on point-charge calculations of A_2^0 in several of host lattices were D for Fe^{3+} is known. Also, the recent work of Lyubimov *et al.*[26] has shown that higher multipole terms which have been neglected in the point-charge calculation can make sizable contributions to the electric field gradients in ionic crystals.

The g value of 2.0019 is slightly less than the free-ion value and is in excellent agreement with the value 2.0020 calculated by Wantanabe.[6] The positive sign of the cubic crystal-field splitting parameter $a=24B_4^4$ is also in agreement with the theoretical predictions of Watanabe[6] (remembering that O_4^4 changes sign on rotating 45° from the susceptibility axis system to the distorted cubic axis system).

ACKNOWLEDGMENTS

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[26] V. N. Lyubimov, Yu. N. Venevtsev and E. Yu. Koiranskaya, Kristallografiya **7**, 949 (1962) [English transl.: Soviet Phys.—Cryst. **7**, 768 (1963)].

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Theory of Absorption of Electromagnetic Radiation by Hopping in n-Type Silicon and Germanium

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The absorption of electromagnetic radiation at 0°K in the wavelength region from 100 to 800 μ and from 500 μ to 2.5 cm in n-type silicon and germanium, respectively, has been investigated. Concentrations of donors up to 2×10^{18} cm^{-3} in Si and 6×10^{16} cm^{-3} in Ge, and compensation ratios up to 0.2, were considered. The model used was that of photon-induced hopping of an electron between the ground states of the donors. The formula for the absorption coefficient is derived and numerical results are presented. The range of validity of our results is also discussed. Absorption coefficients of the order of 10^2 cm^{-1} in Si and 10^1 cm^{-1} in Ge were obtained.

INTRODUCTION

THE ac impurity hopping conduction has been studied, both experimentally and theoretically, up to the frequencies of the order of 10^9 cps.[1–4] The model used was that of phonon-induced hopping of a carrier from the neutral majority impurity center to the ionized one. Both Coulomb potential of the nearest ionized minority center and the external field were taken into account to obtain the energy differences for these transitions.

The purpose of the present work is to study another mechanism of hopping, namely, the photon-induced transitions and their effect on the absorption of electromagnetic radiation in n-type Si and Ge at 0°K. We are interested in the wavelength region from 100 to 800 μ and from 500 μ to 2.5 cm in Si and Ge, respectively. In these wavelength regions at 0°K other absorption mechanisms (lattice vibrations, excitations of neutral impurity centers, free carriers) are, in principle, absent. The occurrence of absorption induced by carriers generated by impact ionization of neutral impurities can be also avoided for low intensities of radiation.

Tanaka and Fan in their paper[4] proposed the photon-induced hopping for explanation of a part of their experimental results concerning the ac impurity conduction in p-type Si at wavelengths larger than 3 cm. Apart from the fact that we are interested in n-type materials, our approach is unapplicable to their case because we consider the electron-phonon interaction to be weak. This is not true, however, if the relaxation energy of the lattice deformed by interaction with the localized carrier is larger than the energy difference $\hbar\omega$ for transition, which is the case in p-type Si at wavelengths larger than about 2 mm.[5,5a]

In the following we shall obtain first the electron states in the two-center Hamiltonian in a nondeformed crystal lattice with an additional electrostatic field. Then we obtain the transition rate for photon-induced

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[1] M. Pollak and T. H. Geballe, Phys. Rev. **122**, 1742 (1961).

[2] M. Pollak, Phys. Rev. **133**, A564 (1964).

[3] S. Golin, Phys. Rev. **132**, 178 (1963).

[4] S. Tanaka and H. Y. Fan, Phys. Rev. **132**, 1516 (1963).

[5] J. Mycielski, Phys. Rev. **125**, 1975 (1962).

[5a] *Note added in proof.* Recently the idea of Tanaka and Fan was developed by S. Tanaka, M. Kobayashi, E. Hanamura, and K. Uchinokura [Phys. Rev. **134**, A256 (1964)] in a way similar to ours. They do not investigate, however, our case $kT\ll\hbar\omega$ and they use several approximations absent in our treatment. They compare their results with the experimental data for Si at 9 Gc/sec and that seems to be unjustified (see above).

hopping, taking into account the weak electron-phonon interaction. At last, the formula for the absorption coefficient is derived and numerical results are presented. The range of validity of our results is also discussed.

