Definition of electron polar scattering angle on ionized impurities for Monte Carlo simulation of charge carrier transport in semiconductors

© V.M. Borzdov, A.V. Borzdov, Yu.G. Vasileuski

Belarusian State University,
220030 Minsk, Republic of Belarus
E-mail: borzdov@bsu.by

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Procedures of polar scattering angle simulation for electron scattering on ionized impurities are examined for Brooks–Herring, Conwell–Weisskopf and Ridley models as the most frequently used in Monte Carlo simulation of charge carrier transport in semiconductors. A more correct procedure for polar scattering angle simulation is proposed for Ridley model. Peculiarities of scattering angle distribution densities calculated in the framework of regarded models are analyzed taking silicon as an example. Comparison of electron mobility calculated by ensemble Monte Carlo method using considered models has been done for doped silicon at 300 K and for constant electric field strength $F = 7 \cdot 10^4$ V/m.

Keywords: ionized impurity, electron scattering, Monte Carlo method.

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1. Introduction

One of the widely known methods of numerical modeling of electrophysical properties and electrical characteristics of semiconductors and semiconductor devices is the Monte Carlo method [1–4]. The most important advantages of this method are the possibility of using precise matrix elements of the charge carrier transition during its interaction with the scatterer for all the main scattering mechanisms in a semiconductor and taking into account the real band structure of the latter [4].

Ionized impurity scattering [5–9] deserves special attention when modeling kinetic phenomena in semiconductors, especially at low temperatures and when highly doped regions of a semiconductor are included in the modeling process. At the same time, despite the rather large number of well-known models of impurity scattering in bulk semiconductors, the Monte Carlo simulation algorithms most often use the Brooks–Herring and Conwell–Weisskopf models, and somewhat less often — the third body exclusion model or the Ridley [6].

This is primarily due to the fact that when modeling the interaction of an electron with an impurity ion by the Monte Carlo method, the issue of determining the state of the charge carrier after the scattering act plays an important role. Considering the interaction of an electron and an impurity ion as absolutely elastic, in the Monte Carlo procedure this process must be characterized by the most important random variable — the polar scattering angle θ, which in each scattering model has its own, different from the others, distribution. In this case, the azimuthal angle φ is usually considered to be a uniformly distributed random variable in the range of values from 0 to 2π [1–4]. In this connection, we should also mention the work [9], in which an isotropic scattering model on a charged impurity center was proposed for transport calculations using the Monte Carlo method.

The formula that can be used to determine the angular distribution for the polar scattering angle in the Brooks–Herring model can be obtained from a general expression for the scattering rate of charge carriers (scattering probability per unit time) on a charged impurity in the first Born approximation for the screened Coulomb potential using the inverse function method [2–4]. At the same time, the act of interaction itself is assumed to be a purely two-particle process. The formula for finding the angle θ for the Conwell–Weiskopf model, as a special case, can also be obtained from the general formula for the probability of scattering per unit time [2,3].

For the Ridley model in the work [10], a two-stage procedure for finding the angle θ was proposed, according to which the impact parameter b is simulated first, and then from the expression for the full scattering cross section — angle θ. In this article, taking into account the screening of the Coulomb field and the results of [10], a more correct procedure (technique) for determining the angular distribution for the polar scattering angle θ in the Ridley model is proposed.

2. Determination of the scattering angle in Brooks–Herring and Conwell–Weiskopf models

According to the classical problem of electron scattering on the Coulomb potential as a purely two-particle interaction, the total scattering cross section $\sigma(k)$ has the following

form [4,11]:

$$\sigma(k) = \pi b^2 = 2\pi \int_{\theta}^{\pi} \sigma_d(k, \theta) \sin\theta d\theta, \tag{1}$$

where $\sigma_d(k, \theta)$ is the differential scattering cross section, k is the modulus of the electron wave vector.

