A large-scale fluctuation potential in a lightly doped compensated semiconductor

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A model of a large-scale fluctuation potential in a lightly doped compensated semiconductor is suggested. The model is used to calculate the chemical potential μ at absolute zero as a function of the degree of compensation K in the interval $0.8 < K < 1$. It is shown that only by allowing for a small-scale potential is it possible to fit the calculated function $\mu(K)$ to the results of numerical modeling. The dependence of the spatial scale of the fluctuation potential on the degree of compensation is established, and the probability density of the large-scale potential, its dispersion, and the density of the impurity states are calculated.

1. INTRODUCTION

At low temperatures the properties of a compensated semiconductor depend primarily on the structure of the impurity bands. To be specific, we will consider a semiconductor of the n-type doped with shallow donors and acceptors with average volume concentrations $\bar N_d$ and $\bar N_a$. We will assume that the conditions of light doping are met, namely $\bar N_{a,d} a^3_{a,d} \ll 1$, where a_a and a_d are the respective Bohr radii. This inequality makes it possible to speak of donor and acceptor impurity bands in the classical sense, when the shift in a level of an impurity center can be assumed equal to the potential energy generated by the other charged impurities in this center. A review of the research into the structure of the impurity band of such semiconductors, that is, the densities of states, the values of the chemical potential, and the configuration of the vacant and filled states in space at absolute zero, can be found in Refs. 1 and 2.

Regarding doped semiconductors it is known[1,2] that the higher the compensation degree $K = \bar N_a / \bar N_d$ the greater the role of the large-scale fluctuation potential, that is, a potential with a characteristic scale R much greater than the average distance between the impurities, $\bar N_{a,d}^{-1/3}$.

What is the current state of affairs in studies of the classical impurity band? On the one hand, there are researchers who employ direct numerical minimization of the Coulomb energy of the interaction of electrons with each other and with the charged impurities. Such work has been carried out primarily by the group of Shklovskiĭ and Éfros, and the main results can be found in Refs. 1–4. An essential drawback of such modeling is the long computing time. In addition, the question of the characteristic spatial scale of fluctuations has yet to quantitatively be resolved. On the other hand, approximate analytical calculations are not in quantitative agreement with the results of numerical modeling.

The most consistent analytical theory of the large-scale fluctuation potential in a lightly doped semiconductor, I believe, has been developed by Chenskiĭ.[5] However, his estimate of the large-scale fluctuation potential (and, respectively, the absolute value of the chemical potential) is half the value obtained by numerical modeling in Ref. 2. Besides, the applicability range of the theory developed in Ref. 5, obtained from the requirement that the number of acceptors in a characteristic fluctuation be greater than one, is restricted to a narrow range of compensation degrees near unity ($0.95 \leqslant K \leqslant 1$).

Using the Chenskiĭ model as a basis, I proceeded from the following assumptions. Since the characteristic scale of fluctuations proves to be relatively small, the Gaussian distribution employed in Ref. 5 for impurities in a fluctuation must be replaced with the more exact Poisson distribution. Also, the characteristic fluctuation amplitude in Ref. 5, that is, the chemical potential μ, was found from an electroneutrality equation in which the small-scale fluctuations of the potential were ignored, and only one of two closely spaced donors proves to be charged by the Coulomb interaction (a similar situation is true for acceptors).

Thus, the aim of the present study is to establish the justification for replacing the Poisson distribution of impurities with a Gaussian distribution. We will see that to exclude the "self-action" of charged centers it is advisable to calculate the electrostatic energy of the system and then use this value to determine the chemical potential. The minimum of the chemical potential determines the characteristic spatial (optimum) scale of potential fluctuations, R, which is expressed here in terms of the average number of donors in a fluctuation as follows: $\bar n_{\rm op} = 4\pi R^3 \bar N_d/3$. This fact makes it possible to refine the $\bar n_{\rm op}(K)$ dependence and "move" the calculations into the region of smaller values of K ($K \geqslant 0.8$). Development of an approximate procedure for allowing for the small-scale potential leads to a substantial increase in μ and makes it possible to reconcile the calculation of μ with the results of numerical modeling.[2]

2. THE CHARGE DISTRIBUTION AND THE FLUCTUATION POTENTIAL

Let us mentally divide the semiconductor into spheres of radius R. For the Poisson distribution, the probabilities of n donors and m acceptors in such a sphere are, respectively,

$$W_d(n) = \frac{(\bar n)^n}{n!}\exp(-\bar n), \tag{1}$$

$$W_a(m) = \frac{(K\bar n)^m}{m!}\exp(-K\bar n), \tag{2}$$

with $\bar n = 4\pi R^3 \bar N_d/3$.

