Electron capture by shallow neutral impurities in semiconductors

E. B. Goldgur[1)] and R. I. Rabinovich

Moscow State Pedagogical Institute and Moscow Institute of Petrochemical and Gas Industry
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We consider electron capture by shallow neutral impurity centers. The center potential is defined by a decay length $a \sim a_B$, a depth $U \sim E_B$, and a binding energy for the "extra" electron $E_i \ll U$ (a_B and E_B are the effective Bohr radius and the Bohr energy). The cross sections are calculated for inelastic capture with emission of an acoustic phonon for electrons with energy $\varepsilon \ll U$ ("slow") and with emission of an acoustic or optical phonon for electrons with $\varepsilon \gg U$ ("fast") at $kT \ll E_i$. It is shown that owing to the inelasticity of the process the lifetime of the slow electrons with respect to capture by neutral centers can, in contrast to the case of cascade capture [M. Lax, Phys. Rev. **119**, 1502 (1960); V. N. Abakumov *et al.*, Sov. Phys. JETP **44**, 345 (1976) and **45**, 354 (1977); Soviet Phys. Semicond. **12**, 1 (1978)], be much smaller than the acoustic relaxation time of the energy. A comparison with the experimental data is made.

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I. INTRODUCTION

In semiconductors doped with shallow impurities, whose degree of compensation (K) is not very small, the electron (hole) lifetime at low temperatures $T \ll E_B$ is usually determined by the capture by the attracting Coulomb centers ($E_B = h^2/2ma_B^2$ is the Bohr energy, a_B is the effective Bohr radius, and T is the temperature in energy units). Several mechanisms of capture by such centers with emission of acoustic and optical (of frequency ω_0) phonons were discussed in the literature (see, e.g., Refs. 1–4). For electrons with wave vector $\mathbf{k}$ and with energy $\varepsilon = \hbar^2 k^2/2m < \hbar\omega_0$, the main contribution to recombination is made by the so-called quasielastic cascade capture mechanism. A model for it was proposed by Lax,[1] who subdivided the capture process in two stages: landing of an electron of energy ε on the center in a state with binding energy $\sim T$, and "sticking" of the electron. Correspondingly, there were introduced the "differential" capture cross sections $\sigma(\varepsilon)$ that depend on the electron energy, and the lifetime $\tau(\varepsilon)$. Abakumov, Perel', and Yassievich[2] have pointed out an error in Lax's arguments. According to them, capture of an electron having an energy $\varepsilon_0 \gg T$ after photoexcitation by a Coulomb center constitutes a continuous descent of the electron in energy as a result of emission of "shallow" acoustic phonons with energy

$$\hbar\omega_q = \hbar sq \sim (ms^2\varepsilon)^{1/2} \ll \varepsilon$$

(s is the speed of sound). In this case the electron drops to the bottom of the band and is captured by one of the highly excited Coulomb states whose distribution is quasicontinuous. Through them it descends to a level with binding energy $\gtrsim T$, from which a return by thermal ejection is unlikely. The capture cross section σ_+ is determined mainly by the classical radius r_T of the orbit, with binding energy $\sim T$, $r_T = e^2/\varkappa T$ ($\varkappa$ is the dielectric constant). Direct capture from a band into bound states is, according to Refs. 2 and 3, relatively small. The carriers manage therefore to become thermalized prior to the capture, and with increase of the density N_+ of the attracting centers the carrier lifetime is limited from below by the energy relaxation time τ_ε, $\tau_\varepsilon(\varepsilon) \propto \varepsilon^{-1/2}$, taken at the energy $\varepsilon = E_n$: $\tau \geqslant \tau_\varepsilon(E_n)$, where $E_n \sim e^2 N^{1/3}/\varkappa$ is the mean squared fluctuation of the impurity potential.[2)] For a quasielastic cascade capture, therefore, a lifetime that depends on the electron energy is meaningless, and the photoelectron distribution energy $F(\varepsilon)$ decreases monotonically with the energy.[2]

On the other hand, it is well known that in semiconductors at $T \ll E_B$ there is possible an inelastic capture of electrons (holes) directly from the band by shallow neutral impurities; this capture leads to formation of H^--like centers (see, e.g., Ref. 5 and the references therein). This capture mechanism has hardly been discussed in theoretical papers. Only one note[6] cites computer-obtained values of the cross section for capture of equilibrium electrons in Ge and Si by shallow neutral donors with emission of acoustic phonons. The experimental data (see, e.g., Refs. 7–10) offer evidence in favor of the assumption that this capture mechanism can exert a substantial influence on the carrier lifetime. Moreover, according to Ref. 11, in doped and weakly compensated n- and p-Si samples such a capture mechanism can bring about a situation wherein the lifetime τ is much shorter than the acoustic energy relaxation time τ_ε, and this leads to an inverse free-carrier distribution function.

