TRANSITION FROM METALLIC TO ACTIVATION CONDUCTIVITY IN COMPENSATED SEMICONDUCTORS

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A theory is developed for describing the transition from the metallic type of conductivity to the activation type occurring in strongly doped semiconductors under the influence of compensation. It is shown that for large degrees of compensation the electrons are distributed very inhomogeneously in space. They form metallic drops which are separated from each other by high, almost impenetrable potential barriers. Under such conditions, the static electric conductivity is of an activational nature in a broad temperature range. The dependence of the activation energy on the degree of compensation and the concentration of the major impurities is found. The critical degree of compensation at which the metal-nonmetal transition occurs is determined. The dependence of activation energy on degree of compensation near the transition point is also found.

1. It is well known that the introduction of compensating impurities into a strongly doped semiconductor can lead to loss of metallic conductivity. Typical experimental data are given, for example, in[1-3]. The samples investigated had metallic conductivity in the absence of compensation, i.e., a conductivity that was high and independent of the temperature. Starting with a certain degree of compensation, their conductivity acquired an activation character. The present paper contains a theory of this phenomenon that makes it possible to calculate the critical degree of compensation and the activation energy arising after the transition.

We consider a semiconductor doped with shallow donors. (For concreteness, we consider an n-type semiconductor.) We assume that the doping is strong, i.e., the Bohr radius of the electron on the isolated donor, a, is much larger than the average distance between donors ($Na^3 \gg 1$). Here N is the donor concentration, $a = h^2\kappa/me^2$, m is the effective mass, κ is the dielectric constant, and e is the electron charge. If the electron concentration n is equal to the donor concentration N (there is no compensation), then in the case of strong doping the electrons form a weakly-nonideal Fermi gas of high density and have metallic conductivity. (The impurity band is merged completely with the conduction band).

The charged impurities distort strongly the electronic states with energies $\epsilon < \gamma$ [4-6], where $\gamma = 2\sqrt{\pi}(e^2/\kappa r_0) \cdot (Nr_0^3)^{1/2}$ is the rms potential of the impurity-concentration fluctuations, and $r_0 = \frac{1}{2}a(\pi/3)^{1/6} \cdot (na^3)^{-1/6}$ is the radius of screening of the impurities by the electrons. If n = N, then at $Na^3 \gg 1$ the Fermi energy is $\mu = (3\pi^2)^{2/3}h^2n^{2/3}/2m \gg \gamma$, i.e., the electronic states close to the Fermi surface can be regarded as free.

If we introduce into the semiconductor acceptors with concentration N_A, then the electron concentration drops. We shall assume that the temperature is low compared with the width of the forbidden band, so that $n = N - N_A$. (We note that in our theory, the compensating impurity need not necessarily be shallow). With decreasing n, the Fermi energy μ decreases, and the potential of the impurities γ increases. We introduce a new parameter

$$\alpha = \mu/\gamma = (3\pi/4)^{3/4}(n/N)^{3/4}(Na^3)^{1/4}. \tag{1}$$

If $\alpha \gg 1$, then the Fermi level lies above the potential relief, and in the opposite case the potential energy of the electron quite frequently exceeds the Fermi energy, so that the electron concentration should be spatially inhomogeneous. This indeed leads to a loss of the metallic conductivity. We shall show in Sec. 3 that if $\alpha \ll 1$, then the electrons are gathered into metallic drops with a density that is almost independent of their average concentration and is determined by high barriers of low penetrability, and therefore the static electric conductivity of such a system has an activation character in a wide temperature interval. The critical concentration of the electrons, at which loss of metallic conductivity occurs, is connected with N by formula (27), which corresponds to the condition $\alpha \approx 1$.

In Secs. 2 and 3 we investigate the electron states at moderate ($\alpha \gg 1$) and very large ($\alpha \ll 1$) degrees of compensation. In Sec. 4 we investigate the static conductivity and find the activation energy at $\alpha \ll 1$.