To find the fluctuation potential in a semiconductor one must determine the potential generated by a separate fluctuation with n donors and m acceptors, $-V^*(r^*, n, m)$, where r^* is the radius vector of the coordinate (an asterisk designates a dimensional quantity). As is the common practice (e.g., see Ref. 1), the concentrations of donors and acceptors are assumed constant within one fluctuation:

$$N_d(\mathbf{r}^*)=3n/4\pi R^3, \quad N_a(\mathbf{r}^*)=3m/4\pi R^3.$$

To determine $V^*(\mathbf{r}^*,n,m)$ we follow a procedure developed and substantiated in Ref. 5, which leads to the following qualitative picture. An average potential $\overline{V}^*$ is established in the semiconductor, it is assumed that outside the fluctuation the potential must tend exponentially to $\overline{V}^*$ with a characteristic screening length R^*_{sc}. This corresponds to a slowly varying density of states near the Fermi level. To find $V^*(\mathbf{r}^*,n,m)$ inside the fluctuation, one must solve the Poisson equation and match the electrostatic potential and the field strength at the fluctuation boundary. In the semiconductor there is a single Fermi level μ_0, and all donors below this level are filled and neutral. Thus, μ_0 is the maximum energy of a neutral donor. It differs insignificantly from the chemical potential (see below) because of the existence in the donor-state density of a Coulomb gap separating vacant states from filled. All fluctuations can be divided into screened and unscreened, depending on the ratio of the energies at the donor level in a fluctuation and on the Fermi level. In unscreened fluctuations the donor level is higher than the Fermi level, all donors are charged, and the fluctuation-charge density ρ^* is $e(N_d - N_a)$, with e the electron charge. In screened fluctuations the donor level reaches the μ_0 level and near the center there is an electroneutrality region where $\rho^* = 0$ (Fig. 1).

Here are the basic equations for the potential. Inside a fluctuation

$$\frac{d^2V^*}{dr^{*2}}=\frac{4\pi e}{\varepsilon}\rho^*, \tag{3}$$

with ε the dielectric constant of the semiconductor. At this point it is expedient to introduce the dimensionless variables

$$r=r^*/R, \quad V=V=V^*/E_R, \quad E_R=e^2/2\varepsilon R, \quad \rho=\rho^*\bar{n}/\varepsilon N_d.$$

Now we take into account the spherical symmetry of a fluctuation and rewrite the Poisson equation (3) in terms of the dimensionless variables:

$$\frac{d^2V}{dr^2}+\frac{2}{r}\frac{dV}{dr}=6\rho. \tag{4}$$

By employing the probability density $P(V)$ of the potential, we can easily write the expressions for the average value of the potential,

$$\overline{V}=\int_{-\infty}^{\infty} VP(V)dV, \tag{5}$$

and for the screening radius R_{sc} outside the fluctuation normalized to R,

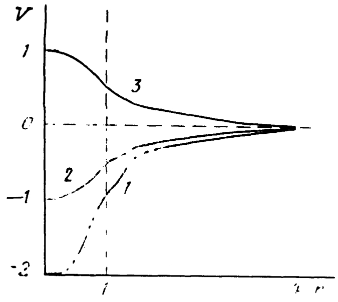

FIG. 1. The qualitative potential patterns for screened (curve *1*) and unscreened (curves *2* and *3*) fluctuations.

$$R_{sc}\approx[6\bar{n}P(V\approx\mu)]^{-1/2}. \tag{6}$$

Here the potential is reckoned from the average value of the potential into the conduction band interior. The solution of the Poisson equation outside the fluctuation is

$$V(r)=(a_1/r)\exp(-r/R_{sc}), \tag{7}$$

where a_1 is a constant determined by the boundary conditions.

The solution for unscreened fluctuations, that is, with ρ = const inside the fluctuation, is

$$V(r)=\rho(r^2-\delta), \tag{8}$$

where

$$\delta=(1+3R_{sc})/(1+R_{sc}).$$

For screened fluctuations ($\rho > -\mu_0/\delta$), which at the center for $r \leqslant r_1$ have an electroneutrality region with $\rho = 0$, solving Eq. (4) yields

$$V(r)=\begin{cases} \mu_0, & 0\leqslant r\leqslant r_1, \\ \rho[-3r_1^2+r^2+2r_1^3/r]+\mu_0, & r_1\leqslant r\leqslant 1. \end{cases} \tag{9}$$

The equation for r_1 can be found from the boundary conditions and has the form

$$(3-\delta)r_1^3-3r_1^2+\delta+\mu_0/\rho=0. \tag{10}$$

It can easily be shown that in terms of dimensionless variables the fluctuation-charge density is equal to the difference between the number of donors and the number of acceptors in the fluctuation:

$$\rho=n-m. \tag{11}$$

The distribution in ρ is given by

$$W_1(\rho)=\sum_{n=\max(0,\rho)}^{\infty} W_d(n)W_a(n-\rho). \tag{12}$$

3. THE ELECTRONEUTRALITY EQUATION AND THE VALUE OF THE CHEMICAL POTENTIAL

The average concentration of the neutral donors in screened fluctuations (only in such fluctuations do neutral donors reside if we do not allow for the small-scale potential) is equal to $\rho r_1^3 N_d/\bar{n}$. Multiplying it by the probable occurrence of such fluctuations and summing over all the fluctuations, we should get the average concentration of neutral donors, that is, impose the electroneutrality condition on the sample,

$$\frac{\overline{N}_d}{\bar{n}}\sum_{\rho=\rho_{min}}\rho r_1^3(\rho)W_1(\rho)=\overline{N}_d(1-K), \tag{13}$$

where $\rho_{\min} = [-\mu_0/\delta] + 1$, with $[-\mu_0/\delta]$ the integral part of $-\mu_0/\delta$.

