Influence of the doping element on the electron mobility in *n*-silicon

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We present a theoretical approach to study the dependence of the electron mobility on the dopant species in n-doped silicon under low electric fields. The electron charge distribution of the impurities is calculated by the Thomas–Fermi theory using the energy functional formulation. Ionized impurity scattering has been treated within the Born approximation. Our model accounts for degenerate statistics, dispersive screening and pair scattering, which become important in heavily doped semiconductors. The dielectric function is accurately approximated by a rational function. A new expression for the second Born amplitude of a Yukawa-like charge distribution is derived, which now depends on the atomic and electron numbers of the impurity ion. Monte Carlo simulations including all important scattering mechanism have been performed in the doping concentration range from 10^{15} to 10^{21} cm^{-3}. The agreement with experimental data is excellent. The results confirm the lower electron mobility in As-doped silicon in comparison to P-doped silicon.
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I. 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, it is less known that the electron mobility in n-type Si depends as well on the chemical nature of the dopant atom.

There is no theoretical model to date which explains the lower mobility data for As-doped samples compared to P-doped Si for impurity concentrations higher than 10^{18} cm^{-3}. The difference between the electron mobility in As- and P-doped samples monotonically increases from 6% at $N_I = 10^{19}$ cm^{-3} up to 32% for $N_I = 4\times10^{21}$ cm^{-3}.[1] Ignoring these phenomena can lead to incorrect interpretation of device data which strongly depend on doping concentration.

There were several attempts in the past to explain these differences by impurity-core effects.[2,3] Ralph *et al.*[4] introduced a central-cell scattering potential determined empirically using bound state energies of donors. Later, El-Ghanem and Ridley[5] employed a square-well impurity core potential. Both approaches cannot explain experimental data sufficiently. Bennett and Lowney made extensive studies of the majority and minority electron mobility in Si[6–8] and GaAs.[9] They used phase shift analysis to calculate the ionized impurity scattering cross sections of minority and majority electron scattering. They introduced different scale factors in the interaction potential for majority and minority electrons. The well-known Brooks–Herring (BH) approach[10] neglects the chemical nature of dopant species by assuming point-like dopant atoms, thus not being able to explain the above mentioned experimental observations.

The basis of our theoretical approach is the Thomas–Fermi (TF) theory.[11,12] This semiclassical treatment of the atom in the energy functional formulation yields the impurity charge density as a function of the atomic and electron number as well as a variational parameter which defines the size of the valence electron charge cloud. Knowing the charge density we obtain analytical expressions for the differential cross section using the Born formalism up to second order to account for the charge sign of the impurity center.[13] This approach from first principles explains the dependence of the electron mobility on the impurity element. To our knowledge this is the first physical based model which explains the lower electron mobility in As-doped silicon than that in P-doped silicon for concentrations higher than 10^{18} cm^{-3}. As all relevant quantities are calculated analytically, the computational burden is only slightly higher than for the simple BH model, so that this approach is well suited for device simulation.

II. CHARGE DENSITY OF IONIZED IMPURITIES

The total electron charge density (in units of the electron charge e) of an unscreened impurity atom with atomic number Z_I and electron number N_I in a solid is given by

$$\rho_I(r) = Z_I\delta(r) - \rho_e^I(r), \tag{2.1}$$

$$N_I = \int \rho_e^I(\mathbf{r})d^3r. \tag{2.2}$$

The first term in Eq. (2.1) describes the nuclear charge density distribution concentrated in the origin, and $\rho_e^I(r)$ is the electron charge density of the impurity ion. There are numerous methods to calculate the electron charge density distribution. As we are interested in analytical solutions, we use the semiclassical TF model. Its basic idea is to treat the valence and core electrons as a degenerate Fermi gas of nonuniform, spherically symmetric electron density in a positively charged background[14] at zero temperature. Under this assumption we get a local relation between the electron charge density and the Fermi energy. The total energy con-