2. In this section we formulate the necessary equations and investigate them in the simpler and more thoroughly investigated case $\alpha \gg 1$. We shall show that in the case of strong doping, all the significant potential fluctuations have a characteristic dimension much larger than the wavelength of the greater part of the electrons localized in these fluctuations. In other words, the potential wells produced by the fluctuations contain many levels. To describe such a system, it is natural to use the Thomas-Fermi self-consistent equation

$$\Delta\Psi = 4\pi e^2\kappa^{-1}[N(\mathbf{r}) - N_A(\mathbf{r}) - n(\mathbf{r})]. \tag{2}$$

Here Ψ is the potential energy of the electron on the curved bottom of the conduction band, and $N(\mathbf{r})$ and $N_A(\mathbf{r})$ are the local values of the donor and acceptor concentrations. The characteristic fluctuations will turn out to have a scale much larger than the mean distance between impurities, i.e., a large number of impurities

participate in the localization of the electrons. The impurity concentrations can therefore be regarded as smooth functions of the coordinates. For the local electron concentration n(r) we have

$$n(\mathbf{r}) = \begin{cases} (2m)^{3/2}(\mu - \Psi)^{3/2}/3\pi^2\hbar^3, & \mu > \Psi, \\ 0 & \mu < \Psi, \end{cases} \quad (3)$$

It is assumed here that $\mu - \Psi$ is so large for the greater part of the electrons that the electron gas can be regarded as ideal both in the sense of interelectron interaction and in the sense of interaction with small-scale fluctuations. It is also assumed that the unperturbed electron spectrum is isotropic and quadratic. We introduce $F(\Psi)$—the probability density of the quantity Ψ. Then the chemical potential μ is determined by the equation

$$n = \frac{(2m)^{3/2}}{3\pi^2\hbar^3} \int_{-\infty}^{\mu} (\mu - \Psi)^{3/2} F(\Psi) d\Psi, \quad (4)$$

which is valid if the main contribution to $F(\Psi)$ at all Ψ that are significant in (4) is made by fluctuations satisfying the conditions indicated above. By definition, we have

$$F(\Psi) = \left(\int e^{-\Omega\{\xi\}} D\xi \right)^{-1} \int e^{-\Omega\{\xi\}} \delta(\Psi - \Psi\{\xi\}) D\xi. \quad (5)$$

Here

$$\xi = N(\mathbf{r}) - N - (N_A(\mathbf{r}) - N_A) \quad (6)$$

and the functional integral is taken over all ξ. The quantity $\exp(-\Omega\{\xi\})$ is the probability of the fluctuation of ξ. We assume that the impurities are randomly distributed. For reasons given below, we are interested only in Gaussian fluctuations, for which

$$\Omega\{\xi\} = \frac{1}{2(N + N_A)} \int \xi^2 d^3r. \quad (7)$$

The functional $\Psi\{\xi\}$ is a solution of Eq. (5), vanishes at infinity, and is taken at a fixed point of space.

We shall show below that the indicated scheme for determining the Fermi level at zero temperature is applicable in case of strong doping for all degrees of compensation, i.e., for all values of α. However, the methods of solving the presented equations for small and large values of α should be entirely different.

In accordance with the statements made in Sec. 1, it can be assumed that $\Psi \ll \mu$ at $\alpha \gg 1$, and Eq. (2) can be linearized. Then its solution takes the form

$$\Psi(\mathbf{r}) = -\frac{e^2}{\kappa} \int \frac{\xi(\mathbf{r}') \exp\{- |\mathbf{r} - \mathbf{r}'|/r_0\} d^3r'}{|\mathbf{r} - \mathbf{r}'|}$$
$$r_0 = \frac{a}{2} \left(\frac{\pi}{3} \right)^{1/6} \frac{1}{(na^3)^{1/6}} \quad (8)$$

In this case the functional integral (5) is calculated exactly by integrating with respect to the Fourier components of the functions ξ. The result obtained in this manner coincides with the result of [4-6], where the case of uncompensated semiconductors was considered:

$$F(\Psi) = \frac{1}{\sqrt{\pi}\gamma} e^{-\Psi^2/\gamma^2}, \quad \gamma = 2\sqrt{\pi}\frac{e^2}{\kappa r_0}[(N + N_A)r_0^3]^{1/2}. \quad (9)$$

Calculating the Fermi energy with the aid of (4) and (9), it is easy to verify that it differs by an amount on the order of $\gamma^2/\mu = \mu/\alpha^2 \ll \mu$ from the Fermi energy of an ideal Fermi gas. It follows from (9) that the rms fluctuation of the potential energy of the electron is equal

to γ. Therefore linearization of (2) is possible only if $\mu \gg \gamma$, i.e., $\alpha \gg 1$. The characteristic dimension of the fluctuations that are significant in the calculation of the chemical potential is of the order of r_0. Such fluctuations can actually be considered with the aid of the Thomas-Fermi equation, since $\hbar^2/mr_0^2 \ll \gamma$, i.e., the typical potential wells contain many levels. Thus we see that at moderate compensation ($\alpha \gg 1$) the electron distribution remains spatially homogeneous and their conductivity has a metallic character.