Simultaneous solution of Eqs. (10) and (13) yields $\mu_0(K,\bar{n})$, where $\bar{n}$, or respectively the fluctuation radius, is the intrinsic parameter of the problem. The solution must be optimized in $\bar{n}$, meaning the possibility of varying the donor occupancy.

In Ref. 5 the optimum radius is found by minimizing $\mu_0(\bar{n})$. Replacing the Gaussian impurity distribution with

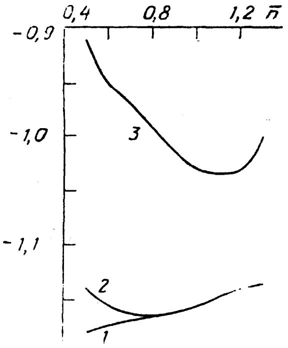

FIG. 2. The Fermi energy μ_0 and the chemical potential μ in units of E_d as functions of the fluctuation size for a compensation degree K equal to 0.9. Curves *1* and *2* correspond to $\mu_0(n)$ at $\rho_{\min} = [-\mu_0/\delta] + 1$ and $\rho_{\min} = \max(2, [-\mu_0/\delta] + 1)$, respectively, and curve *3* to $\mu(n)$ at $\rho_{\min} = \max(2, [-\mu_0/\delta] + 1)$.

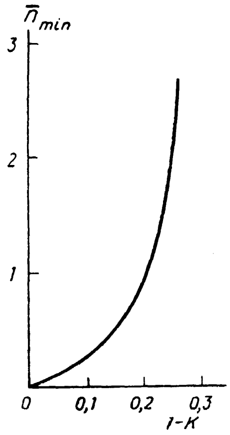

FIG. 3. The minimum size of a fluctuation, $\bar{n}_{\min}$, plotted against the compensation degree K.

the more exact Poisson distribution alters the way in which $\mu_0(\bar{n})$ varies (Fig. 2). First, letting $\bar{n}$ tend to zero, we find that $\mu_0(\bar{n}) \propto -\bar{n}^{-1/3}$ (recall that for the Gaussian distribution $\mu_0(\bar{n}) \propto -\bar{n}^{1/6}$, see Refs. 2 and 5), which follows from the fact that the characteristic charge in a fluctuation proves to be of the order of unity and not $\bar{n}^{1/2}$, as is the case for the Gaussian distribution. This charge is actually equal to K, since employing the Poisson distribution makes it possible to operate with an averaged fractional charge. As $K \to 1$, the plot of μ_0 against $\bar{n}$ acquires an additional minimum at relatively large values of $\bar{n}$ coinciding with the value of $\bar{n}_{\text{op}}$ obtained for the Gaussian distribution.[5] This appears, specifically, at $R_{\text{sc}} = 1$ for $K > 0.98$. The tendency of $-\mu_0(\bar{n})$ to become infinite as $\bar{n} \to 0$ can be arrested by imposing a restriction on $\rho_{\min}$ and assuming that $\rho_{\min} = \max(2, [-\mu_0/\delta] + 1)$ (see Fig. 2). Physically this means ruling out the possibility of a fraction of the donor charge creating a potential for itself. However, the "repercussions" of such self-action are sure to be retained even under such a restriction as soon as $|\mu_0|$ becomes smaller than δ, since the charge of the screened fluctuations, $\rho[1 - r_1^3(\rho)]$, becomes of the order of unity.

Actually, for any degree of compensation one can define a partitioning of minimal size, $\bar{n}_{\min}$, at which the solution to Eq. (13) still has physical meaning. The value of $\bar{n}_{\min}$ can be found by the following reasoning. The minimum charge in screened fluctuations cannot be smaller than unity, that is, the maximum number of neutral donors is $\rho - 1$. As a result, by analogy with Eq. (13), we arrive at an equation for $\bar{n}_{\min}$:

$$\frac{\bar{N}_d}{\bar{n}_{min}} \sum_{\rho=2}^{\infty} (\rho-1) W_1(\rho, \bar{n}_{min}, K) = \bar{N}_d (1-K). \tag{14}$$

The solution to Eq. (14) in the form of $\bar{n}_{\max}$ plotted against K is depicted in Fig. 3. For a definite value of K the range of admissible values of $\bar{n}$ is restricted by the inequality $\bar{n} > \bar{n}_{\min}$. At $K = 0.74$ the value of $\bar{n}_{\min}$ tends to infinity, that is, the solution to Eq. (14) in this range of K loses all meaning.