Unfortunately, as far as we know, no experimental data complete enough are available (although the infrared transmission of n-Ge at helium temperatures was measured up to wavelength of 1.4 mm[6]), and thus our results cannot be compared with experiment at the present time.

ELECTRON STATES IN THE TWO-CENTER HAMILTONIAN

Because of the valley-orbit splitting, the ground state of an isolated shallow donor in silicon and germanium is a singlet.[7] The valley-orbit splitting in silicon[7] is 1.2×10^{-2} eV, 1.5×10^{-2} eV, and 2.2×10^{-2} eV for Sb, P, and As donors, respectively. For germanium, we have 5.7×10^{-4} eV, 2.9×10^{-3} eV, and 4.15×10^{-3} eV for Sb, P, and As donors, respectively.[8–10] Because of the rather large values of this splitting, we can take into account in our wavelength regions only the ground singlet state of the donor, at least for P and As impurities. The wave function of the electron on this state is[11]

$$u(\mathbf{r})=n^{-1/2}\sum_{p=1}^{n}F_p(\mathbf{r})\phi_p(\mathbf{r}).$$

Here n denotes the number of conduction band minima (6 and 4 for Si and Ge, respectively), $\phi_p(\mathbf{r})$ is the Bloch function at the pth minimum, and $F_p(\mathbf{r})$ is the effective-mass envelope function for the pth minimum. The functions $F_p(\mathbf{r})$ can, to a good approximation, be represented by the functional form

$$F_p(\mathbf{r})=(\pi a^2b)^{-1/2}\exp\{-[(x_p^2+y_p^2)/a^2+z_p^2/b^2]^{1/2}\}.$$

The constant a is the transverse orbit radius while b is the longitudinal radius of the orbit. The coordinates x_p, y_p, z_p are taken in a coordinates system in which the z axis is parallel to the axis containing the pth minimum.

Now we are interested in obtaining the two lowest electron states in the two-center Hamiltonian in a nondeformed crystal lattice. The total Hamiltonian has the form

$$H=T+V-e^2/\epsilon r_a-e^2/\epsilon r_b. \tag{1}$$

Here V denotes the potential due mainly to the negatively charged acceptor nearest to the donors a and b, T denotes the Hamiltonian for an electron in an ideal crystal, ϵ is the static dielectric constant and $\mathbf{r}_a$ and $\mathbf{r}_b$ are

$$\mathbf{r}_a=\mathbf{r}-\mathbf{R}_a,\quad \mathbf{r}_b=\mathbf{r}-\mathbf{R}_b,$$

where $\mathbf{R}_a$ and $\mathbf{R}_b$ are the positions of the two donor ions. Without reducing the generality we can assume that

$$\Delta=\langle u(\mathbf{r}_a)|V|u(\mathbf{r}_a)\rangle-\langle u(\mathbf{r}_b)|V|u(\mathbf{r}_b)\rangle\geqslant0.$$

Following the variational procedure applied to this problem by Miller and Abrahams,[12] we obtain the two lowest orthonormal states of the Hamiltonian (1) in the form

$$\psi_a(\mathbf{r})=c_a{}^{+}u(\mathbf{r}_a)+c_b{}^{+}u(\mathbf{r}_b), \tag{2}$$

$$\psi_b(\mathbf{r})=c_a{}^{-}u(\mathbf{r}_a)+c_b{}^{-}u(\mathbf{r}_b), \tag{3}$$

where $c_a{}^{\pm}$ and $c_b{}^{\pm}$ are

$$c_a{}^{\pm}=z^{\pm}[1+(z^{\pm})^2+2Sz^{\pm}]^{-1/2},$$
$$c_b{}^{\pm}=[1+(z^{\pm})^2+2Sz^{\pm}]^{-1/2}.$$