We consider in this paper inelastic capture of electrons (holes) by shallow hydrogenlike neutral impurity centers. From the analogy with the hydrogen atom and with its negative ion H^- it follows that the neutral-center potential has a depth $U \sim E_B$ and a decay length $a \sim a_B$, and that in such a potential there is one "ionic" level for the "extra" electron, with binding energy E_i:

$$E_i \equiv \hbar^2/2ma_i^2 \approx 0.055 E_B \ll U, \tag{1}$$

where a_i is the decay length of the wave function of the extra electron.[12,13] In experiment, donors with an "extra" electron (D^-) and acceptors with an extra hole (A^+) were observed in a number of studies (see the review[5]). We consider below the capture of an "extra" carrier directly into a bound "ionic" state as a result of an inelastic process, namely spontaneous emission of one acoustic or optic phonon with energy

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$\hbar\omega_q = \varepsilon + E_i$.

We assume that the temperature is low enough,

$$T \ll E_i, \tag{2}$$

so that the thermal return of the captured electrons to the conduction band is insignificant. We restrict from above the density N of the neutral centers by the condition that the overlap of the extra-electron wave functions be small:

$$Na_i^3 \ll 1. \tag{3}$$

In addition, we assume that the influence of the Coulomb potential of the charged centers on the free and bound electrons, as well as the binding energy of the ion state, can be neglected, i.e., that

$$e^2 N_+^{1/3}/\varkappa \ll E_i. \tag{4}$$

Depending on the electron energy, two cases will be considered: capture of "slow" electrons with $ka \ll 1$ (i.e., $\varepsilon \ll \hbar^2/2ma^2$) upon emission of acoustic phonons, and capture of "fast" electrons with $ka \gg 1$ upon emission of acoustic or optical phonons. We calculate the cross sections $\sigma_0^{(A)}, \sigma_0^{(0)}$ corresponding to these processes, and the lifetimes $\tau_0^{(A)}, \tau_0^{(0)}$. It is shown that when (2)–(4) are satisfied for electrons with $ka \ll 1$ the relative contribution of the capture by neutral centers increases with increasing N (at $K = \text{const}$) and in the case of small compensations ($K \ll 1$) and low temperatures the capture by neutral centers becomes predominant. It will also be shown that, owing to the inelasticity of the capture process, the time $\tau_0^{(A)}$ due to the inelasticity of the capture process can be much less than the energy relaxation time τ_ε for electrons with $ka \ll 1$ at sufficiently large N but satisfying (3). It makes sense therefore to introduce for this mechanism an energy dependent lifetime $\tau_0(\varepsilon)$, so that the form of the photoelectron distribution function $F(\varepsilon)$ is determined, in contrast to the case of cascade capture,[1,2] by the value and energy dependence of $\tau_0(\varepsilon)$ (see, e.g., Ref. 14). In the last section we discuss the possibilities of observing capture by neutral centers and the available experimental data.

We note that in Ref. 6 the cross section $\sigma_0^{(A)}$ was calculated with a variational function of the bound state. The wave function of the free electron was taken to be a plane wave. An equilibrium electron distribution was assumed. No analytic expressions were obtained in Ref. 6 for $\sigma_0^{(A)}$. Our results and those of Ref. 6 will be compared below.

II. CAPTURE OF SLOW ELECTRONS WITH EMISSION OF ACOUSTIC PHONONS

1. We consider capture of electrons having a wave vector such that $ka \ll 1$. We assume here that $a \ll a_i$, so that the condition $ka \ll 1$ is valid not only at $\varepsilon \lesssim E_i$ but also at $\varepsilon > E_i$. The effective mass is assumed scalar, and the multivalley character of the band structure (Ge,Si) and the degeneracy of the valence band are neglected. The dispersion law of the acoustic phonons is assumed linear, and the impurity centers hydrogenlike.