The calculations can be improved in the region of "small" K by defining the electrostatic energy of the semiconductor in such a way that the self-action of a charge is automatically excluded. This "renormalized" energy can then be used to find the chemical potential.

The expression for the electrostatic energy F of the system, has the following form:

$$F = \frac{\bar{N}_d}{2\bar{n}} \sum_{\rho=-\infty}^{\infty} W_1(\rho) \int_{r_1(\rho)}^{1} 3\rho V(\rho', r) r^2 \, dr. \tag{15}$$

Here $r_1(\rho)$ vanishes for $\rho < \rho_{\min}$ and is found from Eq. (10) for $\rho > \rho_{\min}$, and potential $V(\rho', r)$ is given by Eqs. (8) and (9) for, respectively, unscreened and screened fluctuations in which the charge density is diminished by unity:

$$\rho' = \{\rho[1 - r_1^3(\rho)] - \text{sign}\,\rho\} / [1 - r_1^3(\rho)]. \tag{16}$$

Substituting (8) or (10) into (15), allowing for the fact that $\rho(r) = \text{const}$, and integrating we find the average potential $\langle V(\rho) \rangle$ acting on the charge in the fluctuation:

$$\langle V(\rho) \rangle = \begin{cases} \rho'(3/5 - \delta), & \rho < \rho_{min}, \\ \rho'\{3/5(1 - r_1^5) + 3r_1^3(1 - r_1^2) \\ \quad + (1 - r_1^3)[\delta + (3 - \delta) r_1^3]\}, & \rho \geqslant \rho_{min}. \end{cases} \tag{17}$$

Having calculated the dependence of F on $\bar{n}$ and K, we can determine the chemical potential μ. For this we must find the derivative of F with respect to the electron concentration $\bar{n}_d$ on donors or, bearing in mind that $\bar{n}_d = \bar{N}_d(1 - K)$, we find that

$$\mu = -\frac{1}{\bar{N}_d} \frac{\partial F}{\partial K}. \tag{18}$$

By calculating μ as a function of $\bar{n}$ for a fixed K and finding on the plot of this function the value $\bar{n}_{\text{op}}$ corresponding to the function's minimum we obtain the optimum partitioning of the sample, that is, the occupancy of the donors at which the ground state of the system is realized. Figure 4a shows the results of calculating μ_0 and μ for the Poisson distribution of impurities, and μ_0 for the Gaussian distribution, as functions of K (see the Appendix). All curves have been calculated with $R_{\text{sc}} = 1$ and the energies have been normalized to the average interaction energy of donors, $E_d = e^2(\frac{4}{3}\pi\bar{N}_d)^{1/3}/\epsilon$. From Fig. 4a one can see that in the region where $K \to 1$ all the curves merge. The difference be-

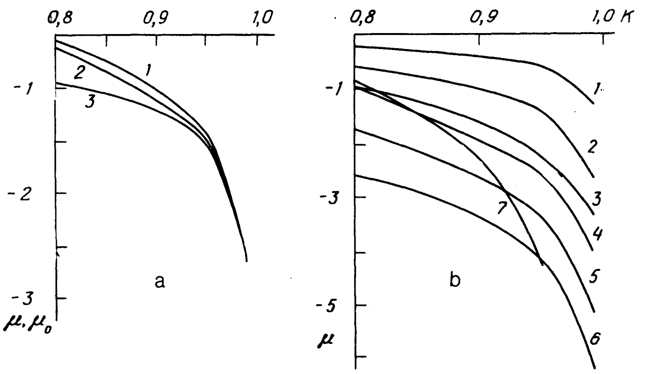

FIG. 4. (a) Diagrams of μ vs K and of μ_0 vs K for the Poisson distribution (curves *1* and *2*, respectively) and of μ_0 vs K for the Gaussian distribution (curve *3*). (b) The chemical potential as a function of the compensation degree without allowance for the small-scale potential (curves *1–3*) and with allowance for such a potential (curves *4–6*). Curves *1* and *4* correspond to $R_{sc} = 0.1$, curves *2* and *5* to $R_{sc} = 1$, and curves *3* and *6* to $R_{sc} = 10$; all energies are given in units of E_d. Curve *7* corresponds to the results of numerical modeling taken from Ref. 2.

tween μ_0 and μ plotted against K for the Poisson distribution in the range of moderate values of K ($0.8 < K < 0.95$) is caused by the existence, between the vacant and filled donor states, of a Coulomb gap where the chemical potential level resides.[2] Note that within the framework of the model considered here the width of the Coulomb gap depends on $\bar n_{op}$ and decreases as $\bar n_{op}$ (and, hence, the degree of compensation) grows. The resulting curves representing the $\mu(K)$ dependence for different screening lengths R_{sc} are depicted in Fig. 4b, and the $\bar n_{op}(K)$ plot is shown in Fig. 5.

Comparison of the absolute values of the Fermi energy with the results of numerical modeling[2] (see curve 7 in Fig. 4b) shows that allowance for only the large-scale potential is insufficient to explain the sharp increase in $\mu(K)$ as $K \to 1$. It is in this region that one must take into account the small-scale potential.