Here

$$z^{\pm}=(\Delta/2W)[1\pm(1+4WS/\Delta+4W^2/\Delta^2)^{1/2}].$$

The following abbreviations were used:

$$W=W_R-\tfrac{1}{2}S\Delta+Z, \tag{4}$$
$$W_R=L-SJ,$$
$$L=-\langle u(\mathbf{r}_a)|e^2/\epsilon r_a|u(\mathbf{r}_b)\rangle,$$
$$J=-\langle u(\mathbf{r}_a)|e^2/\epsilon r_b|u(\mathbf{r}_a)\rangle,$$
$$S=\langle u(\mathbf{r}_a)|u(\mathbf{r}_b)\rangle,$$
$$Z=\langle u(\mathbf{r}_a)|V|u(\mathbf{r}_b)\rangle-\tfrac{1}{2}S[\langle u(\mathbf{r}_a)|V|u(\mathbf{r}_a)\rangle+\langle u(\mathbf{r}_b)|V|u(\mathbf{r}_b)\rangle].$$

W_R is the resonance energy; L, S, and Z will be real in our materials at least if both the donor ions have the positions in the elementary cells of the crystal. Of same course, Δ and J are also real.

The function $\psi_a(\mathbf{r})$ has a larger amplitude near the ion a and the function $\psi_b(\mathbf{r})$ near the ion b. The higher energy corresponds to the state $\psi_a(\mathbf{r})$; the energy difference between the two states is

$$\Delta E=(1-S^2)^{-1}(\Delta^2+4W^2+4WS\Delta)^{1/2}. \tag{5}$$

We shall not assume that $\Delta\gg|W_R|$ as was done by Miller and Abrahams[12] in the theory of dc impurity hopping conduction.

Now we shall investigate the photon-induced transitions between the states $\psi_b(\mathbf{r})$ and $\psi_a(\mathbf{r})$, i.e., hopping of the electron from the donor b to the donor a.

TRANSITION RATE

We assume that the dielectric constant appropriate for our wavelength regions is equal to the static dielectric constant ϵ. We take into account the weak interaction of electrons with longitudinal acoustic phonons. A single deformation potential constant and a

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[6] A. Hadni, J. Claudel, E. Décamps, X. Gerbaux, and P. Strimer, Compt. Rend. **255**, 1595 (1962).

[7] D. K. Wilson and G. Feher, Phys. Rev. **124**, 1068 (1961).

[8] H. Fritzsche, Phys. Rev. **120**, 1120 (1960).

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[10] H. Fritzsche, Phys. Rev. **115**, 336 (1959).

[11] W. Kohn, in *Solid-State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1957), Vol. 5, p. 257.

[12] A. Miller and E. Abrahams, Phys. Rev. **120**, 745 (1960).

Debye spectrum of phonons will be assumed. The transition rate at 0°K from an arbitrary electron bound state b to the electron bound state a with absorption of a photon is according to the formalism developed for weak electron-phonon interaction by Lax, Burstein, and Gummel[13,14]

$$W_{ab}=(4\pi^2e^2/c\hbar^2\epsilon^{1/2})\exp(-\beta)|\langle a|\mathbf{r}|b\rangle\mathbf{n}|^2I(-\omega_0). \quad (6)$$

We neglect here the processes consisting of simultaneous absorption of a photon and emission of phonons; these will be investigated in another paper.

We denote by $\mathbf{n}$ the unit vector parallel to the electric vector of radiation and by $I(\omega)$ the intensity of the radiation per unit interval of the angular frequency ω. At 0°K,

$$\beta=\int_0^\infty f(\omega')d\omega', \quad (7)$$

where $f(\omega')$ is the distribution function for the lattice relaxation phonons; for $\omega'>0$:

$$f(\omega')=(E_1{}^2\omega'/16\pi^3\hbar v^5d)\int|\langle a|\exp(i\omega'\mathbf{\Omega}\mathbf{r}/v)|a\rangle - \langle b|\exp(i\omega'\mathbf{\Omega}\mathbf{r}/v)|b\rangle|^2d\Omega.$$

E_1 denotes the deformation potential constant, v is the sound velocity and d is the density of the crystal. $\mathbf{\Omega}$ is a unit vector parallel to the wave vector of the phonon; we perform the integration over all directions of this vector.

ω_0 is given by

$$-\hbar\omega_0=\Delta E+(E_1{}^2/16\pi^3v^2d)\times\int_0^\infty d\tau\tau^2\int d\Omega[|\langle b|\exp(i\tau\mathbf{\Omega}\mathbf{r})|b\rangle|^2 - |\langle a|\exp(i\tau\mathbf{\Omega}\mathbf{r})|a\rangle|^2], \quad (8)$$

where ΔE is a positive electronic energy difference between the states a and b (in nondeformed crystal lattice). The second term in (8) represents the difference of the lattice relaxation energies in the two electronic states.

