A New Approach to Ionized-Impurity Scattering

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***Abstract*—The Brooks-Herring (BH) approach to ionized impurity scattering overestimates the low-field mobility of electrons in doped semiconductors. We present a consistent ionized-impurity scattering model which, in addition to the BH model, accounts for degenerate statistics, dispersive screening, two-ion scattering and the atomic form factor of the impurity atom. The dielectric function is accurately approximated by a rational function. From the Schwinger scattering amplitude a correction to the first Born amplitude is derived. The charge distribution of the impurities is described by the Thomas-Fermi theory in the energy functional formulation. Despite the various physical effects added an analytical expression for the scattering rate is retained which allows for efficient usage in Monte Carlo transport calculations. Results of such calculations are presented for majority and minority electron mobility in silicon. The results not only confirm the experimental data of the mobility enhancement of minority electrons in degenerate silicon but also the lower electron mobility in As-doped silicon in comparison to P-doped silicon.**

I. Introduction

Most of todays Monte Carlo device simulators focus on accurate modeling of hot carrier dynamics governed by electron-phonon interaction and band structure. For the low-field transport, however, which is dominated by ionized-impurity scattering, often considerably less sophisticated models are used. The frequently employed Brooks-Herring (BH) model overestimates the low-field mobility in the whole doping range significantly (Fig. 4). This model relies on the following assumptions:

- screening is momentum-independent
- independently acting scattering centers
- first Born approximation
- impurity center is treated as a point charge

We developed a new scattering model which firstly includes those physical effects necessary to reproduce measured mobilities and secondly is suitable for application in Monte Carlo device simulations.

II. Scattering Rate

He weakness of the plain Brooks-Herring model cannot be overcome by just adding one dominant effect. Instead several nearly equally important effects have to be added. In our model the scattering rate λ is finally given by:

$$\lambda_{B1}(k) = C(k) \int_0^{2k} \left(\frac{Z - F(q)}{q^2 + \beta_s^2 G(q)} \right)^2 \left(1 + \frac{\sin(qR)}{qR} \right) q \, \mathrm{d}q$$

$$C(k) = \frac{N_I e^4}{2\pi \hbar^2 (\epsilon_0 \epsilon_r)^2 v_g(k)}$$

$$\lambda(k) = \lambda_{B1}(k) + \lambda_{B2}(k) \qquad (1)$$

The first term on the right hand side of (1), λ_{B1}, is consistently derived within the first Born approximation and represents the dominant contribution to the scattering rate, whereas λ_{B2} is a correction accounting for higher terms of the Born series [6]. In the following (1) will be discussed in detail. Before doing so it should be noted that the BH model can formally be recovered from (1) by setting $G(q) = 1$, $F(q) = N$, where N is the number of valence electrons of the impurity center, and neglecting pair scattering and the second Born correction by imposing the limit $R \to \infty$ and $\lambda_{B2} = 0$, respectively.

A. Momentum-Dependent Screening

The inverse Thomas-Fermi screening length β_s is dfined as

$$\beta_s^2 = \frac{e^2 n}{\epsilon_0 \epsilon_r k_B T} \cdot \frac{\mathcal{F}_{-1/2}(\eta)}{\mathcal{F}_{1/2}(\eta)} \qquad (2)$$

The Fermi integrals with the reduced Fermi energy η as argument account for degenerate statistics. $G(q)$ denotes the screening function ($G(q) \leq 1$) which is responsible for the description of momentum-dependent screening. G is closely related to the Lindhard dielectric function [8]. This means that G is defined as an integral not analytically solvable, and hence we adopt a rational approximation of G to avoid time-consuming numerical integration (Fig. 1). In contrast to GaAs, momentum-dependent screening plays an important role in silicon, especially in the upper electron concentration range.