4. THE EFFECT OF A SMALL-SCALE POTENTIAL

Let us consider a fluctuation with n donors and m acceptors. The probability of finding k donors and not a single acceptor in a region of volume r^3 is

$$C_n^k r^{3k}(1-r^3)^{n-k+m}, \tag{19}$$

where C_k^n is the number of combinations of k objects from a set of n. Multiplying this number by $k-1$, summing over k from 2 to n, and dividing by r^3, we obtain the number of donors residing within the given fluctuation at distances from one of the donors ranging 0 to r:

$$N(r)=\frac{(1-r^3)^m}{r^3}[(1-r^3)^n+nr^3-1]. \tag{20}$$

Note that as $r \to 0$ this dependence yields the number of donor pairs residing at distances ranging 0 to r; that is, the dependence corresponds to the nearest-donor approximation.[1]

To determine the potential whose effect the donors "feel," we average the large-scale potential within the fluctuation region:

$$\bar V_{nm}=3\int_0^1 V(n, m, r)r^2\,dr. \tag{21}$$

Substituting the expression for the potential of unscreened or screened fluctuations, (8) or (9), we find that

$$\bar V_{nm}=\begin{cases}\rho(-\delta+{}^3/_5), & \rho<\rho_{min},\\ \mu_0+3\rho(1-r_1)^3(1+3r_1+r_1^2)/5, & \rho\geq\rho_{min}.\end{cases} \tag{22}$$

Recall that $r_1(n,m)$ is determined by Eq. (10). Using the value of $\bar V_{nm}$, we can express the energy in the fluctuation region at a distance r from a charged donor in the form

$$E(r)=\bar V_{nm}-2/r. \tag{23}$$

To find the number of donors with an energy below the Fermi level, we use formula (20) for $N(r)$ with $r=r_{nm}=\min[2/(\bar V_{nm}-\mu_0),1]$. However, for fluctuations with a potential close to the Fermi level ($\bar V_{nm}-\mu_0<1/2$), where it would seem easiest to force a donor to sink below the Fermi level, Eq. (20) yields $N(r=1)=0$. For such fluctuations we find the position of the $N(r)$ maximum attained at $r=r_{max}$, and assume that the number of donors occurring below the Fermi level is still determined by Eq. (20) with $r=r_{max}$. Thus, the number of donors that prove to be neutral in the given fluctuation as a result of interacting with the nearest charged donor is given by Eq. (20) with $r=r_{mn}$, where

$$r_{nm}=\begin{cases}2/(\bar V_{nm}-\mu_0), & E(r_{max})\geq\mu_0,\\ r_{max}, & E(r_{max})<\mu_0.\end{cases} \tag{24}$$

As a result, the fluctuation's charge density diminishes:

$$\rho(n, m)=n-m-N(r_{nm}). \tag{25}$$

Thus, the "small-scale" fraction of the neutral donors is

$$\frac{\bar N_d}{\bar n}\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}W_d(n)W_a(m)N(r_{nm}). \tag{26}$$

This term must be added to the left-hand side of the electroneutrality equation:

$$\frac{1}{\bar n}\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}W_d(n)W_a(m)[N(r_{nm})+\rho r_1^3(\rho)]=1-K. \tag{27}$$

We have thus arrived at a self-consistent and closed system of equations (10), (25), and (27). Carrying out the necessary calculations, we find $\mu_0(\bar n,K)$. To determine the

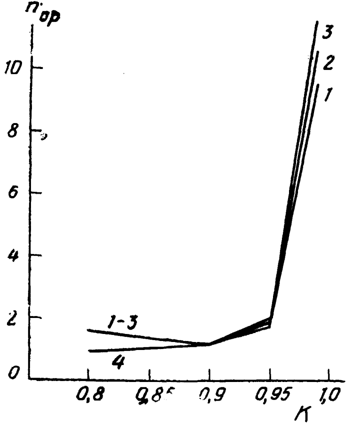

FIG. 5. The optimal fluctuation size $\bar n_{op}$ as a function of the compensation degree K with (curve *4*) and without (curves *1–3*) allowance for the small-scale potential. Curve *1* corresponds to $R = 0.1$, curve *2* to $R = 1$, and curve *3* to $R = 10$.

optimal fluctuation size, we also calculate the electrostatic energy and, via (18), find $\bar{n}_{\text{op}}$. The minimum of μ is attained at values of $\bar{n}_{\text{op}}$ that approximately agree with those obtained earlier without allowing for small-scale fluctuations (see Fig. 5). However, the value of μ_0 increases substantially in the region where $K \to 1$ (see Fig. 4b). Figure 4b shows how the $\mu_0(K)$ curve can be fitted to the numerical-modeling results by varying the screening parameter R_{sc} outside the fluctuation. The screening radius increases with K, owing both to the increase in the fluctuation potential and to the decrease in the electron concentration on the donors.