Let us now identify the state a with the state $\psi_a(\mathbf{r})$ and the state b with the state $\psi_b(\mathbf{r})$. If

$$S<0.03, \quad (9)$$

$$\omega'R/v>3, \quad (10)$$

where $\mathbf{R}=\mathbf{R}_b-\mathbf{R}_a$, we obtain

$$f(\omega')\cong(E_1{}^2\omega'/2\pi^2\hbar v^5d)(\Delta^2+4S^2W^2)(\Delta^2+4W^2)^{-1}\times U(\omega'/v). \quad (11)$$

Here

$$U(\tau)=(4\pi)^{-1}\int|\langle u(\mathbf{r})|\exp(i\tau\mathbf{\Omega}\mathbf{r})|u(\mathbf{r})\rangle|^2d\Omega.$$

In the derivation of (11) we neglected, because of (10), the expression $\langle u(\mathbf{r})|\exp(i\omega'\mathbf{\Omega}\mathbf{r}/v)|u(\mathbf{r}-\mathbf{R})\rangle$ in comparison with $S\langle u(\mathbf{r})|\exp(i\omega'\mathbf{\Omega}\mathbf{r}/v)|u(\mathbf{r})\rangle$ and the contribution from the oscillating term proportional to $\cos(\omega'\mathbf{\Omega}\mathbf{R}/v)$. From (7) and (11) we obtain

$$\beta=(\Delta^2+4S^2W^2)(\Delta^2+4W^2)^{-1}\beta_0$$

where by definition

$$\beta_0=(E_1{}^2/2\pi^2\hbar v^3d)\int_0^\infty U(\tau)\tau d\tau.$$

$f(\omega')$ in the form (11) was used here for all $\omega'>0$ because in view of (9) the contribution to (7) from ω''s nonfulfilling (10) is negligible.

Inserting (2) and (3) into (8) and using (9) we can see that the second term in (8) is at most of the order of SE_{LR} where E_{LR} is the relaxation energy of the lattice deformed by interaction with an electron localized on an isolated donor[5]

$$E_{\mathrm{LR}}=(E_1{}^2/4\pi^2v^2d)\int_0^\infty U(\tau)\tau^2d\tau.$$

As mentioned above, we can use the formalism of Lax, Burstein, and Gummel (i.e., treat the electron-phonon interaction as a weak one) if the energy of lattice relaxation is small compared with the electronic energy difference between the two states. Accordingly, we shall assume

$$\Delta E>2E_{\mathrm{LR}}. \quad (12)$$

Hence, from (12), (9), and (5)

$$\omega_0\cong-\Delta E/\hbar,\quad \Delta E\cong(\Delta^2+4W^2)^{1/2}.$$

Using (2), (3), and (9) we have

$$|\langle a|\mathbf{r}|b\rangle\mathbf{n}|^2=(\mathbf{Rn})^2(W+\tfrac{1}{2}S\Delta)^2(\Delta^2+4W^2)^{-1}.$$

Summarizing, under the assumptions (9) and (12) the hopping rate is

$$W_{ab}=(4\pi^2e^2/c\hbar^2\epsilon^{1/2})\exp[-\beta_0(\Delta^2+4S^2W^2)\times(\Delta^2+4W^2)^{-1}](W+\tfrac{1}{2}S\Delta)^2(\Delta^2+4W^2)^{-1}\times(\mathbf{Rn})^2I[(\Delta^2+4W^2)^{1/2}/\hbar]. \quad (13)$$

ABSORPTION COEFFICIENT

We shall investigate the case of small compensation

$$K<0.2. \quad (14)$$

Only the donors nearest to the compensating ionized acceptors are ionized at 0°K. Let us investigate at the moment the electron jumps to an ionized donor situated (at the point $\mathbf{R}_a$) in the vicinity of a given compensating center. These jumps occur from the neutral donors (we denote the position of a neutral donor by $\mathbf{R}_b$).