For slow electrons, the short-range potential of a neutral atom can be approximated by a zero-radius potential (δ potential). This is equivalent to the following boundary condition on the functions of the free and bound states[12,13]:

$$\lim_{r\to 0} \frac{1}{r\psi}\frac{d}{dr}(r\psi) = -\frac{1}{a_i}. \tag{5}$$

The bound-state wave function $\psi_i(\mathbf{r})$ is then

$$\psi_i(\mathbf{r}) = (2\pi a_i)^{-1/2}\frac{\exp(-r/a_i)}{r}. \tag{6}$$

The plane-wave approximation cannot be used for the wave function of a free electron. The reason is, as will be shown below, that the main contribution to the capture is made by the region of distances $r < a_i$, where the influence of the potential of the center is significant. In the δ-potential approximation this influence reduces to the fact that only the phase $\delta_0(k)$ of the s component of the wave function $\psi_k(\mathbf{r})$ differs from zero[13]:

$$\delta_0(k) = \operatorname{arctg}(-ka_i). \tag{7}$$

The wave function for the free electron, orthogonal to (6) and corresponding to boundary condition (5), is of the form

$$\psi_k(\mathbf{r}) = V^{-1/2}\left[e^{i\mathbf{kr}} + \frac{f}{r}e^{ikr}\right], \tag{8}$$

where

$$f = \frac{\exp(2i\delta_0(k)) - 1}{2ik} = \frac{-a_i}{1+ika_i} \tag{9}$$

is the scattering amplitude,[13] and V is the normalization volume; the second term of (8) describes the scattered wave.

2. We assume that capture takes place only with spontaneous emission of the deformation acoustic phonons (see Ref. 2). Then the probability of a transition from the state $\psi_k(\mathbf{r})$ (8) into a state $\psi_i(\mathbf{r})$ (6) is given by

$$W_{ki} = \frac{2\pi}{\hbar}\frac{V}{(2\pi)^3}\int d\mathbf{q}\,|M_q|^2\delta(\hbar\omega_q - \varepsilon - E_i), \tag{10}$$

where

$$M_q = iE_c\left(\frac{\hbar\omega_q}{2Vs^2\rho}\right)^{1/2}\int \psi_k^*(\mathbf{r})\,e^{i\mathbf{qr}}\psi_i(\mathbf{r})\,d\mathbf{r}, \tag{11}$$

E_c is the deformation-potential constant and ρ is the crystal density.

Before we calculate the matrix element (11), we estimate certain characteristic parameters. The phonon emitted after capture has a wave vector $q = (E_i + \varepsilon)/\hbar s$, so that the parameter qa_i is large:

$$qa_i = \frac{E_i + \varepsilon}{\hbar s}a_i = \left(\frac{E_i}{2ms^2}\right)^{1/2}\left(1 + \frac{\varepsilon}{E_i}\right) \gg 1. \tag{12}$$

Actually, the quantity $(E_i/2ms^2)^{1/2}$ for hydrogenlike centers does not depend on the effective mass and can be rewritten in the form

$$\left(\frac{E_i}{2ms^2}\right)^{1/2} = \frac{1}{2}\frac{a_B}{a_i}\frac{e^2}{\varkappa\hbar s}.$$

For typical semiconductors (Ge,Si), the "fine-structure constant" $e^2/\varkappa\hbar s$ is large, ~ 25. It follows then from (1) that $(E_i/2ms^2)^{1/2} \sim 3$, so that qa_i is several times larger than unity even at $\varepsilon < E_i$. It is also easy to verify that the ratio k/q is

small,

$$\frac{k}{q}=\left(\frac{2ms^2}{E_i}\right)^{1/2}\begin{cases}(\varepsilon/E_i)^{1/2}, & \varepsilon\ll E_i\\ (E_i/\varepsilon)^{1/2}, & \varepsilon\gg E_i\end{cases}. \tag{13}$$

At $\varepsilon\sim E_i$ we have

$$\frac{k}{q}\sim\frac{1}{2}\left(\frac{2ms^2}{E_i}\right)^{1/2}. \tag{13a}$$

M_q was calculated accurate to terms of zeroth and first order in $(qa_i)^{-1}$ and k/q. For the integral in (11)

$$I_{ki}=\int\psi_{\mathbf{k}}^{*}(\mathbf{r})\,e^{i\mathbf{q}\mathbf{r}}\psi_i(\mathbf{r})\,d\mathbf{r};$$

we then obtain

$$|I_{ki}|=\frac{(2\pi^3a_i^3)^{1/2}}{V^{1/2}}\frac{1}{qa_i}\left(1-\frac{4}{\pi qa_i}\right), \tag{14}$$

where qa_i is given by (12). The first term in (14) takes into account the contribution to the matrix element from the scattered wave, and the second from the plane wave. It can be seen that $|I_{ki}|$ (14) is determined principally by the scattered wave. The reason is that the main contribution to I_{ki} is made by the distance region $r\lesssim q^{-1}$, where $|f/r|\sim|qa_i/(1+ika_i)|$. According to (12) and (13), $|qa_i/(1+ika_i)|\gg 1$ at all values of ka_i.