3. We now consider the case of strong compensation $\alpha \ll 1$. We start from qualitative considerations that make it possible to determine the Fermi energy in this case. Since the Bohr radius of an isolated impurity is much larger than the mean distance between impurities, it is natural to assume that the electron wavelength extends over many impurities, and the impurity density can be regarded as a smooth function of the coordinates. This function contains fluctuations of all possible scales. The rms fluctuation of the number of impurities in a volume R^3 is $(NR^3)^{1/2}$, and the corresponding fluctuation of the potential energy of the test electron is $\gamma(R) \approx (e^2/\kappa R)(NR^3)^{1/2}$. We see therefore that the larger the scale of the fluctuations of the electron potential energy, the larger their amplitude. This estimate, however, does not take into account the electron redistribution, which cancels almost completely the impurity charge of the large-scale fluctuations. Indeed, the large-scale fluctuations have a low excess-charge density, on the order of $\sqrt{NR^3}/R^3$. If $n > (NR^3)^{1/2}/R^3$, then the electrons, becoming slightly redistributed over the crystal, neutralize the charge of the fluctuation and smooth out its potential completely. Consequently, fluctuations with dimension $R > R_c = N^{1/3}/n^{2/3}$ can have a space charge provided only the excess number of impurities is $Z \gg (NR^3)^{1/2}$. But the probability of such fluctuations is exponentially small, they make no contribution to the electron balance, and they can be disregarded in the calculation of the chemical potential.

At zero temperature, the electrons occupy the deepest regions of the potential relief, up to the Fermi level μ. In order to calculate μ, it is necessary to understand first how many electrons can be contained in an attracting fluctuation having a dimension R and an excess number Z of impurities. This number is limited for two reasons. First, it cannot exceed Z, otherwise the fluctuation is no longer attractive but repulsive. Second, it is limited as a result of the Pauli principle. The depth of the potential well is of the order of $e^2Z/\kappa R$, and the number of quantum states in it is $Z_q = Z^{3/2}(R/a)^{3/2}$. The ratio $Z_q/Z = Z^{1/2}(R/a)^{3/2}$ increases with Z. In the rms fluctuation $Z \approx (NR^3)^{1/2}$. Therefore for fluctuations having a scale $R > R_q$, where R_q is determined by the equations

$$(NR_q^3)^{1/4}(R_q/a)^{3/2} = 1, \quad R_q = a/(Na^3)^{1/5}, \quad (10)$$

the charge limitation is more important than the quantum limitation. It is easy to verify that $R_q \ll R_c$ when $\alpha \ll 1$.

We can now determine the chemical potential obtained if all the electrons are placed in potential wells having dimensions not larger than R, with $R_q \ll R \ll R_c$. It follows from this double inequality that wells of dimension R have a space charge and the quantum

limitation for them is unimportant. We break up the entire crystal into small cubes of volume R^3. The fraction of the cubes in which the excess number of impurities Z lies in the interval dZ is equal to $(NR^3)^{-1/2} \exp(-Z^2/NR^3)dZ$, and their number per unit volume is

$$g(Z)dZ = \frac{1}{(NR^3)^{1/2}} \exp\left\{-\frac{Z^2}{(NR^3)}\right\}\frac{dZ}{R^3} \qquad (11)$$

(These calculations are only estimates and do not take numerical factors into account.) If the small cube contains Z_e electrons, then the work that must be performed to remove one of them is of the order of $(Z - Z_e)e^2/\kappa R$. We have taken into account here the fact that the inhomogeneities with dimension smaller than R make no significant contribution to the potential. In equilibrium in all the cubes in which $Z_e > 0$, this work should be the same and equal to $-\mu$. Thus, we obtain for the number of electrons

$$Z_c = \begin{cases} Z - Z_\mu, & Z > Z_\mu, \\ 0 & Z < Z_\mu, \end{cases} \qquad (12)$$