5. THE PROBABILITY DENSITIES OF THE POTENTIAL AND OF THE DONOR STATES

Having determined the ground state of the system, it is expedient to compare the density of donor states, obtained within the framework of the developed model, with numerical-modeling results taken from Ref. 2. To this end we calculate the probability densities of the large-scale fluctuation potential and of the donor states.

Recall that by employing the probability density of the fluctuation potential, $P(E)$, it is relatively easy in the quasiclassical approximation to calculate the "tails" of the state densities of the conduction and valence bands[1] and the dispersion of the fluctuation potential. We can assume, to first approximation, that the densities of the donor and acceptor states are proportional to $P(E)$ (see Ref. 5). However, knowing the structure of the fluctuations, we can calculate these functions more accurately.

In an individual fluctuation the potential probability density is

$$P(E^{\cdot},\rho)=\frac{3}{4\pi R^3}\int \delta(E^{\cdot}-V^{\cdot}(\mathbf{r}^{\cdot}))\,d\mathbf{r}^{\cdot}. \tag{28}$$

Integrating and going over to dimensionless variables yields

$$P(E,\rho)=3r^2\Big/\frac{dV}{dr}\Big|_{V(r)=E}. \tag{29}$$

Substituting the expression (8) for the potential of an unscreened fluctuation into (29), multiplying the result by the probability of such a fluctuation, and summing over all the fluctuations that produce the potential E, we find the probability density of the potential generated by unscreened fluctuations:

$$P_1(E)=\frac{3}{2}\sum_n\sum_m\left[\delta+\frac{E}{\rho(n,m)}\right]^{1/2}\frac{W_d(n)W_a(m)}{\rho(n,m)}, \tag{30}$$

where the summation is over all the fluctuations that satisfy the inequalities $\rho_1<\rho(n,m)<\rho_2$, with $\rho_1=-E/\delta$ and $\rho_2=-E/(\delta-1)$.

Similar calculations with the expression (9) for the screened fluctuation potential substituted for (8) yield the probability density of the potential generated by screened fluctuations:

$$P_2(E)=\frac{3}{2}\sum_n\sum_m\frac{r^4(E,\rho)W_d(n)W_a(m)}{\rho(n,m)[r^3(E,\rho)-r_1^3(\rho)]}, \tag{31}$$

where $r_1(p)$ is found by solving Eq. (10) with a known μ_0, the function $r(E,\rho)$ is found by solving (9) and (10), and the summation is over all the fluctuations that obey the inequalities $\rho_{\min}\leqslant\rho(n,m)\leqslant\rho_3$, with ρ_3 the maximum charge density at which the potential at the boundary of a screened fluctuation still attains the value E, or

$$V(r=1,\rho_3)=E. \tag{32}$$

Note that the function $V_1(\rho)=V(r=1,r_1(\rho))$ monotonically decreases as ρ grows.

The total probability density of the potential is the sum of the probability densities for screened and unscreened fluctuations,

$$P(E)=P_1(E)+P_2(E), \tag{33}$$

and is shown in Fig. 6. Allowance for small-scale fluctuations (Fig. 6b) leads to a decrease in the number of screened fluctuations and flattens the "excessive" peak (excessive from the standpoint of numerical simulation) that is near the Fermi level and is caused by the contribution $P_2(E)$ of the screened fluctuations.

In the model developed here the probability density of the large-scale potential has two delta-like peaks. The first lies near the Fermi level ($E=\mu_0$) and has the amplitude

$$P(E=\mu_0)=\sum_n\sum_m r_1^3(n,m)\,W_d(n)W_a(m), \tag{34}$$

while the second corresponds to $E=0$ and has the amplitude

$$P(E=0)=\sum_n\sum_m W_d(n)W_a(m). \tag{35}$$

The summation here is over all fluctuations with $\rho(n,m)=0$.

From the standpoint of physics it is clear that the two peaks must spread out, the first largely because of small-scale fluctuations, and the second because of fluctuations of the boundary conditions. For one thing, the spreading of the peak at $E=0$ balances the dip in the potential's probability-density caused by the fact that this energy region corresponds to the screening potential outside the fluctuation and is not taken into account when $P(E)$ is calculated.

Knowing the probability density of the potential, we can calculate the dispersion γ of the large-scale potential as a function of the compensation degree K of the semiconductor:

$$\gamma(K)=\left[\int_{-\infty}^{\infty}V^2P(V,K)\,dV\right]^{1/2}. \tag{36}$$

Note that in comparison to μ_0, the dispersion γ proves to be less sensitive to whether or not the small-scale potential is taken into account (Fig. 7).