The Brooks–Herring approach, as is known, takes into account the screening of the Coulomb potential of the two-particle interaction by replacing it with the Yukawa potential $V(R)$:

$$V(R) = \frac{Ze^2}{4\pi\varepsilon\varepsilon_0 R} \exp(-R\beta_s), \tag{2}$$

where the inverse radius of the Debye screening is

$$\beta_s = \left(\frac{e^2 n_0}{\varepsilon\varepsilon_0 k_B T}\right)^{1/2}. \tag{3}$$

In (2) and (3) R — distance to the impurity center, e — electron charge, Ze — ion charge, ε_0 — dielectric constant, ε — relative permittivity of a semiconductor, k_B — Boltzmann constant, T — temperature, n_0 — concentration of free charge carriers. Next, for certainty, we will consider a donor semiconductor and assume that the doping impurity is completely ionized. In this case, it is possible to assume that $n_0 = N_I$, where N_I is the concentration of the ionized impurity.

Then the equation (1) for the Brooks–Herring model, it is written as

$$\sigma_{\mathrm{BH}}(k) = \pi b_{\max}^2 = 2\pi \int_{\theta_{\min}}^{\pi} \sigma_{d\mathrm{BH}}(k, \theta) \sin\theta d\theta, \tag{4}$$

where $\theta_{\min}$ — the minimum value of the scattering angle θ corresponding to the maximum value of the $b_{\max}$ of the impact parameter b.

It is easy to show that the density of the distribution of the polar angle when scattering by impurities for the non-parabolic dispersion law in the first Born approximation in the case of the Yukawa potential and the overlap integral equal to one [12] can be represented as

$$f(\theta) = A \frac{\sin\theta}{\left(\frac{4(1-\cos\theta)}{h^2} m_d^* E(1+\alpha E) + \beta_s^2\right)^2}, \tag{5}$$

where A — normalization constant, E — electron energy, m_d^* — the mass of the density of states, $\hbar$ — reduced Planck constant.

Then, based on the method of inverse functions, we have the following expression for determining the angle θ using the Monte Carlo method:

$$r_1 = \frac{\int_{\cos\theta}^{\cos\theta_{\min}} f(\theta) d\theta}{\int_{-1}^{\cos\theta_{\min}} f(\theta) d\theta}, \tag{6}$$

where r_1 — a random number evenly distributed over the interval [0,1]. Solving (6), we proceed to the expression for explicit simulation of the angle θ [2,3]:

$$\cos\theta = 1 - \frac{2(1-r_1)}{1 + 4r_1 \frac{E(1+\alpha E)}{E_\beta}}, \tag{7}$$

where α — the coefficient of nonparabolicity, $E_\beta = \hbar^2\beta_s^2/2m_d^*$.

For the Conwell–Weiskopf model, in accordance with the remark made above in the Introduction, it is possible to obtain [2,3]:

$$\cos\theta = \frac{\left(\frac{E(1+\alpha E)}{E_\beta(1+2\alpha E)}\right)^2 r_1 - 1}{\left(\frac{E(1+\alpha E)}{E_\beta(1+2\alpha E)}\right)^2 r_1 + 1}. \tag{8}$$

Formulas (7) and (8) were used by many authors to determine the angle θ in the Monte Carlo procedure for the Brooks–Herring and Conwell–Weiskopf models.

3. Determination of the scattering angle and the impact parameter in the Ridley model

Since the Brooks–Herring model is obtained under the assumption that a two-particle interaction takes place at the nearest impurity center during scattering, it does not take into account the possible participation of some other, more distant, third center of impurity scattering in the electron scattering act. To eliminate this disadvantage, Ridley [6] introduced a weighting factor, which can be considered as the probability that this scattering act is a purely two-particle scattering process at the nearest scattering center.

According to Ridley, the probability of the absence of scattering centers with a parameter less than b is equal to

$$P(b) = \exp\left(-\pi a N_I b^2\right), \tag{9}$$

where a is the average distance between the ions.