where $Z_\mu = -\mu R\kappa/e^2$. We now obtain μ from the condition

$$n = \int_{Z_\mu}^{\infty} (Z - Z_\mu)g(Z)dZ. \qquad (13)$$

Substituting (11) in (13), we obtain

$$\mu = -\gamma(R)\left[\ln(R_c/R)^{3/2}\right]^{1/2}. \qquad (14)$$

We assume that the distribution of the impurities is correlated in such a way that there are no fluctuations with $R > R_0$. Then, if $R_q \ll R_0 \ll R_c$, we obtain from (14)

$$\mu = -\gamma(R_0)\left[\ln(R_c/R_0)^{3/2}\right]^{1/2}. \qquad (15)$$

If $R_0 < R_q$, all that changes in (16) is the factor under the logarithm sign. A logarithmic factor appears in (14) and (15) because the number of electrons that can be contained in an average cube is of the order of its charge, i.e., $(NR^3)^{1/2}$. But there are on the average nR^3 electrons for each cube. When $R \ll R_c$, the second number is smaller than the first and there are enough electrons only for a small number of cubes with the lowest potential. We shall henceforth consider only the case when there is no correlation in the arrangement of the impurities, or $R_0 \gg R_c$. It is seen from (14) that in this case the main lowering of the chemical potential is due to fluctuations with $R \approx R_c$ and

$$\mu = \delta\mu_0, \ \mu_0 \equiv \gamma(R_c) = e^2 N^{1/3}/\kappa n^{1/3}, \ \delta > 0, \qquad (16)$$

where δ is a numerical coefficient for which a calculation procedure will be given below. Electrons are contained in this case, roughly speaking, in half of the cubes with dimension R_c. Within the fluctuation of the dimension R_c, the distribution of the electrons is highly inhomogeneous (see the figure). If the cube of dimension R_c in which there are electrons is broken up into cubes of dimension $R \ll R_c$, then the greater part of the smaller cubes turns out to be empty.

In the foregoing arguments we took into account only Gaussian fluctuations having a scale larger than the average distance between the impurities. The probability of producing a potential well through a non-Gaussian fluctuation of the donor concentration is proportional to
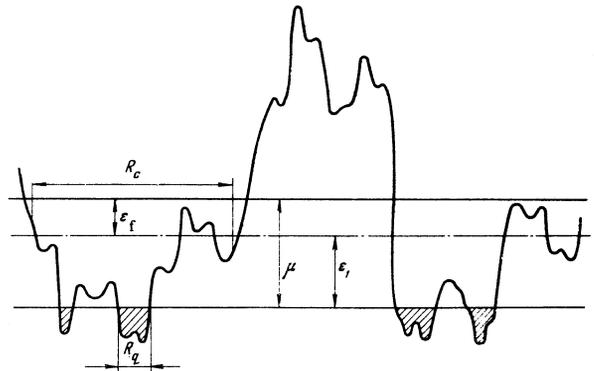
Energy scheme of compensated semiconductor. The sinuous line represents the bending of the bottom of the conduction band. The upper solid straight line is the mean value of the energy of the bottom of the conduction band. The lower solid line is the Fermi level. The dash-dot line is the flow-through region. The regions occupied by electrons are shown shaded.

$\exp(-Z\ln(Z/NV))$, where Z is the number of donors participating in the fluctuation and V is the volume of the fluctuation. Most probable among such fluctuations is a fluctuation representing a cluster of donors forming an almost pointlike nucleus of a multiply charged impurity atom[7,8]. In our case the energy of the singly-charged impurity center (donor) is small compared with μ_0. Therefore in order for a non-Gaussian fluctuation to give rise to a state lying below the Fermi level, it is necessary to have $Z \gg 1$. Such fluctuations have an exponentially small probability and can be disregarded.

In accord with the foregoing, the quantitative theory should be constructed with the aid of Eq. (2), in which it is meaningful to introduce the dimensionless variables

$$\chi = \frac{\Psi}{\mu_0}, \quad x = \frac{r}{R_c}, \quad \delta = \frac{\mu}{\mu_0}, \quad f(x) = \frac{\xi}{n}. \qquad (17)$$

In terms of these variables we obtain

$$\Delta_x\chi = 4\pi[f + 1 - \rho(x)], \qquad (18)$$

where

$$\rho(x) = \begin{cases} \dfrac{3^{1/2}}{2\pi^{1/2}\gamma^2\alpha^2}(\delta - \chi)^{1/2} & \chi < \delta, \\ 0 & \chi > \delta. \end{cases} \qquad (19)$$