Substituting (14) in (11) and (10), we obtain the capture coefficient $\alpha_0^{(A)}(\varepsilon)=v(\varepsilon)\sigma_0^{(A)}(\varepsilon)$:

$$\alpha_0^{(A)}(\varepsilon)\equiv W_{ki}V=\frac{\pi^2E_c^2}{\rho\hbar s^2}\left(\frac{E_i}{2ms^2}\right)^{1/2}\varphi\left(\frac{\varepsilon}{E_i},\beta\right), \tag{15}$$

where

$$\beta=\frac{4}{\pi}\left(\frac{2ms^2}{E_i}\right)^{1/2},\quad \varphi(x,\beta)=(1+x)\left(1-\frac{\beta}{1+x}\right)^2,$$

and $v(\varepsilon)=(2\varepsilon/m)^{1/2}$ is the velocity of an electron with energy ε. It follows from (15) that the capture coefficient increases almost linearly with the electron energy at $\varepsilon>E_i$, and is practically independent of ε at $\varepsilon\ll E_i$. Following Ref. 2, we introduce the characteristic length l_0, which is connected with the mean free path l and with the energy-relaxation time $\tau_\varepsilon(\varepsilon)$:

$$l_0=\frac{\pi\rho\hbar^4}{2m^3E_c^2}=\frac{T}{2ms^2}l=v(\varepsilon)\tau_\varepsilon(\varepsilon). \tag{16}$$

The capture cross section for electrons with energy ε takes then the form

$$\sigma_0^{(A)}(\varepsilon)=\frac{2\pi^3}{l_0}a_i^3\left(\frac{E_i}{2ms^2}\right)^{1/2}\left(\frac{E_i}{\varepsilon}\right)^{1/2}\varphi\left(\frac{\varepsilon}{E_i},\beta\right). \tag{17}$$

Accordingly we obtain from (17) an expression for the "differential lifetime" of electrons with energy ε:

$$\frac{1}{\tau_0^{(A)}(\varepsilon)}=\frac{2\pi^3}{\tau_\varepsilon(\varepsilon)}Na_i^3\left(\frac{E_i}{2ms^2}\right)^{1/2}\left(\frac{E_i}{\varepsilon}\right)^{1/2}\varphi\left(\frac{\varepsilon}{E_i},\beta\right). \tag{18}$$

The possibility of introducing a lifetime independent of the electron energy will be confirmed below (cf. Ref. 2).

3. We analyze now expressions (17) and (18). To this end we put $\varepsilon\sim E_i$ in (17), so that

$$\sigma_0^{(A)}\sim\frac{2\pi^3}{l_0}a_i^3\left(\frac{E_i}{2ms^2}\right)^{1/2}.$$

In the case of cascade capture of equilibrium electrons by attracting centers, cross section $\sigma_+^{(A)}$ takes the form $\sigma_+^{(A)}=4\pi r_T^3/3l_0$ (r_T as defined in the Introduction). It can be seen that $\sigma_0^{(A)}$, just as $\sigma_+^{(A)}$, is determined by the sphere of the radius of the capturing orbit and by the ratio of this radius to l_0. The cross section $\sigma_0^{(A)}$, however, in contrast to $\sigma_+^{(A)}$, contains also the factor $(E_i/2ms^2)^{1/2}$, which amounts to several times ten for typical semiconductors. It stems from the following. Owing to the "condensation" of $\psi_k(\mathbf{r})$ near the δ center (see Ref. 12) there appears in the matrix element, as already mentioned, an additional factor $\sim qa_i$ compared with the plane-wave case. It is this which increases the cross section by $(qa_i)^2\sim E_i/2ms^2$ times. In addition, the factor r_T/l_0 in $\sigma_+^{(A)}$, which is the ratio of the time of flight of the electrons through a sphere of radius r_T to the energy-relaxation time $\tau_\varepsilon(T)$, corresponds to $\sigma_0^{(A)}$ to the factor $(a_i/l_0)(E_i/2ms^2)^{1/2}$. Expressing l_0 in terms of the time $\tau_c(\varepsilon)$ of the spontaneous emission of acoustic phonons:

$$\tau_c(\varepsilon)=\left(\frac{4ms^2}{\varepsilon}\right)^{1/2}\tau_\varepsilon(\varepsilon)\approx l_0\frac{2^{1/2}ms}{\varepsilon},$$

and for the electrons with $\varepsilon\sim E_i$ we obtain

$$\frac{a_i}{l_0}\left(\frac{E_i}{2ms^2}\right)^{1/2}\sim\frac{a_i}{v(E_i)\tau_c(E_i)},$$

i.e., this is the ratio of time of flight through the sphere to the time of spontaneous emission of acoustic phonons. For transitions from the free state into the bound one, the time τ_c is in essence the time of energy relaxation, since the electron loses all its energy at once.

It follows from (18) that even at $Na_i^3\ll 1$ the time of direct capture of an electron from the band by the impurity centers can be much shorter than the energy relaxation time $\tau_\varepsilon(\varepsilon)$, i.e., an electron optically excited to energies $\varepsilon_0\gg T$ can be captured before it manages to "cool off" substantially as a result of collisions with acoustic phonons. It is this which justifies the introduction of the energy-dependent cross section $\sigma_0^{(A)}$ (17) and the lifetime $\tau_0^{(A)}(\varepsilon)$ (18).

We recall that in the case of quasielastic cascade capture the electron "cooling" is faster than the capture, and no introduction of energy-dependent cross sections and times is possible; the photoelectron distribution function then coincides with the energy (Ref. 2). If the direct capture of the electrons directly from the band is faster than their cooling, the form of the photoelectron distribution function is determined by the value and energy dependence of the ratio $\tau_\varepsilon(\varepsilon)/\tau(\varepsilon)$, where $\tau(\varepsilon)$ is the lifetime of an electron with energy ε.[14] In particular, if $\tau_\varepsilon(\varepsilon)/\tau(\varepsilon)>1$ at $\varepsilon\gg T$, an inverse distribution function is possible.[14,11] (The mechanism of the capture was not specified in Ref. 14.)

4. We compare now the coefficients of capture by neu-

tral ($\alpha_0^{(A)}$) and attracting ($\alpha_+^{(A)}$) centers in the case of low density $N_+, N_+ \ll r_T^{-3}$. We shall assume that the carriers have an equilibrium distribution, and use for $\alpha_0^{(A)} = \sigma\langle v\rangle$ an interpolation formula[2] that gives correct expressions at $T \gg ms^2$ and $T \ll ms^2$ ($\langle v\rangle$ is the velocity averaged over the distribution):

$$\alpha_+^{(A)} \approx \frac{4}{3}\pi\frac{\langle v\rangle}{l_0}\left(\frac{e^2}{\varkappa T}\right)\left[\frac{e^2}{\varkappa(T+2{,}74ms^2)}\right]^2. \qquad (19)$$

From (15) and (19) we obtain for electrons with $\varepsilon \sim T$

$$\frac{\alpha_0^{(A)}}{\alpha_+^{(A)}} \sim 0.1\left(\frac{T}{E_B}\right)^{1/2}\frac{(T+2.74ms^2)^2}{E_B^{1/2}(2ms^2)^{1/2}}. \qquad (20)$$

It was indicated above the real values of the ratio $E_i/2ms^2 \lesssim 10$. The upper bound (2) on the temperature means then in fact that capture by neutral centers is significant only at $T \lesssim 2ms^2$. The right-hand side of (20) is then $\lesssim 10^{-2}$, so that the lifetime is determined by capture by neutral centers only at degrees of compensation $K < 10^{-2}$.