Then, if the differential cross section $\sigma_{d\mathrm{BH}}$ calculated by the Brooks–Herring model is multiplied by the probability (9), then a simple formula is obtained for determining the corresponding differential cross section in the Ridley model [6]:

$$\sigma_{d\mathrm{R}}(k, \theta, b) = P(b)\sigma_{d\mathrm{BH}}(k, \theta). \tag{10}$$

A procedure was described for calculation of the parameters θ and b in the work [10] that allows for determining these parameters in the Ridley model by generating one random number using the Monte Carlo method. According to this procedure the impact parameter b is simulated first, and then the parameter θ is simulated using „inversion“

equation (4) (i.e., its solutions). The method of inverse functions was used to determine the parameter b in [10]:

$$r_2 = \frac{\exp(-\pi a N_I b^2) - \exp(-\pi a N_I b_{\max}^2)}{1 - \exp(-\pi a N_I b_{\max}^2)}, \qquad (11)$$

where r_2, as well as r_1, — a random number with a uniform distribution over the interval $[0, 1]$.

Thus, in [10] it was assumed that the parameter b is initially the only random variable with a normalized distribution density equal to

$$f(b) = 2\pi b a N_I \exp(-\pi a N_I b^2), \qquad (12)$$

and the parameter θ is a random function of the parameter b, the explicit form of which is determined by the solution of the equation (1). In [12], the solution of this equation is given with respect to $\cos\theta$:

$$\cos\theta = 1 - \frac{1}{2k^2}\left[\left(\frac{2k^2\pi b^2}{K^2} + \frac{1}{4k^2 + \beta_s^2}\right)^{-1} - \beta_s^2\right], \qquad (13)$$

where

$$K^2 = \frac{Z^2 e^4 (1 + 2\alpha E) m_d^* k}{4\pi h^2 \varepsilon^2 \varepsilon_0^2 \nu(k)}, \qquad (14)$$

where $\nu(k)$ is the group velocity of electrons.

It can be noted that the distribution density (12) is the Rayleigh distribution density with a constant density of impurity centers in the plane $\lambda = aN_I$.

It is known that the distribution of the distance l can be described using this density from any point of the plane to the nearest neighboring point for the Poisson field of points on the plane with constant density λ [13]. It follows from this that the random behavior of the parameter b with a density of the form (12) is determined only by the geometric arrangement of impurities in the plane and does not take into account the features of the random character of the parameter θ, which has a distribution density of (5) in the two-particle quantum mechanical interaction in the Brooks–Herring model. In this case, the type of density (5) is directly determined by the type of matrix element, which is calculated in the first Born approximation for the electron scattering process on a charged impurity center.

Taking into account the above, in the framework of the Ridley model, for a more correct and accurate Monte Carlo simulation of the parameters θ and b, it is proposed to consider the process of electron scattering on an impurity atom as a two-particle interaction in which the electron is scattered by a certain angle θ, which is a random variable with a distribution density (5) taking into account the probability $P(b)$ that there is no third nearest scattering center. The probability of such a process will depend on two random variables θ and b, each of which is characterized by its own probability density. Assuming that the random parameters θ and b are statistically independent, and using the method of inverse functions, based on (5) and (12) for two joint random events:

$$r_1 r_2 = \frac{\int_{\cos\theta}^{1} \frac{d\cos\theta'}{\left(\frac{4(1-\cos\theta)}{h^2} m_d^* E(1+\alpha E) + \beta_s^2\right)^2}}{\int_{-1}^{1} \frac{d\cos\theta'}{\left(\frac{4(1-\cos\theta)}{h^2} m_d^* E(1+\alpha E) + \beta_s^2\right)^2}} \times \frac{\exp(-\pi a N_I b^2) - \exp(-\pi a N_I b_{\max\,\mathrm{BH}}^2)}{1 - \exp(-\pi a N_I b_{\max\,\mathrm{BH}}^2)}. \qquad (15)$$

Thus, it is possible to connect two random parameters θ and b in a probabilistic way using the formula (15). Note that, in a deterministic (non-random) way, analytically these two parameters remain connected using the formula (13). In this case, the Ridley differential section $\sigma_{d\mathrm{R}}(k, \theta, b)$ is a function of two independent random parameters θ and b. Indeed, using the classical connection between the impact parameter b and the differential cross section $\sigma_{d\mathrm{BH}}(\theta)$ in the form (see, for example, [14])

$$\sigma_{d\mathrm{BH}}(\theta) d\Omega = 2\pi b db, \qquad (16)$$

where $d\Omega = 2\pi \sin\theta d\theta$ is the element of the solid angle into which the electron is scattered, the formula (10) for the Ridley differential cross section can be rewritten as follows:

$$\sigma_{d\mathrm{R}}(k, \theta, b) = \frac{P(b) b db}{\sin\theta d\theta}, \qquad (17)$$

which confirms the validity of the above.