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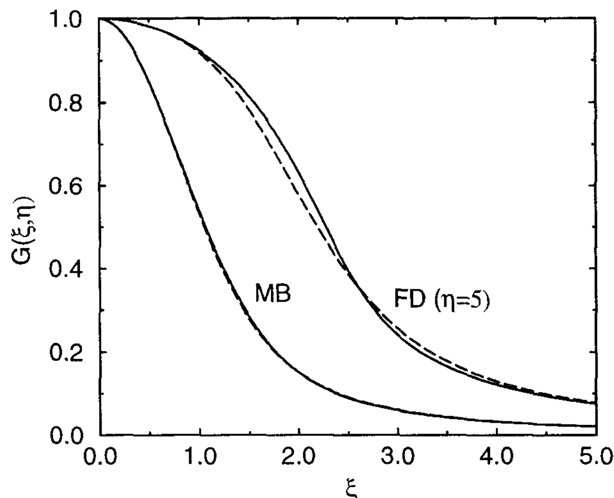

Fig. 1. Screening function for the non-degenerate case (MB) and the degenerate case for $E_F = 5kT$. Solid lines: exact, dashed lines: rational approximation.

B. Multi-Potential Scattering

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.

Pair-scattering models have been widely used to describe dipole scattering in compensated semiconductors [4][5][14]. In this work we deal with uncompensated silicon and have thus to consider pairs of equally charged ions. Pair-scattering is accounted for by the term $\sin(qR)/qR$. The parameter of interest, R, represents the average distance between the impurity centers. Note that in the limit $R \to 0$ equally charged pairs of impurities scatter up to twice as effectively as independent monopoles [12].

C. The Atomic Form Factor

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

$$\rho_{ion}(r) = Z\delta(r) - \rho_e(r) \tag{3}$$

$$N = \int \rho_e(\vec{r}) d^3r \tag{4}$$

The first term in (3) 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 distribution of the valence electrons in momentum space, is defined as the Fourier transform of the charge density [13]:

$$F(q) = \int d\vec{r} \, \mathrm{e}^{-i\vec{q}\cdot\vec{r}} \rho_e(\vec{r}) \tag{5}$$

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 Thomas Fermi atomic 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 [15] 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 Coulomb potential energy of electron-electron and electron-nucleus interactions, the kinetic energy, an inhomogeneity correction [17] for the kinetic energy, and a quantum mechanical exchange energy correction [7].

For the form factor we chose some function containing one free parameter. In principle any function is suitable as long as it vanishes at infinity and the integral over a certain domain remains finite. Two widely used charge density distributions (atomic form factors) are the normalized hydrogen-like exponential charge distribution

$$\rho_e(r) = \frac{N\,\alpha^3}{8\pi} \mathrm{e}^{-\alpha\, r} \tag{6}$$

$$F(q) = \frac{N\alpha^4}{(q^2+\alpha^2)^2} \tag{7}$$

and the normalized screened Coulomb charge distribution:

$$\rho_e(r) = \frac{N\,\alpha^2}{4\pi} \frac{\mathrm{e}^{-\alpha\, r}}{r} \tag{8}$$

$$F(q) = \frac{N\alpha^2}{q^2+\alpha^2} \tag{9}$$

By minimizing the energy functional the variational parameter is obtained as function of both N and Z. Calculated ground state energies of different ions and neutral atoms with a hydrogen-like density function give extremely accurate results (within 2%) in comparison with experimental data.

The momentum-dependent form factor strongly influences the scattering strength of the ionized impurity. Fig. 2 shows $(Z - F(\theta))^2$ for P-doped Si for different energies assuming a screened Coulomb charge density. Only in the forward direction ($q = 0$) $F(q)$ becomes a constant equal to the number of electrons (BH limit). Yet, with increasing doping concentraton and carrier energy the angle-dependence of the atomic form factor becomes important. From Fig. 3 we see the more complicated functional behavior of the form factor in B-doped Si which emphasizes the importance of the atomic form factor for the correct description of minority electron transport. Note that $(Z - F(\theta))^2$ is smaller than unity in case of acceptor ions in contrast to donor ions where this factor is greater than one. At a scattering angle of $\theta = \frac{\pi}{2}$ the scattering cross section is even zero.