When calculating the density of charged donor states, we must exclude self-action (just as we did when calculating the electrostatic energy); that is, we must replace ρ with ρ' when calculating the potential of charged centers. In addition, in the case of screened fluctuations we must bear in mind that the density of vacant donor states, ρ_d, is inhomogeneous over the fluctuation volume,

$$\rho_d=\begin{cases} n, & r_1<r\leqslant 1,\\ m, & 0\leqslant r\leqslant r_1.\end{cases} \tag{37}$$

As a result, for the density of donor states we have

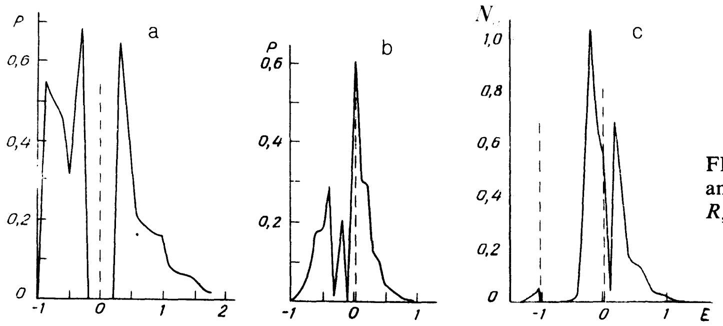

FIG. 6. The probability density of the potential without allowance (a) and with allowance (b) for the small-scale potential at $K = 0.95$ and $R_{sc} = 1$, and the donor-state density (c) at $K = 0.9$ and $R_{sc} = 1$.

$$N_d(E)=\frac{3}{2}\frac{\bar{N}_d}{\bar{n}_{op}}\sum_n\sum_m\frac{\rho_d}{\rho-1}W_d(n)\,W_a(m)\times\left\{\left(\delta+\frac{E}{\rho-1}\right)^{1/2}+\frac{r^4(E,\rho-1)}{[r^3(E,\rho-1)-r_1^3(\rho-1)]}\right\},\tag{38}$$

where summation is carried out over all fluctuations with potential E.

For the density of neutral donors we obtain a delta-like peak at μ_0 with the amplitude

$$N_d(E=\mu_0)=\frac{\bar{N}_d}{\bar{n}_{op}}\sum_n\sum_m\rho(n,m)r_1^3(n,m)\,W_d(n)\,W_a(m),\tag{39}$$

and the term caused by small-scale fluctuations,

$$N_d(E)=\frac{dN(r)}{dr}\frac{dr}{dE},\tag{40}$$

where $N(r)$ is defined by (20), and $r(E)$ is obtained by solving Eq. (23). The total density of donor states at $K = 0.95$ is depicted in Fig. 6c, where the presence of a Coulomb gap between neutral and charged donors is evident.

6. CONCLUSION

The calculations show that the large-scale fluctuation potential for a strongly compensated semiconductor can be calculated by allowing for the fact that a small-scale potential may exist simultaneously with the large-scale potential. Moreover, it was found that when $K < 0.74$, allowing only for the large-scale potential cannot satisfy the sample's electroneutrality equation. Here it is assumed that a fluctuation becomes screened, that is, the potential reaches the Fermi level, if only one donor is excessively charged.

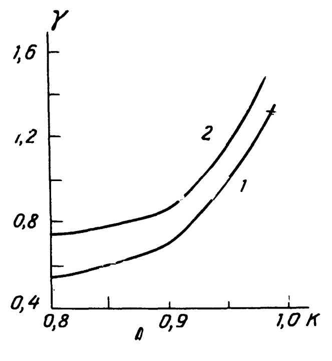

FIG. 7. The dispersion of the large-scale potential as a function of the compensation degree without allowance for the small-scale potential (curve 1) and with allowance for such a potential (curve 2) ($R_{sc} = 1$).

We have also established that the characteristic spatial size of a fluctuation potential coincides with $\bar{n}_{op}$ for the Gaussian distribution of impurities when $K\to 1$ (see the Appendix). For moderate compensation degrees ($0.8 < K < 0.95$) it is necessary to employ the Poisson distribution of impurities and to calculate the chemical potential μ using the value of the electrostatic energy of the semiconductor. At $K\approx 0.8$ the characteristic spatial scale approaches the average distance between impurities; that is, the potential ceases to be large-scale.

The density of the donor states has a Coulomb gap near the Fermi level and is close to the results of numerical modeling.[2]

Let us discuss the assumptions used in the model.

1. It was assumed that outside a fluctuation the potential tends to its average value $\bar{V}$ exponentially. In the present model this question can be evaded more precisely. Namely, by using the densities of donor and acceptor states we solve outside the fluctuation a Poisson equation in which the spatial distribution of the charge is determined by these densities.[5] This, however, would complicate the model considerably, since for each fluctuation we would have to solve numerically the Poisson equation outside the fluctuation with the parameters of n donors and m acceptors and then achieve additional self-consistency in the density of states.

The calculation results show that the value of the chemical potential greatly depends on the outer screening radius of a fluctuation, R_{sc}, and that the characteristic spatial size is practically independent of R_{sc}, except in the region where $K\to 1$ (Fig. 5).