Thus, considering formulas (13) and (15) as a system of two equations with two unknowns θ and b, it is possible to calculate the distributions of $f(\theta)$ and $f(b)$ by simulating the product of two pseudorandom numbers r_1 and r_2. In this case, the equation (15) is solved numerically.

4. Results of modelling and discussion

Figure 1 shows as an example the results of calculating the density of angular distributions of $f(\theta)$ in silicon with a concentration of donor impurity $N_I = 10^{23}\,\mathrm{m}^{-3}$ for the electron energy $E = 10^{-2}\,\mathrm{eV}$ for the Brooks–Herring and Ridley models with the procedure of simulating the angle θ described in [10] and proposed in this paper. It can be seen from this figure that all three density curves differ markedly in their shape and the value of the angle θ corresponding to the maximum of the functions $f(\theta)$.

Figure 2 shows similar dependences for the electron energy $E = 10^{-1}\,\mathrm{eV}$. It follows from the figure that these distributions were subject to significant changes compared to the distributions shown in Fig. 1. In particular, it can be seen that the maximum value of $f_{\max}(\theta)$ for this energy corresponds to the Ridley model with the procedure we proposed.

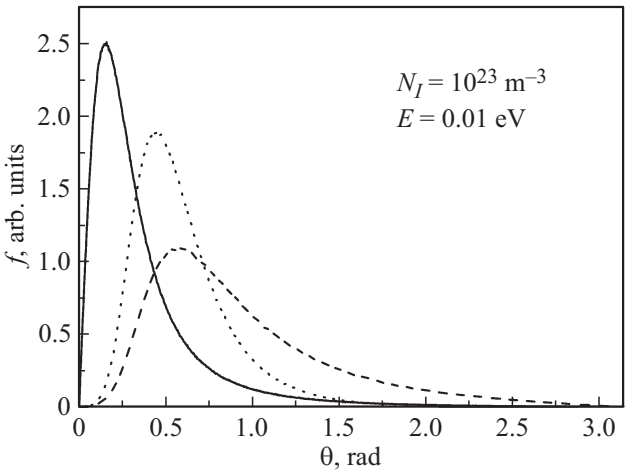

Figure 1. Distribution densities of the polar scattering angle θ for the concentration of ionized impurity $N_I = 10^{23}\,\mathrm{m}^{-3}$ and electron energies $E = 0.01\,\mathrm{eV}$. Solid curve — Brooks–Herring model, dashed — Ridley model [10], dotted — Ridley model with our proposed procedure.

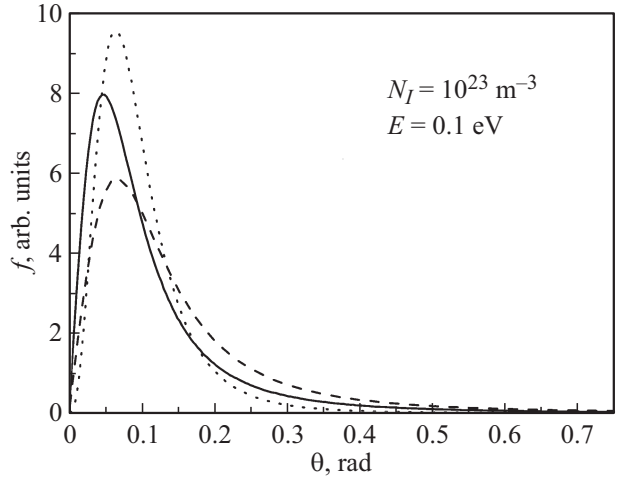

Figure 2. Distribution densities of the polar scattering angle for the concentration of ionized impurity $N_I = 10^{23}\,\mathrm{m}^{-3}$ and electron energies $E = 0.1\,\mathrm{eV}$. Solid curve — Brooks–Herring model, dashed — Ridley model [10], dotted — Ridley model with our proposed procedure.