We proceed now to compare the lifetimes $\tau_0^{(A)}$ and $\tau_+^{(A)}$ for the case when the impurity density and the degree of compensation K are such that the density of the attracting centers is $N_+ = KN_D > r_T^{-3}$ (we have in mind an n-type semiconductor, and N_D is the donor density). Then $\tau_+^{(A)}$ takes on the minimum value $\tau_{+\min}^{(A)} \sim \tau_\varepsilon(E_n)$. Let for the sake of argument $E_n \sim T$ and $\tau_{+\min}^{(A)} \sim \tau_\varepsilon(T)$; further increase of E_n, i.e. of the density of the attracting centers, decreases $\tau_+^{(A)}$ insignificantly, $\tau_+^{(A)} \propto N_+^{-1/6}$ (Ref. 2). For electrons with energy $\varepsilon \sim T \ll E_i$ we then have $\tau_0^{(A)}(T) \ll \tau_+^{(A)}(T)$ at

$$Na_i^3 \equiv N_D(1-K)a_i^3 \gg \left(\frac{2ms^2}{E_i}\right)^{1/2}\frac{1}{2\pi^3}\left(\frac{T}{E_i}\right)^{1/2}\left(\frac{1}{1-\beta}\right)^2. \qquad (21)$$

At $(2ms^2/E_i)^{1/2} \sim 0.3$, $T/E_i \sim 0.2$, $\beta \sim 0.5$ the right-hand side of (21) is $\sim 10^{-3}$. Thus, when the density of the principal impurity is increased and the condition $N_+ = KN_D \sim r_T^{-3}$ is reached, capture by neutral centers becomes substantial also in the case of moderate compensation.

III. CAPTURE OF FAST ELECTRONS WITH EMISSION OF ACOUSTIC AND OPTICAL PHONONS

1. We consider capture of electrons whose energy satisfies the condition $ka \gg 1$, with spontaneous emission of acoustic phonons. We assume here that M_q satisfies as before expression (11) with a linear dispersion law. For electrons with $ka \gg 1$ the wave function $\psi_k(\mathbf{r})$ can be chosen to be a plane wave. We then get from (10) and (11)

$$(\tau_0^{(A)})^{-1} = \alpha_0^{(A)}N \approx 32\pi\frac{1}{l_0}Na_i^3\left(\frac{E_i}{\varepsilon}\right)\left(\frac{E_i}{2ms^2}\right)^{1/2}\left(\frac{2E_i}{m}\right)^{1/2}. \qquad (22)$$

Introducing again the time $\tau_\varepsilon(\varepsilon)$, we obtain from (22)

$$(\tau_0^{(A)})^{-1} \cong \frac{32\pi}{\tau_\varepsilon(\varepsilon)}Na_i^3\left(\frac{E_i}{\varepsilon}\right)^{1/2}\left(\frac{E_i}{2ms^2}\right)^{1/2}. \qquad (23)$$

Since the energy of electrons with $ka \gg 1$ exceeds E_i considerably, the lifetime (23) is much longer than that of the "slow" electrons (18) at the same values of Na_i^3). In addition, when (3) is satisfied, $\tau_0^{(A)}$ (23) exceeds τ_ε. The fast electrons are thus cooled more rapidly than they are captured.[3)]

2. We proceed to consider capture of fast electrons with emission of optical phonons. We neglect the dispersion of the optical phonons and assume that their frequency $\omega(q) \approx \omega(0) \approx \omega_0$. We recognize that $\hbar\omega_0$ is usually several times larger than the Bohr energy, so that the wave function of an electron with energy $\varepsilon \sim (\hbar\omega_0 - E_i)$ can be taken in the form of a plane wave. The corresponding matrix element of the transition can be obtained from (7) and (8) by making the substitutions $\hbar\omega_q \to \hbar\omega_0$, $E_c \to E_{\text{opt}}$, where E_{opt} is the constant of the deformation interaction with the optical phonons.

After simple calculations we obtain in analogy with Ref. 3

$$W_{ki} = \frac{\pi E_{\text{opt}}^2\omega_0}{\rho s^2 V}\delta(\varepsilon - \hbar\omega_0 + E_i). \qquad (24)$$

In the case of dispersionless optical phonons, capture is possible only for electrons with energy $\varepsilon \approx \hbar\omega_0 - E_i$. The capture probability turns out to be the same as in the case of capture by the ground state of a Coulomb center (see Ref. 3). We obtain the lifetime with respect to capture with emission of optical phonons, assuming that the density $\rho(E')$ of the impurity levels is smeared near the energy $(-E_i)$:

$$\rho(E') = V\frac{N}{\pi}\frac{\gamma}{\gamma^2 + (E' + E_i)^2}, \quad E' \sim (-E_i), \qquad (25)$$

and the distribution $F(\varepsilon)$ of the photoelectrons in the band is described by a δ function:

$$F(\varepsilon) \propto \delta(\varepsilon - \hbar\omega_0 - E'). \qquad (a)$$

For the lifetime we obtain

$$(\tau_0^{(0)})^{-1} = \frac{E_{\text{opt}}^2\omega_0}{\rho s^2}\frac{N}{\gamma}. \qquad (26)$$