Using the results of numerical modeling taken from Ref. 2 and comparing $\mu(K,R_{sc})$ with $\mu(K)$ obtained in Ref. 2, we can solve the inverse problem of finding $R_{sc}(K)$. Three characteristic points of the μ vs K dependence can be found from the points of intersection of curves 4–6 with curve 7 representing the results of numerical modeling (Fig. 4b). The values of R_{sc} obtained in the process range from 0.1 to 10 and are in my opinion reasonable. Note in this connection that it is wrong to use outside the fluctuation an unscreened potential that decreases like r^{-1} and corresponds to $R_{sc} = \infty$, as is often done in calculations of the probability density and the density of states of a potential (see Refs. 1 and 6).

2. It is usually assumed that the concentration is constant within a fluctuation. In Ref. 5 the effect of the concentration inhomogeneity of μ was calculated. A fluctuation of radius R was "partitioned" into two concentric regions of equal volume; in each region the concentration was assumed constant. It was found that the difference in the values of μ amounts to less than one percent. Allowance for small-scale fluctuations has practically no effect on the sensitivity of the calculation to the structure of the large-scale potential, that is, allowance for inhomogeneities in the concentration inside a fluctuation can be said to lead to deviations in μ of the order of one percent.

3. In allowing for small-scale fluctuations we limited our discussion to the case of two closely spaced donors. The case of two closely spaced acceptors is clearly unimportant when the parameter $|\mu/\Delta E_{d,a}|$ is much less than unity, with $\Delta E_{d,a}$ the energy interval between the donor and acceptor levels. The case of a pair of closely spaced donor and acceptor may lead to the violation of electroneutrality in the center of screened fluctuations. However, when the condition $1-K \ll 1$ is met, the "center of gravity" in the sample's electroneutrality equation (27) is shifted to the "small-scale" fraction of the neutral donors. Actually, as $K \to 1$, the small-scale fraction also tends to unity. This is directly corroborated by our calculations. For small-scale fluctuations it is easy to obtain a parameter that permits neglect of the probability of an acceptor landing in the region of closely spaced donors. The maximum separation r_μ, between a neutral donor and the nearest charged donor is determined by the sample's electroneutrality equation and is equal to[1]

$$r_\mu \approx [(1-K)/\bar{N}_d]^{1/3}. \tag{41}$$

According to Eqs. (1) and (2), the ratio of the probability W_3 of finding two donors and one acceptor in a volume of radius r_μ to the probability W_2 of finding only two donors in the same volume is

$$W_3/W_2 = K(1-K). \tag{42}$$

It is the smallness of this parameter that permits neglect of the direct effect of an acceptor on the charged state of a donor in small-scale fluctuations.

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APPENDIX

In Ref. 5 only the case with $R_{sc} = \infty$ was studied in detail. For this reason we now calculate R_{sc} for a Gaussian distribution in an interval of practical interest, $0.1 \leqslant R_{sc} \leqslant 10$.

Since the Poisson equation contains the difference (11) between the donor and acceptor concentrations, this difference can also be shown to be given by the Gaussian distribution:[5]

$$W_1(x) = \pi^{-1/2} \exp[-(x-x_0)^2], \tag{A1}$$

where

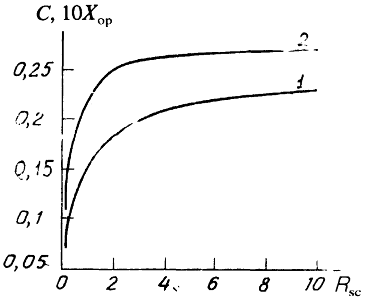

FIG. 8. C vs R_{sc} (curve *1*) and X_{op} vs R_{sc} (curve *2*) for a Gaussian distribution of impurities.

$$x_0 = \bar{n}^{1/2}(1-K)[2(1+K)]^{-1/2}, \quad x = (n-m)x_0/(1-K)\bar{n}.$$

According to (11), the charge density in terms of the x variables has the form $\rho = \bar{n}(1-K)x/x_0$. Substituting Eq. (A1) into the electroneutrality equation yields

$$\int_{x_1}^{\infty} x r_1^3(x) W_1(x)\, dx = x_0, \tag{A2}$$

where

$$x_1 = C/\delta x_0^{1/3}, \quad C = -\mu_0/E_d[(1+K)^2/2(1-K)]^{1/3}.$$

As in the case of the Poisson distribution, by solving Eqs. (10) and (A2) simultaneously we determine the dependence of the maximum energy μ_0 of a neutral donor (the Fermi level) on the partitioning radius x. The minimum of this quantity corresponds to the optimum partitioning radius X_{op}. The calculated dependences of X_{op} and C on R_{sc} are illustrated in Fig. 8. Using these calculations, we find the asymptotic behavior of the optimal size and the position of the Fermi level in the absence of the small-scale potential as $K \to 1$:

$$\bar{n}_{op} = 2X_{op}^2(1+K)/(1-K)^2, \tag{A3}$$

$$\mu_0 = -CE_d[(1+K)^2/2(1-K)]^{1/3}. \tag{A4}$$

Note that according to our calculations, the $\bar{n}_{op}(K)$ dependence defined by Eq. (A3) represents the asymptotic behavior of $\bar{n}_{op}$ as $K \to 1$ with allowance for the small-scale potential.

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