To verify the adequacy of the Conwell–Weisskopf, Brooks–Herring and Ridley models (taking into account the simulation of the angle θ according to the work [10] and using our proposed methodology), the mobility of μ electrons in silicon doped with a single-charge donor impurity in a constant electric field with a strength of $F = 7 \cdot 10^4\,\mathrm{V/m}$ at 300 K, was calculated using the ensemble Monte Carlo method [1] taking into account all the main mechanisms of electron scattering: phonon acoustic intra-valley and intervalley scattering (all g- and f-phonons were taken into account), as well as plasmon and impurity scattering. In this case, a nonparabolic model of the band structure with a nonparabolicity coefficient $\alpha = 0.5\,\mathrm{eV}^{-1}$ was used. Mobility was determined according to the formula $\mu = v_{dr}/F$, where v_{dr} is the drift velocity, the average value of which was calculated using ensemble Monte Carlo method.

Figure 3 shows the results of calculating electron mobility using the Monte Carlo method for three impurity scattering models (Conwell–Weiskopf, Brooks–Herring and Ridley) in the concentration range of ionized impurity $N_I = 10^{21} - 10^{24}\,\mathrm{m}^{-3}$. The same figure shows the experimental data obtained in [15] corresponding to the modeling conditions.

An analysis of the behavior of the curves provided in this figure allows drawing the following conclusions. First, it can be seen that for the concentration of impurities of $N_I < 10^{22}\,\mathrm{m}^{-3}$ the best match of the simulation and experimental results is provided by the Ridley model, in which the polar angle θ was simulated using the method proposed in this article. Secondly, for the doping levels of a semiconductor $N_I > 3 \cdot 10^{23}\,\mathrm{m}^{-3}$, the Conwell–Weiskopf model provides the best match with the experimental model, which, as is known, rather roughly describes the process of two-particle interaction and the impurity center without taking into account the screening effect. Thirdly, it can be noted that the curves corresponding to the Brooks–Herring model and the Ridley model, for which the polar angle θ is simulated according to [10] in the entire range of concentration changes N_I, differ slightly. In addition, the discrepancy of all models under consideration with the experiment increases with an increase in the concentration of impurity ions up to the value of $N_I = 10^{24}\,\mathrm{m}^{-3}$.

To further analyze the results of the calculation and experiment on the mobility of μ, Fig. 4 shows the results of calculating the angular distributions we made for the Brooks–Herring and Ridley models for the electron energy

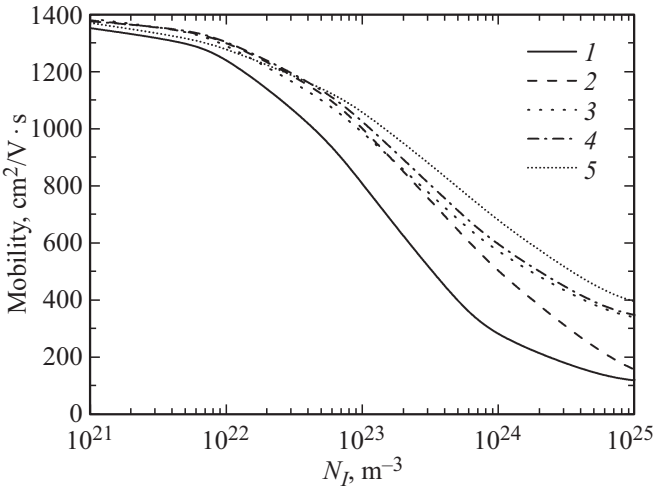

Figure 3. Dependences of electron mobility on the concentration of ionized donor impurity in silicon for various models of scattering on ionized impurity at a temperature of 300 K. Curve *1* is an interpolation of experimental data [15], *2* is Conwell–Weiskopf model, *3* is Brooks–Herring model, *4* is Ridley model [10], *5* is Ridley model with our proposed procedure.