Because of (14) we can assume that all donors except the one nearest to our acceptor are neutral and that the potential V is the Coulomb potential of this ionized

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[13] M. Lax and E. Burstein, Phys. Rev. **100**, 592 (1955).

[14] H. Gummel and M. Lax, Ann. Phys. (N. Y.) 2, 28 (1957).

acceptor. We shall therefore neglect the dipole potentials of other ionized acceptor-ionized donor pairs present in the crystal. This assumption will be discussed later.

If the origin of the spatial coordinates is at the acceptor ion, the probability that the donor nearest to this ion is in the element of volume dv_a and that there is a neutral donor in the element $dv_b(R_b>R_a)$ is equal to $N^2\exp(-4\pi NR^3{}_a/3)dv_a dv_b$, N being the concentration of donors.

Multiplying by W_{ab}, integrating over $\mathbf{R}_a$, $\mathbf{R}_b(R_b>R_a)$ and multiplying by the concentration KN of acceptors we obtain the total number of jumps per unit of time and volume. Using $I(\omega)$ in the form of δ function and multiplying by the energy $\hbar\omega$ of photons we have the following formula for the absorption coefficient:

$$\alpha=\hbar\omega KN^3\int dv_a\exp(-4\pi NR_a{}^3/3)\int_{R_b>R_a}dv_b W_{ab}. \quad (15)$$

W_{ab} is given by the formula (13) where

$$I[(\Delta^2+4W^2)^{1/2}/\hbar]$$

is replaced by $\delta[\omega-(\Delta^2+4W^2)^{1/2}/\hbar]$. The assumption (12) can now be rewritten as

$$\hbar\omega>2E_{\mathrm{LR}}. \quad (16)$$

If β_0 is not much larger than unit, we can, using (9), replace in the exponent in (13) $\Delta^2+4S^2W^2$ by Δ^2. Assuming that in the region of the two donors a and b the field of the acceptor is homogeneous enough we can neglect Z in (4). This assumption will be discussed later. It enables us also to put

$$\Delta\cong(e^2/\epsilon)(1/R_a-1/R_b).$$

Now we make the following approximation. We replace in formula (15) $W_R{}^2$ and S^2 by their values $\langle W_R{}^2\rangle_{\mathrm{av}}$ and $\langle S^2\rangle_{\mathrm{av}}$ averaged over all directions of the vector $\mathbf{R}$. According to Miller and Abrahams,[12] for n-type Si and Ge we obtain

$$\langle S^2\rangle_{\mathrm{av}}=(\pi^{1/2}/18n\eta^{1/2})(R/a)^{7/2}\exp(-2R/a),$$
$$\langle W_R{}^2\rangle_{\mathrm{av}}=(2\pi^{1/2}e^4/9\epsilon^2a^2n\eta^{1/2})(R/a)^{3/2}\exp(-2R/a).$$

Here

$$\eta=(a/b)^2-1.$$

These formulas are correct, if (9) in the form

$$\langle S^2\rangle_{\mathrm{av}}{}^{1/2}<0.03 \quad (17)$$

holds. Using (17), changing the variables in (15) and integrating over four of them we obtain finally (R and R_a have the same meaning as before)

$$\begin{aligned}\alpha=&(32\pi^4\epsilon^{1/2}KN^3/3c\hbar)\\ &\times\int_{R(\omega)}^{\infty}R^3\langle W_R{}^2\rangle_{\mathrm{av}}(\hbar^2\omega^2-4\langle W_R{}^2\rangle_{\mathrm{av}})^{-1/2}\\ &\times\exp[-\beta_0(\hbar^2\omega^2-4\langle W_R{}^2\rangle_{\mathrm{av}})/\hbar^2\omega^2]\\ &\times l[R,(\hbar^2\omega^2-4\langle W_R{}^2\rangle_{\mathrm{av}})^{1/2}]dR, \quad (18)\end{aligned}$$

with

$$l(R,E)=\int_{R_{a1}}^{R_{a2}}R_a{}^4(1-\epsilon R_aE/e^2)^{-3}\times\exp(-4\pi NR_a{}^3/3)dR_a, \quad (19)$$

where

$$R_{a1}=e^2/\epsilon E+\tfrac{1}{2}R-(e^4/\epsilon^2E^2+\tfrac{1}{4}R^2)^{1/2},$$
$$R_{a2}=(e^2R/\epsilon E+\tfrac{1}{4}R^2)^{1/2}-\tfrac{1}{2}R.$$

$R(\omega)$ is larger of the two solutions of the equation

$$2(\langle W_R{}^2\rangle_{\mathrm{av}})^{1/2}=\hbar\omega$$

if these solutions exist, or equals a if these solutions do not exist or when the larger of them is smaller than a.