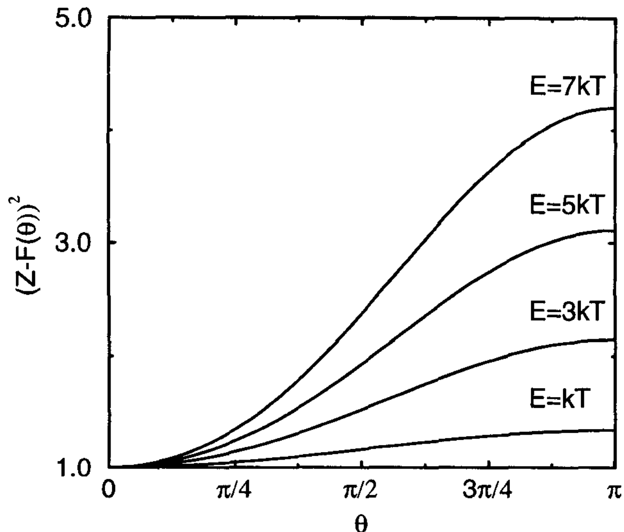

Fig. 2. The factor $(Z - F(\theta))^2$ for phosphorus doped silicon. For comparison, in the BH model $(Z - F(\theta))^2 \equiv 1$.

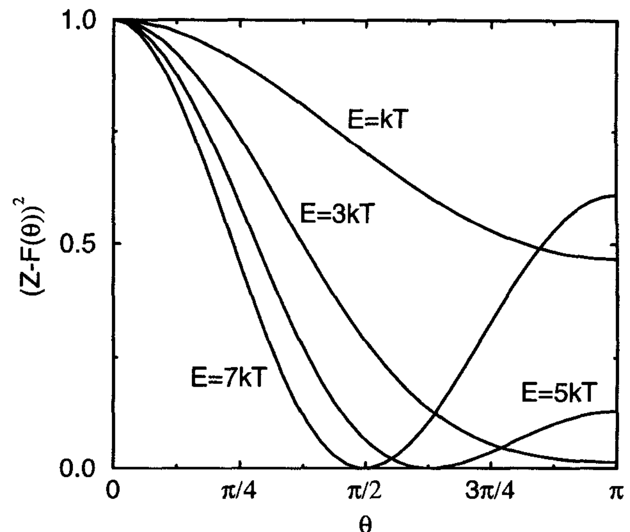

Fig. 3. $(Z - F(\theta))^2$ for boron doped silicon.

The situation to date is that there is no theoretical model which explains the different mobility data observed for As- and P-doped silicon at high impurity concentrations. The difference between the electron mobility in As- and P-doped samples monotonically increases from 6 % at $N_I = 10^{19}\,\mathrm{cm}^{-3}$ up to 32 % for $N_I = 4{\cdot}10^{21}\,\mathrm{cm}^{-3}$ [11]. Bennett and Lowney made extensive studies of the majority- and minority electron mobility in Si [1][2][3]. They used phase shift analysis to calculate the ionized impurity scattering cross sections of minority and majority electron scattering. As they introduced many parameters to explain experimental data for different donors, the theoretical situation remained unsatisfactorily from a physical point of view.

D. Second Born Correction

The second term of the Born series for the scattering amplitude is considered as a correction to the dominant first term. For the derivation of the second Born scattering amplitude not all above mentioned effects can be included consistently. Therefore, constant screening ($G(q) = 1$), point-like ion charge ($F(q) = N$) and independent scattering centers ($\sin qR/qR \to 0$) have to be assumed in order to get analytical expressions. To obtain the final correction λ_{B2} we employ the variational method of Schwinger [9]. A discussion on the second Born correction can be found in [10].

III. Results and Discussion

The proposed scattering model has been employed in a Monte Carlo transport calculation. Both the minority and majority electron mobility in silicon was simulated at room temperature. In addition to ionized impurity scattering, which is the main scattering process in a heavily doped semiconductor, we take into account phonon scattering and electron-plasmon scattering.