The energy smearing of the impurity level γ, $\gamma \ll E_i$, can be due to the finite time τ_i, $\gamma \sim \hbar/\tau_i$, of the electron on this level, as a result of jumps to the neighboring central center,[5] or to the broadening of the levels on account of the fields of the charged centers. The behavior of the capture coefficient

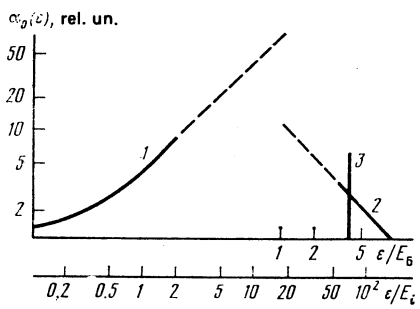

FIG. 1. Capture coefficient vs electron energy. Curve 1—plot of $\alpha^{(A)}(\varepsilon)/\alpha_0^{(A)}(0)$ according to (15) at $\beta = 0.5$; curve 2—plot of $\alpha_0^{(A)}(\varepsilon)/\alpha_0^{(A)}(10E_B)$ according to (22). The peak at $\varepsilon = 4E_B$ (3) corresponds to the coefficient of capture with emission of optical phonons (in relative units $10^{-3}\alpha_0^{(0)}/\alpha_0^{(A)}(0)$, see the text).

as a function of the electron energy, in accord with (15), (22), and (26), is shown in the figure for $(E_{opt}/E_c)^2 = 10$, $\gamma = 0.2\ E_i$, $\hbar\omega_0 = 4\ E_B$. The data on $\alpha_0^{(A)}(\varepsilon)$ are listed in the table (their calculation is discussed in Sec. IV). In the calculation of $\alpha_0^{(A)}(\varepsilon)$ it was assumed that $a \approx 0.5a_B$, while relations (15) and (22) are valid for $qa \lesssim 1$ [i.e., $\varepsilon \lesssim 2E_i$, see Eq. (12)] and for $\varepsilon > 3E_B$. The dashed lines are extrapolations of Eqs. (15) and (22) to regions of higher and lower energies, respectively.

IV. NUMERICAL ESTIMATES. COMPARISON WITH EXPERIMENT

1. Numerical estimates of the coefficients for capture by neutral centers with emission of acoustic phonons were obtained for the case of electron capture by donors in Ge and Si and of holes by acceptors in Si. The deformation-potential constants were expressed in terms of the experimentally known (see Ref. 2) length l_0. The obtained values of $\alpha_0^{(A)}$ for $\varepsilon \ll E_i$ together with the data of Ref. 6 are given in the table. The first line corresponds to the case when the wave function in the band is plane, and the second to the wave function (8). The following experimental values of E_i were used in the calculations (see Ref. 5): $E_i = 0.57$ meV (Sb) and 0.75 meV (As) for donors in Ge, $E_i = 1.7$ meV (P) for donors in Si, and $E_i = 2$ meV (B) for acceptors in Si. It can be seen from the table that allowance for the correct behavior of the wave function at $r \lesssim a_i$ increases $\alpha_0^{(A)}$ by 3–10 times and changes the dependence of $\alpha_0^{(A)}$ on E_i [see the data on Ge(Sb) and Ge(As)].

2. The experimental data on the influence of the density of the neutral centers on the lifetime are available for n-Si and p-Si.[7-11] For electrons and holes in Si, according to (1), $a_i \sim 80$–100 Å, so that the conditions (2) and (3) are satisfied at $N \ll 10^{18}$ cm^{-3} and $T \ll 20$ K. The capture coefficients obtained in Refs. 7, 8, and 10 at $T = 4.2$ K amount to $\sim 10^{-7}$ cm^3/sec, or several times smaller than the theoretical values in the table. It must be noted, however, that the experimental data of Ref. 8 were reduced using for the extra carrier a binding energy 4.7–5 meV, which is much higher than E_i. This may be due to violation of condition (4) in the investigated samples. A detailed study of the lifetime as a function of the densities of the attracting (N_-) and netural centers was carried out in Ref. 9 on p-Si with impurity photoexcitation. It was observed that in samples with $N = 5\times10^{15}$–1.2×10^{16} cm^{-3} and with compensation 0.1–1.7% the lifetime at $T = 4.2$ K is much shorter than in samples with the same N_- but larger N. This proves, in our opinion, that capture by neutral centers predominates. We note also that the values of τ obtained in Ref. 9 for these samples are lower than $\tau_\varepsilon(T)$. The dependences of τ on N were measured in Ref. 11 for samples of weakly compensated n-Si and p-Si. It was observed that starting with certain values $N > N_1$ the weak $\tau(N)$ dependence typical of cascade capture[2] gives way to an abrupt decrease of τ to values much less than $\tau_\varepsilon(E_n)$. This was attributed to the fact that at $N > N_1$ a new recombination channel via neutral centers is "turned on" (see below).