The assumption (17) was essential for the derivation of the formula (18). Therefore, we can use this formula, if the contribution from the range of R in which (17) is not fulfilled does not play the main role in the absorption.

In formula (18) we neglected the contribution from the pairs for which the distance between donors is smaller than a. We are in the position to do so because, on the one hand, the assumption (17) is not fulfilled for such Rs and, on the other hand, such pairs do not really give any contribution to the absorption. The reason for this is that the energy difference between the two lowest electron states in the case $R<a$ will be of the order of the ionization energy of an isolated donor.[15] Of course we are not interested in the case of such high photon energies.

We shall now discuss the assumption used before that the field of the acceptor is homogeneous so that we can neglect Z in (4). This, as well as the whole procedure of obtaining the two-center electronic states, cannot be justified in the case of jumps "through" the acceptor (Z is then of the order of W_R). One can show that in (19) the values of R_a close to R_{a1} corresponds to such jumps. Because $\langle W_R{}^2\rangle_{\mathrm{av}}$ decreases rapidly with increasing R, the main contribution to the absorption is given by R's not far from $R(\omega)$. For such R's the value of R_{a1} is not higher than about $\frac{1}{2}R(\omega)$. Therefore, if the function $R_a{}^4\exp(-4\pi NR_a{}^3/3)$ has the maximum at $R_a>\frac{1}{2}R(\omega)$ we can suppose that the contribution from the jumps "through" the acceptor can be neglected. There from the restriction

$$N<8/\pi R^3(\omega). \quad (20)$$

Now we show that for the most important region of R's, i.e., these not far from $R(\omega)$, the main contribution is given by $R_a\lesssim(\pi N)^{-1/3}$, $(\pi N)^{-1/3}$ being the position of the maximum of the function $R_a{}^4\exp(-4\pi NR_a{}^3/3)$. Under the condition (20) we have $R_{a1}\lesssim(\pi N)^{-1/3}$. If also $R_{a2}\lesssim(\pi N)^{-1/3}$, our supposition is obviously true. Therefore, we shall study the case $R_{a2}\gg(\pi N)^{-1/3}$.

Using the facts that, on the one hand, we are interested in the case of photon energies much smaller than the ionization energy of the donor and, on the other

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[15] D. R. Bates, K. Ledsham, and A. L. Stewart, Phil. Trans. Roy. Soc. London A246, 215 (1953).

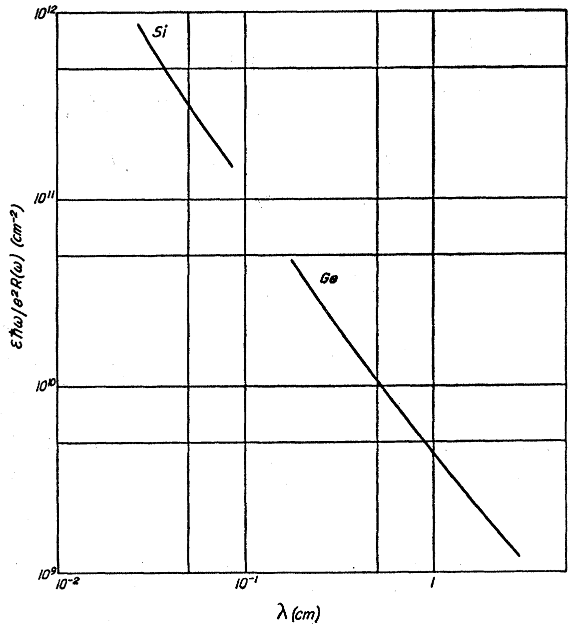

FIG. 1. The dependence of $\epsilon\hbar\omega/e^2R(\omega)$ [see assumption (21)] on the wavelength of radiation for n-Si and n-Ge.