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sists of the classical Coulomb potential energy of electron-electron E_{e-e} and electron-nucleus interactions E_{e-n}, and the kinetic energy E_k. Hence we define the total energy functional

$$E_0 = E_k + E_{e-n} + \lambda E_{e-e}, \tag{2.3}$$

$$E_k = c_k e^2 a_0 \int \rho_e(r)^{5/3} d^3r, \tag{2.4}$$

$$E_{e-n} = -\frac{Ze^2}{\epsilon} \int \frac{\rho_e(r)}{r} d^3r, \tag{2.5}$$

$$E_{e-e} = \frac{e^2}{2\epsilon} \int \int \frac{\rho_e(r)\rho_e(r')}{|\mathbf{r}-\mathbf{r}'|} d^3r d^3r' \tag{2.6}$$

with the Bohr radius a_0, $c_k = (3/10)(3\pi^2)^{2/3}$ and a correlation parameter λ. Let

$$\rho_e^I(r) = \frac{N_I \alpha^2}{4\pi} \frac{e^{-\alpha r}}{r}. \tag{2.7}$$

be the electron charge density distribution. Its Fourier transform

$$F_I(q) = \frac{N_I \alpha^2}{q^2 + \alpha^2} \tag{2.8}$$

is called the atomic form factor of the charge distribution. The variational parameter α has to be determined by minimizing E_0. Calculating the first derivative of the total energy with respect to the variational parameter α and N_I we get two equations for α and λ:

$$0 = \frac{\partial E}{\partial \alpha}, \tag{2.9}$$

$$0 = \left.\frac{\partial E}{\partial N_I}\right|_{N_I = Z_I}. \tag{2.10}$$

Condition (2.10) makes the chemical potential vanish for a neutral atom. Solving Eqs. (2.9) and (2.10) with respect to λ and α, we obtain finally

$$\alpha = \frac{Z_I^{1/3}}{c_k^* a_0 \epsilon} \frac{\left[1 - 2\left(\frac{Z_I}{N_I}\right)\right]}{\left[\frac{5}{3} - 4\left(\frac{Z_I}{N_I}\right)^{1/3}\right]}, \tag{2.11}$$

$$c_k^* = \frac{\Gamma(4/3)}{2} \left(\frac{3\pi}{4}\right)^{2/3} \left(\frac{3}{5}\right)^{7/3}. \tag{2.12}$$

Deriving (2.11) we assumed a spatially constant permittivity ϵ. In this way an approximation is introduced since ϵ depends on the wave number and varies between the vacuum value for large q and the static dielectric constant of the host material for small q.

In addition, there is experimental evidence of a strong increase of ϵ approaching the critical donor concentration in n-Si.[15] Even a dopant dependence has been observed near the Mott transition at very low temperatures.[16] We can understand this effect quantitatively by noticing that the ionization energy of dopants depends both on the doping concentration and on the dopant species. The ionization energy goes to zero, as soon as the donor level merges the conduction band. As a consequence the dielectric constant, which is a measure of the polarization of a solid in an electric field, increases in value.

To our knowledge there is still no theoretical explanation for these effects, nor any experimental studies of these dependencies at room temperature could be found. Considering all these uncertainties and for efficiency reasons we used the usual background value $\epsilon = 11.7\epsilon_0$ (in units of the vacuum permittivity ϵ_0) for the dielectric constant in Si. However, if further studies on the dependencies of ϵ on concentration and wavenumber show significant differences to the background value, it will have a strong impact on the size parameter α. In case, that ϵ is in the order of the vacuum permittivity, the parameter α will increase by an order of magnitude. Then the influence of the q dependence of the atomic form factor decreases strongly, so that the finite size of the charge density cannot sufficiently explain the differences in the mobility. Thus, the physical origin of the dependence of the electron mobility on the dopant species would still remain unclear.

III. SCATTERING POTENTIAL

The scattering potential is induced by an effective charge density ρ_{eff}, which can be expressed by Eq. (2.1) minus the total charge density of the host material,

$$\rho_{\text{eff}}(r) = \rho_I(r) - \rho_{\text{si}}(r) = (Z_I - Z_{\text{si}})\delta(r) - (\rho_e^I - \rho_e^{\text{si}}). \tag{3.1}$$

Equation (3.1) ensures that, if a Si atom is placed on a lattice site, the scattering potential vanishes.