3. We have not discussed above the subsequent fate of an electron captured by a neutral center. The point is that at temperatures satisfying Eq. (2), in the absence of photoexcitation, there are no "extra" electrons on the neutral centers. Therefore the electrons captured in the "ionic" state are those excited either from the valence band (interband brightening, see Ref. 7), or from the ground state of the impurity (impurity brightening, see Refs. 5 and 9), so that capture by the neutral center is only the first stage of recombination. For the density of the neutral centers not to decrease in stationary photoexcitation, the "extra" electrons captured by them must recombine with the hole rapidly during the interband brightening. In the case of impurity photoexcitation in samples with low compensation, the electron can return to the "initial" state in the following way: By hopping over neutral centers with emission of acoustic phonons, the electron approaches a positively charged donor D^+, forms a complex $D^- - D^+$ which is the analog of the hydrogen molecule in the ionic state, and then recombines.[5,10] The corresponding recombination channel can be called "indirect," in contrast to the "direct" one, which is captured by an attracting center. It is clear that an indirect recombination channel can be realized only in the case when the hopping probability

TABLE I. Coefficients of captures by neutral centers (cm^3/sec) at $\varepsilon \ll E_i$

Material and type of carrier	Ge	Si	
	electrons	holes	electrons
$\psi_k(\mathbf{r})$ – plane wave	$3.1\cdot10^{-7}$ (Sb) $2.9\cdot10^{-7}$ (As)	$0.95\cdot10^{-7}$ (B)	$1.45\cdot10^{-7}$ (P)
$\psi_k(\mathbf{r})$ – plane + scattered wave (8)	$2.6\cdot10^{-6}$ (Sb) $3.5\cdot10^{-6}$ (As)	$3.15\cdot10^{-7}$ (B)	$7.45\cdot10^{-7}$ (P)
According to Ref. 6 at T = 2K*	$3\cdot10^{-7}$		$0.8\cdot10^{-7}$

*Note. The value of $\sigma_0^{(A)}$ in accord with Ref. 6 was obtained from the plots given in that reference for the temperature dependence of the capture cross sections, averaged over the equilibrium distribution.

$W_h \propto \exp(-t/N^{1/3}a_i)$, $t \sim 1$, greatly exceeds the probability $W_T \propto \exp(-E_i/T)$ of the reverse thermal ejection of the electron into the conduction band, and there is a sufficiently large probability W_R of recombination of a $D^- - D^+$ complex with distance $R \sim N^{-1/3}$ between the "nuclei."[5] It follows therefore that an indirect recombination channel can be realized at helium temperature only if the neutral-center density is high enough, $N > N_1$. It is impossible to indicate the theoretical value of N_1 since there are no theoretical estimates of W_R; Experimental data on N_1 are given in Ref. 11.

It must be noted that a decrease of τ with increasing N is possible at $N \ll N_1$ when the ionic states of the neutral centers are almost completely isolated. In this case capture by the neutral centers leads to an increase of the density of the attracting centers and by the same token to a decrease of τ_+ (Refs. 15 and 16).

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[1)]Moscow Institute of Petrochemical and gas industry.
[2)]The function $\tau_\varepsilon(\varepsilon)$ as written here pertains to electron interaction with only strain-induced acoustic phonons.
[3)]If it is assumed that $a \sim a_B$ and Eqs. (18) and (23) are valid at $ka \sim 1$, the ratio of the lifetimes of the fast and slow electrons at $ka_B \sim 1$ turns out to be $(E_i/2ms^2)(E_B/E_i)^2$. This is simply $(qa_i)^2$ at $q \sim E_B/\hbar s$.

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