Calculated average values of the polar scattering angle θ at different concentrations of ionized impurity for three scattering models

Concentration impurities, m^{-3}	Average angle value θ		
	Model Brooks–Herring, π	Model [10], π	Proposed by us model, π
10^{22}	0.0199	0.0460	0.0242
10^{23}	0.0610	0.0967	0.0572
10^{24}	0.1680	0.2080	0.1460

$E = 4 \cdot 10^{-2}$ eV. This energy in the numerical experiment is close to the energy of an electron in a weak field, in which the value of the low-field mobility of electrons at a temperature of 300 K [15] was experimentally determined.

At the same time, since the results of calculating the drift velocity by the Monte Carlo method presented in Fig. 3, in addition to angular distributions, largely depend on the scattering rate for this mechanism, it is also necessary to refer to the dependences of the impurity scattering rate on the energies shown in Fig. 5 for a correct explanation of the behavior of the curves shown in Fig. 3. The intensities are calculated for silicon doped with a single-charge donor impurity according to the formulas taken from [1–3,10].

A comparison of the results presented in Figs. 3, 4 and 5 allows explaining rather close arrangement of the curves $\mu(N_I)$ corresponding to the Brooks–Herring and Ridley models [10] by a formal coincidence of the mobility values obtained due to large scattering angles θ (see fig. 4), but at the same time a lower scattering rate for the electron energy $E = 4 \cdot 10^{-2}$ eV in the Ridley model [10] compared to the Brooks–Herring model. The slightly higher mobility, which was determined by calculations using our method for concentrations of $N_I > 5 \cdot 10^{22}\,m^{-3}$, can be explained by smaller scattering angles that fall out when they are simulated according to this method. The above is confirmed by the average values of the angles θ calculated according to the formula for the average value of the angle:

$$\bar{\theta} = \int_0^{\pi} \theta f(\theta) d\theta, \qquad (18)$$

which are given in the table.

Regarding the procedure [10], it should be noted that, compared to the Brooks–Herring model and our model, it is characterized by a higher probability of scattering to more obtuse angles for all three values of the impurity concentration (see the table). This can be explained by the fact that, as already noted above, the form of the distribution of $f(\theta)$ for this procedure depends primarily on the nature of the distribution of $f(b)$, which describes the random nature of the location of impurities in the lattice cross-section plane and does not take into account the quantum mechanical sharp-angle nature of the interaction of the charge carrier with a separate impurity center. The importance of this latter fact was, in particular, pointed out in the work [9], in which critical comments were reasoned regarding the description of the process of two-particle interaction using „static screening“ by impurity ions in the Ridley model. In this connection, it should be noted that the

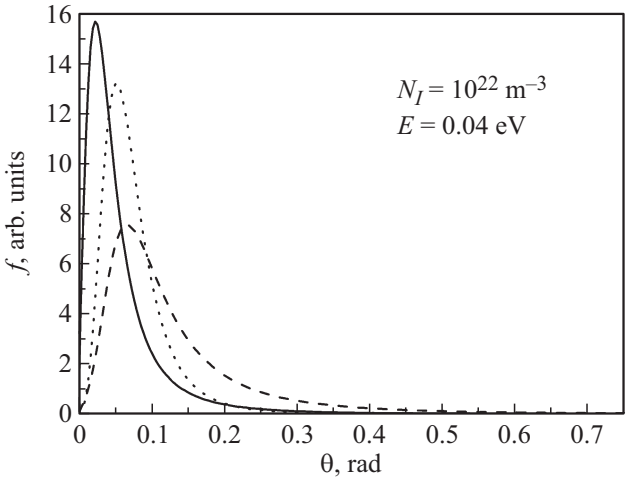

Figure 4. Distribution densities of the polar scattering angle for the concentration of ionized donor impurity $N_I = 10^{22}\,m^{-3}$ and electron energies $E = 0.04$ eV. Solid curve is the Brooks–Herring model, dashed curve is the Ridley model [10], dotted curve is the Ridley model with our proposed procedure.