As an external charge in a solid is screened by free carriers, the effective scattering potential with $U_0 = e^2/\epsilon$ is reduced to

$$\mathscr{U}(q) = \frac{\rho_{\text{eff}}(q) U_0}{q^2 \epsilon(q)}. \tag{3.2}$$

Let us assume M randomly located ionized impurities in silicon. With increasing M the average distance R between two impurities decreases such that scattering processes become important in which two or even more ions are involved simultaneously. Assuming linear superposition the Fourier potential of M impurities located at $\mathbf{r}_i$ becomes

$$\mathscr{U}(\mathbf{q}, \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_M) = \frac{\rho_{\text{eff}}(q) U_0}{q^2 \epsilon(q)} \sum_{j=1}^{M} e^{-i\mathbf{q}\cdot\mathbf{r}_j}. \tag{3.3}$$

The squared scattering potential (3.3) after averaging over a unit sphere is essentially given by

$$|\mathscr{U}(q, R_{ij})|^2 = 2U_0^2 \left[\frac{\rho_{\text{eff}}(q)}{q^2 \epsilon(q)}\right]^2 \times \left(M + 2\sum_{i,j} \frac{\sin(qR_{ij})}{qR_{ij}}\right) \quad M \geq 2 \tag{3.4}$$

with $1 \leq i \leq M-1$, $2 \leq j \leq M$ and $i < j$. The Lindhart dielectric function is given by[17]

$$\epsilon(q) = 1 + \frac{\beta^2}{q^2} G(\xi, \eta), \tag{3.5}$$

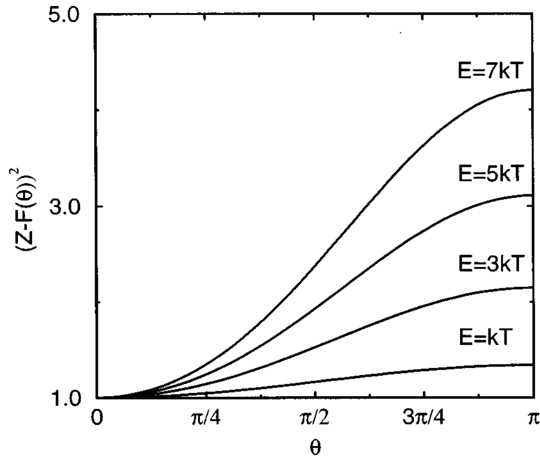

FIG. 1. The squared effective charge in momentum space $[Z-F(\theta)]^2$ of P with the atomic number Z and the atomic form factor F is shown using Eqs. (2.8) and (2.11). Note, that with increasing kinetic electron energies and scattering angles (at higher doping) one obtains values well above unity (BH limit).

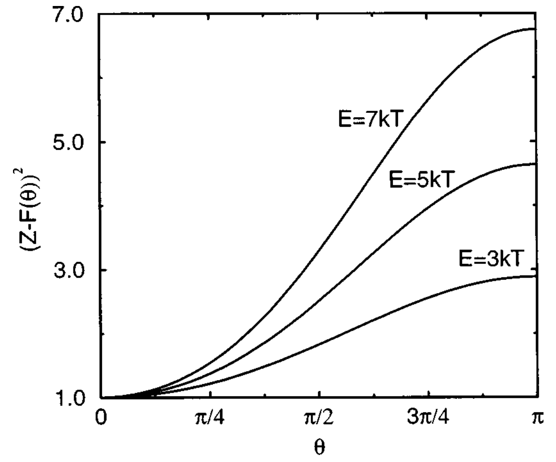

FIG. 2. An even stronger increase of the effective charge is obtained for As due to the higher atomic number. Again, Eqs. (2.8) and (2.11) is used for the atomic form factor F with the variational parameter α.

where the inverse Thomas–Fermi screening length for an uncompensated semiconductor is defined by

$$\beta^2=\frac{ne^2}{\epsilon k_BT}\frac{\mathscr{F}_{-1/2}(\eta)}{\mathscr{F}_{1/2}(\eta)}. \tag{3.6}$$

k_BT is the thermal energy and n the free carrier concentration. $\mathscr{F}_j$ denotes the Fermi integral of order j and η is the reduced Fermi energy. The screening function[17]

$$G(\xi,\eta)=\frac{1}{\mathscr{F}_{-1/2}(\eta)}\frac{1}{\xi\sqrt{\pi}}\int_0^\infty\frac{x}{1+\exp(x^2-\eta)}\ln\left|\frac{x+\xi}{x-\xi}\right|dx, \tag{3.7}$$

$$\xi^2=\frac{\hbar^2q^2}{8m^*k_BT},\quad \eta=\frac{E_F-E_C}{k_BT}$$

represents the dielectric response of the conduction electrons to an external potential.