Taking the foregoing into account, we shall regard $f(x)$ as a Gaussian random function with correlator

$$\langle f(x)f(x')\rangle = 2\delta(x - x'). \qquad (20)$$

(Higher correlators split into products of paired correlators). It follows from Eqs. (18) and (19) that when $\alpha \ll 1$, in the regions with $\rho(x) > 0$, the potential energy χ is very close to δ. It follows from (18) that, accurate to terms containing powers of α, the following condition should be satisfied in these regions:

$$\rho(x) = f + 1, \chi = \delta, \qquad (21)$$

i.e., in the regions where electrons are present, they neutralize fully the charge of the impurities. As a result, our problem has reduced in our approximation to the following:

Given a continuous charge density $f + 1$ in the entire crystal, find regions such that when the charge contained in them is completely neutralized, the potential produced by the remaining charge will be constant and equal to

$\delta(\chi = \delta)$ at all points of these regions, but larger than δ ($\chi > \delta$) at the remaining points of the crystal. In addition, the initial charge at all the points of the neutralized regions should be positive ($f + 1 > 0$). The chemical potential δ is determined from the neutrality condition, which states that the total uncompensated charge of the crystal is equal to zero. It is obvious from the very outset that if $f + 1 > 0$ in the entire crystal, then neutralization occurs likewise in the entire crystal and (21) is satisfied at all its points $\chi \equiv 0$ and $\delta = 0$. In fact, however, there exist such regions in which the random function $f < -1$. Consequently, complete neutralization is impossible, and if it is assumed that the mean value of χ is equal to zero, then the chemical potential $\delta < 0$.

The obtained system of equations (18) and (21) is purely classical and can be obtained from the condition that the Coulomb energy of the electron interaction with the impurities and with one another be minimal. This energy is given by

$$E\{q\} = -\iint \frac{q^2(x)(f(x')+1)}{|x-x'|} d^3x d^3x' \qquad (22)$$
$$+ \frac{1}{2}\iint \frac{q^2(x)q^2(x')}{|x-x'|} d^3x d^3x'.$$

To take into account the positiveness of the electron concentration $\rho(x)$ and at the same time impose no limitations on the class of the varied functions, we have introduced the notation $q^2(x) = \rho(x)$. Taking into account the constancy of the total number of electrons by the condition

$$\frac{1}{V}\int q^2(x) d^3x = 1, \qquad (23)$$

we should vary the functional $E\{q\} - \delta \int q^2(x)d^3x$. Here V is the volume of the integration region in (22) and (23), and δ is the Lagrange multiplier (in this case the chemical potential). The corresponding Euler equation is of the form

$$q(x)(\delta - \chi(x)) = 0, \qquad (24)$$

where

$$\chi(x) = \int \frac{f(x')-1-\rho(x')}{|x-x'|} d^3x'. \qquad (25)$$

It follows from (24) that in the regions where $\rho(x) \neq 0$, the energy $\chi(x) = \delta$, and consequently $\rho(x) = f(x) + 1$. It is easy to show that when (24) is satisfied the second variation is negative, provided only $\chi(x) > \delta$ wherever the density $\rho(x)$ vanishes. We have thus obtained an equivalent system of equations. The presence of a minimum of the functional (22) follows from the fact that this functional is bounded from below.

The characteristic dimension of the regions with potential δ is determined by the smallest scale used in simulating the function f. Let, for example, the δ function in (20) be smeared out over a length of order L (in dimensional units). Then the electrons form drops with dimension L and with a number of particles equal to the excess impurity charge of the drop, i.e., $(NL^3)^{1/2}$. The potential produced in the drop by a charge that is external with respect to it depends, of course, on the spatial distribution of the drops. It is produced, however, by large-scale fluctuations with a total charge on the order of $(NR_c^3)^{1/2}$, and the discreteness of the electron charge of the order of $(NR^3)^{1/2}$ has a negligible influence. Thus, when $L \ll R_c$ the chemical potential δ is independent of L. Since δ is determined from Eqs. (18), (19),

and (21), which contain no parameters, it is clear that $|\delta|$ is of the order of unity. We have thus obtained the result (16) and equations for the determination of the coefficient δ.