hand, $\langle W_R{}^2\rangle_{\text{av}}\sim\langle S^2\rangle_{\text{av}}(e^2/\epsilon R)^2$ and $\langle S^2\rangle_{\text{av}}$ is small, one can prove that $\hbar\omega\epsilon R(\omega)/e^2\ll 1$. This yields, if $R\approx R(\omega)$ and $E\lessgtr\hbar\omega$, $\epsilon ER_{a2}/e^2\ll 1$. Since in our integrations $E\lessgtr\hbar\omega$, we can see that in the case $R_{a2}\gg(\pi N)^{-1/3}$ the derivative of the integrand in (19) is negative at the point R_{a2}. Thus again the main contribution is given by $R_a\lesssim(\pi N)^{-1/3}$.

Using now (14) and (20) we obtain that R_a's and R's giving the main contribution to the absorption fulfill even in the case of K close to 0.2 the inequalities $R_a<1/2(KN)^{1/3}$ and $R<1/(KN)^{1/3}$. Thus we can say that the hopping takes place predominantly between the donors within the volume including one acceptor. Jumps across two such volumes are less frequent.

The first assumption used in deriving the formula for absorption coefficient was that we can neglect the dipole potentials of ionized acceptor-ionized donor pairs. The dipole fields cancel themselves partially; moreover dipoles have various positions and orientations with respect to the two-donor pair. Let us now take on the same straight line one two-donor and one ionized acceptor-ionized donor pair, the distance between these pairs being $(KN)^{-1/3}$ (about the mean distance between acceptors). Let the distance between the two donors be $R(\omega)$ and the dipole moment of the ionized acceptor-ionized donor pair be equal to the mean value of the dipole moment of such pairs in the crystal. If even in this situation the difference of the dipole potential between the two donors is smaller than $\hbar\omega$, i.e., if

$$K<[\epsilon\hbar\omega/e^2R(\omega)]N^{-2/3}, \qquad (21)$$

we are in the position to neglect the dipole potentials in the derivation of α.

TABLE I. Values of the material constants.

Material	ϵ	a (Å)	η	β_0	E_{LR} (eV)
n-Si	11.7	22.1	4.2	0.43	8.0×10^{-4}
n-Ge	16.0	70.8	18.8	0.059	2.5×10^{-5}

Summarizing, our formula for the absorption coefficient is valid, if the assumptions (16), (20), (14), and (21) are fulfilled and the main contribution to (18) is given by R's fulfilling (17). The assumption $T=0$°K should be interpreted as $kT\ll\hbar\omega$. $\hbar\omega$ must be much smaller than the ionization energy of a donor and the intensity of radiation must be small enough to avoid the "saturation effect," i.e., a serious change of electron states occupation.

NUMERICAL RESULTS

In the Table I we give the values of the material constants used by us. The values of β_0 and E_{LR} were taken from the paper by Myszkowski and Gómułka.[16]

In Fig. 1 we give the dependence of the expression $\epsilon\hbar\omega/e^2R(\omega)$ from the assumption (21) on the wavelength λ of radiation for both materials. One can see that, for example, if N is 10^{18} cm^{-3} and 3×10^{16} cm^{-3} in Si and Ge, respectively, then for $\lambda<700\ \mu$ in Si and $\lambda<3$ mm in Ge the maximal value of K fulfilling our assumptions

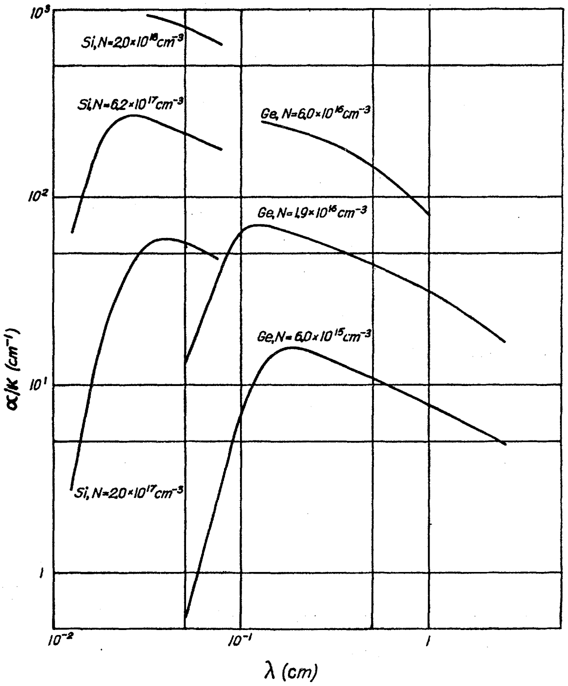

FIG. 2. The dependence of the absorption coefficient per unit compensation on the wavelength of radiation for n-Si and n-Ge at various concentrations of donors.