In principle, Eq. (3.4) can be calculated, if one has an information of all distances $R_{ij}=r_i-r_j$ between two arbitrary impurities. Note, that to first order only the average distance R between neighboring impurities has to be known. Having no information about the R_{ij} and noting that the contributions of higher order decrease with R_{ij}^{-1}, we consider in our further discussion only the case $M=2$. Using Eq. (3.5) we finally obtain for Eq. (3.4)

$$|\mathscr{U}(q,R)|^2=2U_0^2\left(\frac{(Z_I-Z_{\mathrm{si}})-(F_I-F_{\mathrm{si}})}{q^2+\beta^2G(\xi,\eta)}\right)^2\left(1+\frac{\sin(qR)}{qR}\right), \tag{3.8}$$

where Z_{si} and F_{si} denote the atomic number and the form factor of Si. Note, if dopant and host atom are identical, there is no perturbation, so that Eq. (3.8) vanishes. At low doping concentration we can set $R\to\infty$, $G(\xi,\eta)\approx G(0,\eta)=1$, and $F(q)\approx F(0)=N$ so that (3.8) reduces to the well-known BH result.

The momentum-dependent form factor strongly influences the scattering strength of the ionized impurity. Figure 1 shows the factor of (3.4)$(Z-F(\theta))^2$ for P for different energies. Only in the forward direction F becomes equal to the number of electrons (BH limit). Yet, with increasing doping concentration and carrier energy the angle dependence of the atomic form factor becomes important. A similar effect is shown in Fig. 2 for As with an even stronger angle dependence of the form factor explaining the lower electron mobility for As-doped Si compared to P-doped samples.

IV. SCATTERING RATE

With a given scattering amplitude $f(q)$ the differential scattering cross section σ is defined as[18]

$$\sigma(q)=\frac{\pi^2\hbar^3}{m^{*2}v_g(k)}|f(q)|^2\rho(E). \tag{4.1}$$

Equation (4.1) is valid for arbitrary density of states ρ and group velocity v_g. Considering low field electron transport only we can assume a nonparabolic dispersion,

$$E(1+\delta E)=\frac{\hbar^2k^2}{2m^*} \tag{4.2}$$

with a nonparabolicity factor δ. Thus ρ can be expressed by

$$\rho(E)=\frac{\sqrt{2}m^{*3/2}}{\pi^2\hbar^3}\sqrt{E(1+\delta E)}(1+2\delta E). \tag{4.3}$$

Using the total cross section

$$\sigma_{\mathrm{tot}}(k)=\frac{2\pi}{k^2}\int_0^{2k}\sigma(q)q\,dq, \tag{4.4}$$

the total scattering rate is given by

$$\lambda(k)=N_p v_g \sigma_{\mathrm{tot}}(k), \tag{4.5}$$

where $N_p=N_I/2$ is the density of impurity pairs. In the first Born approximation the scattering amplitude is related to the scattering potential by[19]

$$f_{B1}(q)=\frac{2m^*}{\hbar^2}\,\mathscr{U}(q). \tag{4.6}$$

As a consistent derivation of the second Born amplitude including dispersive screening is impossible, we set the screening function equal to unity. For the same reason we drop the two-ion correction in the following discussion. After several transformations and tedious integrations (see, e.g., Ref. 20) the second Born amplitude for a charge distribution (2.7) can be written as

$$\begin{aligned} f_{B2}(k,\mathbf{k}_1,\mathbf{k}_2)&=\frac{V_0^2}{2\pi^2}\lim_{\epsilon\to 0}\int d\boldsymbol{\kappa}\,\frac{[Z-F(\boldsymbol{\kappa}-\mathbf{k}_1)][Z-F(\boldsymbol{\kappa}-\mathbf{k}_2)]}{(\kappa^2-k^2-i\epsilon)(\beta^2+|\boldsymbol{\kappa}-\mathbf{k}_1|^2)(\beta^2+|\boldsymbol{\kappa}-\mathbf{k}_2|^2)}\\ &=\frac{V_0^2}{2\pi^2}\,[(Z-N^*)^2\mathscr{T}_{\beta\beta}(q)+2N^*(Z-N^*)\mathscr{T}_{\alpha\beta}(q)+N^{*2}\mathscr{T}_{\alpha\alpha}(q)] \end{aligned} \tag{4.7}$$