The proposed method for investigating Eq. (18) is based on the fact that the charge limitation is more important than the quantum limitation. Only a negligible fraction of the quantum states contained in each well are filled, and we are justified in assuming that the Fermi level coincides with the bottom of the well ($\delta = \chi$). As mentioned earlier, when $R < R_q$ the quantum limitation is important, and consequently χ cannot be regarded as constant in regions occupied by the electrons. This is seen formally from the fact that for a scale $R \approx R_q(x = \alpha^{8/9})$, in accordance with (18)—(20), we have $f \approx \alpha^{-4/3}$, $\chi - \delta \simeq \alpha^{4/9}$ and $\Delta\chi \approx \alpha^{-4/3}$, i.e., $\Delta\chi$ turns out to be of the same order as the remaining terms of (18). This circumstance, however, does not influence the calculation of δ, since $R_c \gg R_q$, and δ in fact ceases to depend on L when $L \ll R_c$. The quantum effects cause only the further breakup of the electron drops to cease when $L < R_q$. Indeed, the density of the electrons in a drop of dimension R_q is of the order of $(NR_q^3)^{1/2}/R_q^3$. It is easy to verify that the corresponding Fermi energy is of the order of the depth of the well $\gamma(R_q)$. The amplitude of the potential fluctuations with scale $L < R_q$, which equals $\gamma(L)$, is small compared with the Fermi energy of the drop reckoned from the local value of the potential (see the figure). Such fluctuations therefore produce little distortion of the electronic states in a drop of dimension R_q. In other words, it can be stated that there is no breaking up of a drop of dimension R_q, since the small drops located in the territory of the old drop do not have enough quantum states to accommodate all the electrons of the old drop.

Thus, the electrons are located in drops having a dimension on the order of R_q, with concentration $\bar{n} \approx (NR_q^3)^{1/2}/R_q^3 = N/(Na^3)^{1/3}$. The drops are very unevenly distributed in space, and there exist inhomogeneities of any dimension from R_q to R_c.

The applicability of Eqs. (18) and (19) to such a system follows from the fact that the number of states in a well of dimension R_q and depth $\gamma(R_q)$ is large, and from the fact that $\bar{n}a^3 \gg 1$, i.e., the electrons form a weakly nonideal Fermi gas. It is also easy to verify that when $\alpha \ll 1$ the concentration in the drop is much larger than the average concentration ($\bar{n} \gg n$) and that $R_q \gg N^{-1/3}$.

4. Let us see now how the static electric conductivity changes as a function of α. It is obvious that when $\alpha \gg 1$ it has a metallic character. When $\alpha \ll 1$ the main obstacle to the conductivity is the large-scale fluctuations of the potential with amplitude μ_0 and dimension R_c. The tunneling transparency of such a relief contains

$$\exp\{-\sqrt{m\mu_0}R_c / \hbar\} = \exp\{-(Na^3)^{1/6}\alpha^{-10/9}\},$$

i.e., it is very small. Therefore an important role is assumed by the question whether an electron with a given energy can pass through the crystal and circumvent the humps of the potential relief. In analogy with[9], we introduce a flow-through energy ϵ_f such that an electron with ϵ_f can pass through the entire crystal and be at all times in the classically accessible region, but at a lower energy this is impossible. The probability-theory prob-

lem of finding ϵ_f should be solved with the aid of the classical equations (18), (20), and (21). (For details concerning the mathematical formulation of the problem see[9].) Inasmuch as these equations do not contain parameters, the result takes the form

$$\epsilon_f - \mu = \nu_0 \mu_0, \tag{26}$$

where ν_0 is the numerical coefficient. Since in the classical problem the potential can in general not be smaller than μ, it is clear that ν_0 is nonnegative. In addition, $\nu_0 \neq 0$, since for any $L \ll R_c$ the regions in which the electrons are located occupy a negligible fraction of the total volume of the crystal and cannot be connected with one another. Thus, $\nu_0 > 0$.

At temperatures $T < \epsilon_1$, where $\epsilon_1 = \nu_0 \mu_0$, the conductivity can be realized as a result of thermal flinging of the electrons onto the flow-through level. This conductivity is proportional to $\exp(-\epsilon_1/T)$. In principle, this mechanism can experience competition on the part of the conductivity of the electrons situated at the Fermi level and resulting from quantum tunneling. As is well known, the very existence of such a conductivity at $T = 0$ is problematic[10]. We shall not discuss this question here, but note only that the conductivity over the Fermi level should contain a tunnel-induced small quantity of the type $\exp\{-(Na^3)^{1/9}/\alpha^{10/9}\}$, and we confine ourselves to the temperature region $T > T_1$, where $T_1 = \epsilon_1 \alpha^{10/9}/(Na^3)^{1/9}$, in which the activation conductivity undoubtedly prevails over the tunnel conductivity.

