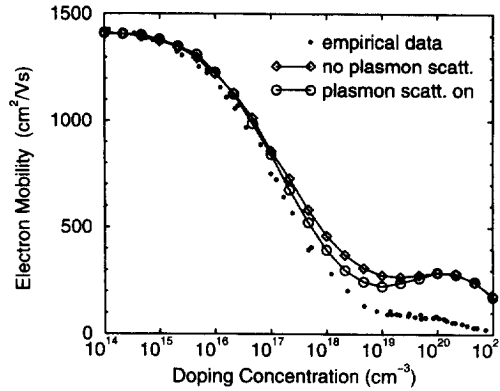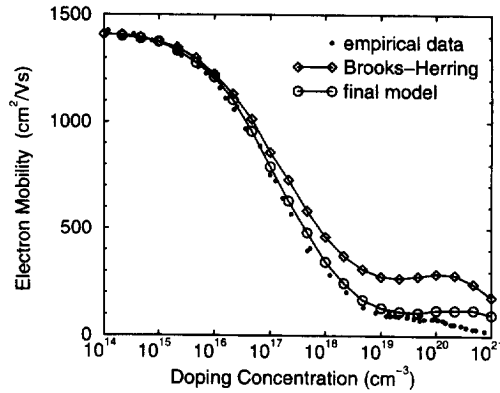

Fig. 6. Evaluation of the full model including momentum-dependent screening, two-ion correction, second Born correction and plasmon scattering.

the doping range $[10^{14}, 10^{20}]$ cm^{-3} where the agreement with experimental data is much better than that of the plain Brooks–Herring model. Only for very high concentrations ($> 10^{20}$ cm^{-3}) additional effects, which are beyond the scope of our model, starts to become dominant. We think that in this region the point-ion approximation breaks down.

6. CONCLUSION

An ionized impurity scattering model was developed which includes three corrections to the widely used Brooks–Herring model. In contrast to GaAs, momentum-dependent screening plays an important role in silicon, especially in the upper electron concentration range. The screening function is approximated by a rational function. Pair scattering is included within the first BA. From the Schwinger scattering amplitude a simple expression for a second Born correction is derived. All these effects are modeled in a way which requires no time consuming numerical integration or tabulation of pre-calcu-

Fig. 4. Electron mobility including the second Born correction in comparison with the Brooks–Herring model and empirical data.

lated functions. Plasmon scattering acts at inter-
mediate doping concentrations and must not be
neglected because of its strong concentration-
dependent nature. The presented model is appli-
cable up to $N_I = 10^{20}$ cm^{-3} and shows very good
agreement with experimental data. The weakness of
the plain Brooks–Herring model cannot be over-
come by just adding one dominant effect but only
by adding several nearly equally important effects.

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