with

$$\begin{aligned} \mathscr{T}_{\mu\nu}(q)&=\frac{\pi^2}{\mathscr{R}_{\mu\nu}(q)}\Bigg[\operatorname{atan}\frac{\mathscr{S}_{\mu\nu}(q)+\mathscr{R}_{\mu\nu}(q)}{\mathscr{T}_{\mu\nu}}-\operatorname{atan}\frac{\mathscr{S}_{\mu\nu}(q)-\mathscr{R}_{\mu\nu}(q)}{\mathscr{T}_{\mu\nu}}+\frac{i}{2}\log\frac{1+\left(\frac{\mathscr{S}_{\mu\nu}(q)+\mathscr{R}_{\mu\nu}(q)}{\mathscr{T}_{\mu\nu}}\right)^2}{1+\left(\frac{\mathscr{S}_{\mu\nu}(q)-\mathscr{R}_{\mu\nu}(q)}{\mathscr{T}_{\mu\nu}}\right)^2}\Bigg],\\ \mathscr{R}_{\mu\nu}(q)&=\sqrt{k^2(q^2+\mu^2+\nu^2)^2-\mu^2\nu^2(4k^2-q^2)},\\ \mathscr{S}_{\mu\nu}(q)&=k[q^2+(\mu+\nu)^2],\quad \mathscr{T}_{\mu\nu}=\mu\nu(\mu+\nu),\\ N^*&=\frac{N}{1-(\beta^2/\alpha^2)},\quad V_0=\frac{m^*e^2}{2\pi\hbar^2\epsilon}. \end{aligned} \tag{4.8}$$

For $\alpha\to\infty$, we obtain the well-known result for a point-like nucleus of charge Z_I-N_I Ref. 19:

$$\begin{aligned} f_2(q)&=\frac{V_0^2(Z_I-N_I)}{qA(q)}\left[\operatorname{atan}\frac{\beta q}{2A(q)}+\frac{i}{2}\log\frac{A(q)+kq}{A(q)-kq}\right],\\ A(q)&=\sqrt{\beta^4+4\beta^2k^2+k^2q^2}. \end{aligned} \tag{4.9}$$

The validity of the Born approximation for impurity scattering in doped semiconductors has been discussed extensively in Ref. 21.

V. MONTE CARLO METHOD

In the following we briefly describe 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 (3.8) when a rational approximation is used for the screening function. An appropriate function is

$$G(\xi,\eta)\approx\frac{1+a\xi^2+b\xi^4}{1+c\xi^2+d\xi^4+e\xi^6} \tag{5.1}$$

with unknowns a,b,c,d,e which have to be chosen such as to match the screening function at zero and for infinity.[22] The two-ion contribution to the scattering rate can then 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 very time intensive. Therefore, we resort to an acceptance/rejection scheme which does not require the scattering rate to be known explicitly.[23]

The total scattering cross section in the Born approximation Eq. (4.4) is

$$\sigma_{\mathrm{tot}}(k)=\sigma_1(k)+\sigma_c(k). \tag{5.2}$$

To first order, σ_1 is essentially the integral of Eq. (3.8) over the solid angle. The correction σ_c is obtained by expanding the second Born amplitude Eq. (4.9) in powers of

$$z(q)=\frac{A(q)+kq}{A(q)-kq}. \tag{5.3}$$

Retaining only the zero order term we obtain

$$\sigma_c(k)\approx a_c(k)\sigma_1(k), \tag{5.4}$$

$$a_c=\frac{\bar{U}(4+\bar{U})}{4(1+4k^2/\beta^2)} \tag{5.5}$$

with $\bar{U}=U_0/\beta$.

Considering Eq. (4.4) we have to construct a supremum p_{sup} holding the inequality

$$p_{\mathrm{sup}}(q)\geqslant\frac{a_c}{[q^2+\beta_s^2G(\xi,\eta)]^2}\left(1+\frac{\sin(qR)}{qR}\right). \tag{5.6}$$

The simple function

$$p_{\mathrm{sup}}(q)=\frac{2a_c}{(q^2+\beta_1^2)^2} \tag{5.7}$$

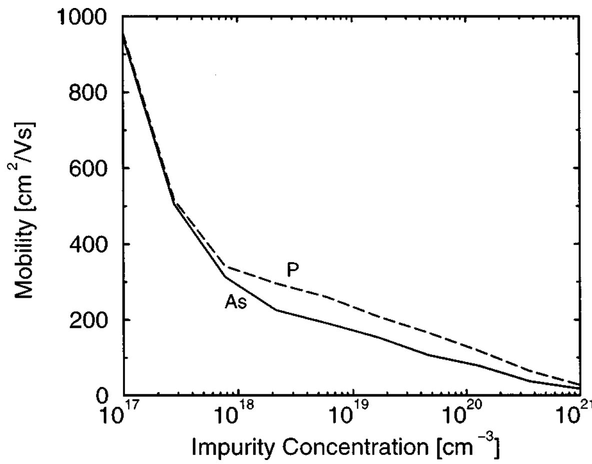

FIG. 3. The majority electron mobility vs the ionized impurity concentration in P and As-doped Si at 77 K. The atomic form factor becomes important above 10^{18} cm^{-3}.