The activation energy ϵ_1, according to (16), is of the order of $e^2 N^{2/3}/\kappa n^{1/3}$, i.e., it increases with increasing degree of compensation and concentration of the main impurities. This result was obtained under the assumption that $Na^3 \gg 1$. The activation energy ϵ_1 in the opposite limiting case, as shown in[9], is equal to $\hbar^2/2ma^2 + \nu_1 \mu_0$, where ν_1 is the numerical coefficient. At $Na^3 = 1$ and $n \ll N$ we have $\hbar^2/2ma^2 \ll \nu_1 \mu_0$. Therefore both results are of the same order of magnitude when $Na^3 = 1$.

We have discussed above the conductivity in the cases $\alpha \gg 1$ and $\alpha \ll 1$. Let us see now how the transition from metallic to the nonmetallic conductivity occurs. Equations (18)–(20) depend only on one parameter α. We have shown that the quasiclassical description is applicable for $\alpha \gg 1$ and $\alpha \ll 1$. However, when $\alpha \approx 1$ we also have $\sqrt{m\mu_0} R_c/\hbar \gg 1$, i.e., the potential wells contain many levels, and the tunneling transparency of the humps is small. We can therefore determine the Fermi level $\mu(\alpha)$ at all values of α with the aid of (18)–(20). In addition, at all α we can introduce the flow-through energy $\epsilon_p(\alpha)$.

Let us define $\nu(\alpha)$ by the relation $\epsilon_f(\alpha) - \mu(\alpha) = \nu(\alpha)\mu_0$. As $\alpha \to 0$, we have $\nu(\alpha) \to \nu_0$, and when $\alpha \gg 1$, it becomes negative. The loss of metallic conductivity occurs at the point α_c at which $\nu(\alpha_c) = 0$, with α_c being, of course, of the order of unity. It follows from (1) that the critical concentration of the electrons is connected with the concentration of the main impurities by the relation

$$n_c = 0.43 N^{1/3} \alpha_c^{4/3}/a. \tag{27}$$

The activation energy is $\epsilon_1 > 0$ at $n < n_c$ and vanishes when $n = n_c$. The number α_c must be determined in accordance with the indicated procedure with the aid of a computer.

It is easy to determine the behavior of the activation energy ϵ_1 near the transition, when $0 < (n_c - n)/n_c \ll 1$. Indeed, the point α_c is not a singular point for each of the functions $\mu(\alpha)$ and $\epsilon_f(\alpha)$. (The point α_c is not a point of thermodynamic phase transition.) Therefore both functions can be expanded in series about the point α_c, and their derivatives at this point, generally speaking, are not equal to each other. We therefore readily obtain

$$\epsilon_1 = (n - n_c) \left[\frac{d\epsilon_f}{dn} - \frac{d\mu}{dn} \right]_{n=n_c}$$

for $(n_c - n)/n_c \ll 1$. We note that the mobility threshold at the energy ϵ_f has a quantum smearing connected with the fact that at energies barely below the threshold the tunneling probability is not small. It is easy to verify, however, that this smearing is of the order of T_1 and can be disregarded in the temperature region $T > T_1$ under consideration.

In conclusion, let us discuss the question of experimental verification of the conclusions of the theory. The experimental data given in[2-3] show how the conductivity of Ge and GaAs changes under the influence of compensation from metallic (independent of the temperature) into activational. The experimentally observed activation energy ϵ_1 increases with decreasing n and reaches very large values (100 meV in[2] and 300 meV in[3]). In[2], the dependence of ϵ_1 on n has been investigated in detail. It is seen that ϵ_1 increases more rapidly than in accordance with the law $\epsilon_1 \sim n^{-1/3}$ predicted by us. This circumstance is possibly connected with the considerable errors that arise in the determination of the electron concentration n in samples with large degrees of compensation[11].

To verify relation (27), which connects the concentrations of the electrons and the impurities at the transition point, it is necessary to perform experiments in which both concentrations would vary. It is then desirable to use semiconductors with small carrier effective masses, so that n and N can vary in wide ranges at the transition point.

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