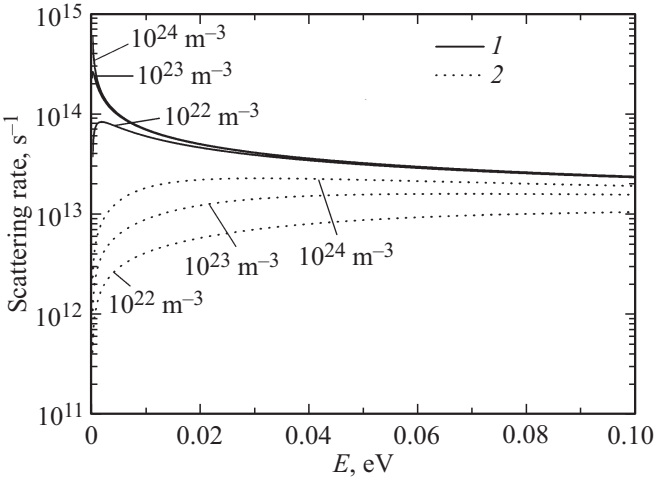

Figure 5. Electron scattering intensities on an ionized donor impurity in silicon at a temperature of 300 K. Curves *1* — the Brooks–Herring model, *2* — the Ridley's third body exclusion model. The scattering intensities are given for three values of the ionized impurity concentration ($N_I = 10^{22}$, 10^{23} and $10^{24}\,m^{-3}$).

increase in popularity of the latter is primarily attributable to the publication of the work [10], in which, a fairly good match was obtained using the example of GaAs with the results of the mobility experiment and, of course, taking into account the fact that this model provides much lower values of the scattering rate than the Brooks–Herring model at low energy values (see Fig. 5), which is very important when modeling transfer processes using the Monte Carlo method. At the same time, calculations for silicon using the Ridley model, taking into account the more correct procedure developed by us for the simulation of the polar scattering angle θ for values $N_I > 5 \cdot 10^{22}\,\mathrm{m}^{-3}$, showed the worse match of the calculation results with the experiment, than for the Brooks–Herring model.

Thus, in this paper, the procedures for simulation of the polar angle of electron scattering on impurity ions were considered and analyzed within the framework of the Brooks-Herring, Conwell–Weiskopf and Ridley models most often used in the Monte Carlo method. An original technique for simulation of this angle was proposed and tested for the Ridley model. Taking into account the fact that, unlike the method described in the work [10], it takes into account both the features of the quantum-mechanical two-particle interaction of an electron with an impurity ion, and the probability of the absence of another nearby ion during this interaction, it is more correct compared to the method described in the work [10].

5. Conclusion

A comparative analysis of the results of the calculation and experiment for determining the low-field mobility of electrons in silicon at a temperature of $T = 300\,\mathrm{K}$ for the three models considered was performed: Brooks–Herring, Conwell–Weiskopf and Ridley. The calculation results showed that the Ridley model with the procedure we developed for simulation of the angle θ provided the best match with the experimental data for the concentration of impurity ions of $N_I < 10^{22}\,\mathrm{m}^{-3}$ and the Conwell–Weiskopf model — for concentrations $N_I > 3 \cdot 10^{23}\,\mathrm{m}^{-3}$ The Brooks–Herring model and the Ridley model with the procedure described in [10] provided similar results in the entire range of concentrations studied $10^{21}\,\mathrm{m}^{-3} \leq N_I \leq 10^{25}\,\mathrm{m}^{-3}$.

Calculations performed using the procedure developed by us for the Ridley model with an impurity concentration of $N_I \geq 5 \cdot 10^{22}\,\mathrm{m}^{-3}$ demonstrated a less good match with the experiment than for the same model with the procedure described in the paper [10]. This indicates that the use of the Ridley model for the accurate calculations of electron mobility using the Monte Carlo method in semiconductors, in particular in silicon, at its doping level $N_I \geq 10^{23}\,\mathrm{m}^{-3}$ requires caution and further critical analysis.

Conflict of interest

The authors declare that they have no conflict of interest.

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