can be used as supremum for the scattering rate (4.5), where $\beta_1^2=\beta_s^2 G_{\min}$, with $G_{\min}$ being the screening function evaluated at $q_{\max}=2k$. The scattering rate employed in the Monte Carlo procedure is calculated from Eq. (5.7), and is thus larger than the physical scattering rate (4.5). To find an appropriate q the so-called combined technique[23] 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.

VI. RESULTS AND DISCUSSION

We present calculated mobilities for silicon at 77 and 300 K. In addition to ionized impurity scattering which is the main scattering process in heavily doped semiconductors, we take into account acoustic intravalley scattering, six different types of phonon intervalley scattering and electron-plasmon scattering following the approach of Ref. 24. We have neglected screening in case of phonon scattering as it seems to be of little importance at finite temperatures.[25,26] Especially at high doping concentrations ionized impurity scattering is the dominate scattering process.

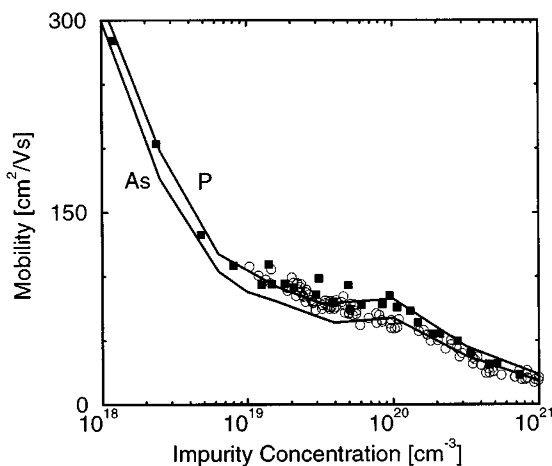

FIG. 4. The majority electron mobility vs the ionized impurity concentration in P- and As-doped Si at 300 K. Simulation: solid lines; experimental data from Ref. 1: open circles (As; filled squares (P). Note the proposed maximum at 10^{20} cm^{-3} caused by different contributions to the total electron mobility.

The Pauli exclusion principle has been included by means of a rejection technique assuming equilibrium Fermi–Dirac statistics $f(\mathbf{k}')$ for the final states $\mathbf{k}'$. Having selected the final state the transition is accepted if $r>f(\mathbf{k}')$ otherwise rejected and treated as self-scattering.[23]

We adopt an isotropic effective mass of $m^*=0.32m_0$ and a nonparabolicity factor of $\delta=0.5\ \mathrm{eV}^{-1}$.[23] As previous work is indicating that binary electron-electron scattering is not significant in n-Si,[27,28] it has been neglected. Figure 1 and Fig. 2 show the effective charge in momentum space as a function of the scattering angle θ for different electron energies. This prefactor of the scattering rate strongly affects the scattering cross section at high doping concentration, where higher scattering angles are more pronounced, so that the q dependence of the atomic form factor cannot be neglected. Only at low doping concentrations the BH model of a constant effective charge is valid. The squared difference between Z and $F(\theta)$ is higher for As than for P at the same energy because the effective charge of As ions is larger than that in P ions (Figs. 1 and 2). Hence, the electron mobility is always lower in As-doped samples than in P-doped samples. In Fig. 3 and Fig. 4 the electron mobility is plotted versus the ionized impurity concentration at 77 and 300 K, respectively. Note the proposed maximum in the electron mobility at 10^{20} cm^{-3} in Fig. 4, which results from the fact, that different physical effects affecting the mobility have a maximum impact at different doping concentrations. Due to the exclusion principle the electron mobility trend to go up, whereas various scattering processes decrease the mobility.

VII. CONCLUSION

We have shown that consideration of the spatial charge distribution of the ionized impurities can explain the dopant-dependent electron mobility in heavily doped n-silicon. Differences in the spatial extended charge distribution result in different effective charges of the ionized dopants. However, if further studies on the dielectric constant in Si show substantially smaller values than the usually used background value, the influence of the q-dependent atomic form factor on the mobility decreases significantly. This, in turn, would mean that the dopant-dependent electron mobility cannot be explained sufficiently by the atomic form factor of the impurity atom.

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