The calculated majority electron mobility is depicted in Fig. 4. The large discrepancy between the BH mobility and the measured one is reduced by the new model mainly due to the inclusion of momentum-dependent screening, pair-scattering and the second Born correction. These effects are of nearly equal importance in the upper concentration range. Furthermore, a variety of experimentally observed effects can be distinguished due to the term $Z - F(q)$. Until now it was commonly believed that the atomic form factor does not play a role for the rather low-energetic scattering processes as they occur in a semiconductor. We found, however, that the inclusion of F explains the dependence of the mobility on the impurity element, e.g. the different electron mobility measured in As- and P-doped silicon.

The atomic form factor is also partly responsible for the enhanced minority mobility compared to the majority mobility (Fig. 5). This can be understood by considering the factor $(Z - F(\theta))^2$ which is smaller than unity in case of acceptor ions and greater than one for donor ions (see Figs. 2 and 3). Another reason for the enhancement is the second Born correction, which has the opposite sign for repulsive potentials compared to attractive ones. Plasmon scattering lowers the mobility in p-type material significantly and is responsible for the dip in the minority mobility at about $N_I = 10^{19}\ \mathrm{cm}^{-3}$ (Fig. 5), which corresponds to the maximum strength of the electron-plasmon interaction.

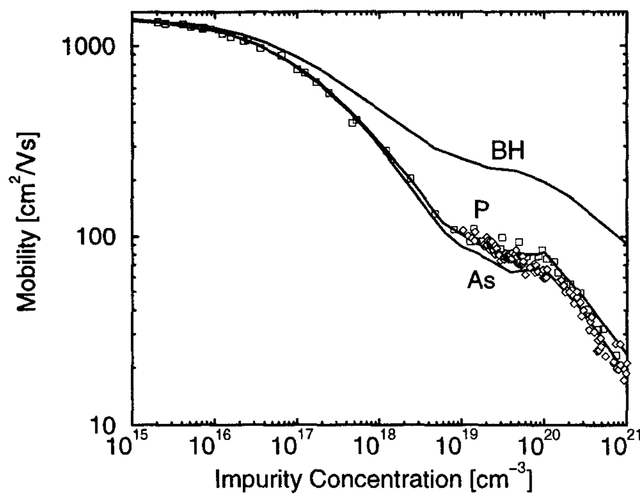

Fig. 4. Majority electron mobility in Si at 300K. Simulation results (solid lines) are shown for the plain BH model, and for the model (1) with parameters for P and As. Experimental data [11] are represented by squares (P) and diamonds (As).

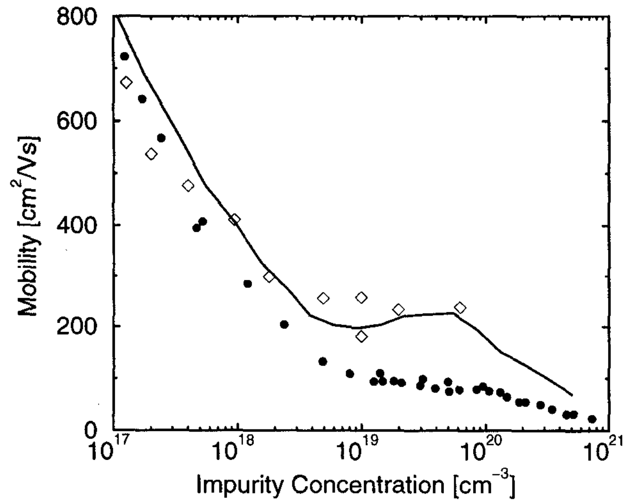

Fig. 5. Minority electron mobility in B-doped Si: Simulation (solid line), experimental data from [16] (open diamonds), and majority mobility after [11] (filled circles).

IV. Conclusion

We have shown that even in the first Born approximation one can differentiate between attractive and repulsive scattering centers, if one takes into account the spatial charge distribution of the ionized impurities. The momentum dependence of the atomic form factor has to be considered to reproduce the dopant-dependent electron mobility in a heavily doped semiconductor. Furthermore, it can be concluded that the two-ion correction, momentum-dependent screening, and the second Born correction are becoming important at $N_I = 10^{18}$. Due to the lack and inconsistency of experimental data for the minority mobility it is difficult to compare the simulation results quantitatively for this particular case.

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