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[16] A. Myszkowski and S. Gómułka, Phys. Rev. 134, A1102 (1964).

is 0.2 [given by the assumption (14)]. For $\lambda = 800\ \mu$ and $\lambda = 2.5$ cm the maximal value of K is 0.16 and 0.014 in Si and Ge, respectively.

The numerical computations of the ratio α/K given by the formula (18) were performed for the concentrations of donors 2.0×10^{17}, 6.2×10^{17}, 2.0×10^{18} cm^{-3} in Si and 6.0×10^{15}, 1.9×10^{16}, 6.0×10^{16} cm^{-3} in Ge. At the two lower concentrations in each material we are interested in $\hbar\omega$ smaller than one-fourth of the ionization energy of a donor. We shall thus avoid the influence of the excited states of donors. At highest concentrations we are in the "intermediate region" of the impurity conduction. Apart from the problem of the conduction mechanism in this region the ground states of donors do not form yet the impurity band and our results should be valid if $\hbar\omega$ is smaller than, say, one half of the concentration-dependent activation energy ϵ_2 of conduction. We take ϵ_2 about 8×10^{-3} eV in Si (rather arbitrarily) and about 2×10^{-3} eV in Ge.[17] At still higher concentrations the ground states of donors form the impurity band and our model cannot be used. The long-wavelength limitations in our computations were given by the assumption (16) except of the highest concentration in Ge where the restriction (20) is stronger.

In the Fig. 2 we give the computed ratio α/K as a function of the wavelength of radiation for the mentioned concentrations of donors in Si and Ge. The maximal values of the absorption coefficient in our ranges of wavelength, concentration, and compensation are 190 cm^{-1} in Si ($N=2.0\times10^{18}$ cm^{-3}, $K=0.2$, $\lambda=310\ \mu$) and 50 cm^{-1} in Ge ($N=6.0\times10^{16}$ cm^{-3}, $K=0.2$, $\lambda=1.3\times10^{-1}$ cm).

At wavelengths larger than about 500 μ and 3×10^{-1} cm in Si and Ge, respectively, the assumption (17) is fulfilled in the whole range of integration over R in (18). For λ smaller than about 450 μ in Si and 2.5×10^{-1} cm in Ge the contribution from R's nonfulfilling (17) is about one-half of the total absorption coefficient. Thus, for such wavelengths, our results are rather semiquantitative.

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Phonon-Induced Relaxation in Excited Optical States of Trivalent Praseodymium in LaF$_3$†

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Phonon-ion interactions have recently been shown to satisfactorily explain the temperature dependence of widths and positions of the R lines of some $3d$ ions in crystals. These interactions give rise to phonon relaxation processes and are investigated here as the mechanisms responsible for the widths and positions of sharp optical transitions in ($4f$) ions, in particular LaF$_3$:Pr^{3+}. The widths of transitions originating or terminating in the metastable $^3P_0$ state and involving the $^3H_4$, $^3H_6$, $^3F_2$, and $^3F_4$ states of Pr^{3+} in LaF$_3$ have been investigated as a function of temperature and are found to be both qualitatively and quantitatively explainable in terms of lifetime broadening of the interacting states via nonradiative processes. Temperature-dependent shifts have also been measured for the above four groups of transitions and are shown to be in qualitative agreement with theoretical predictions. Additional features of the LaF$_3$:Pr^{3+} spectrum, including several unreported weak transitions and vibrational sidebands, are also reported.

I. INTRODUCTION

THE thermal behavior of the widths and positions of sharp optical transitions of ($3d$) ions in solids has recently been actively investigated by a number of authors[1–10] and successfully interpreted in terms of interactions between lattice vibrations (phonons) and ions. Similar studies on ($4f$) ions in solids have been

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