Model of a deep impurity center in a many-valley semiconductor

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It is shown that the wave function of a highly localized impurity state with a given symmetry can be constructed using a small number of parameters and the **k·p** expansion of the wave function in the vicinity of various critical points of the Brillouin zone. This method is used to obtain the wave function of a deep acceptor state with t_2 symmetry in germanium and silicon. The cross sections for direct and indirect optical transitions are calculated in the impurity absorption region of Ge. The possibility of determination of the parameters of the wave function by modulation spectroscopy methods is discussed.

Deep impurity centers in semiconductors are currently described mainly using two approaches. In the first approach the wave function of an electron state of an impurity center is constructed by hybridization of an atomic wave function with wave functions of the lattice ions.[1] Although progress has recently been made in such quantum-mechanical calculations, considerable computational difficulties are encountered in this approach.

The second, semiphenomenological, approach is based on the fact that in describing a large number of processes involving deep impurity centers we need to know the wave function only at a large distance from an impurity center (i.e., for small values of the quasimomentum). Then, using the short-range nature of the impurity potential, we can construct the wave function of an impurity state using the zero-radius potential model in the range $r \gg R_0$ (R_0 is the characteristic radius of action of the impurity potential).[2-4] In this model the energy of a level is deduced from experimental results and employed as a parameter of the theory.

Our aim will be to develop further this semiphenomenological approach in order to provide a description of electron transitions involving an impurity center in the vicinity of various points in the Brillouin zone. By way of application, we shall calculate the photoionization cross sections of direct and indirect transitions from a deep acceptor center in a many-valley semiconductor of the Ge type.

1. WAVE FUNCTION OF A DEEP IMPURITY CENTER IN A MODEL OF A SHORT-RANGE POTENTIAL

We shall construct the wave function of a bound state for the specific case of a deep acceptor center. In doing this we make substantial use of the hypothesis of the short-range nature of the impurity potential. Moreover, we shall assume that the position of the impurity level in the band gap and the symmetry of the impurity state are known. We shall consider only states with t_2 symmetry. Such a state can be formed, for example, as a result of d-shell splitting of a transition metal impurity ion in a crystal lattice field having T_d symmetry.

We shall begin our discussion with silicon. It is known that the spin–orbit splitting of the energy bands is small compared with the energy of a deep level,[1)] which makes it possible to ignore the spin–orbit interaction. In this case the states of the center with symmetry t_2 are characterized by an index m, which can assume three values: $m = -, +, 0$, corresponding to three projections of the "angular momentum" $L = 1$.

We shall write down the wave function of a state of an impurity center in the form of a series:

$$|m\rangle = V^{-1/2} \sum_{\mathbf{k},\alpha} C_\alpha^m(\mathbf{k})\, e^{i\mathbf{kr}} |\alpha, \mathbf{k}_0\rangle, \tag{1}$$

where the expansion is in terms of the basis functions of the **k·p** method $V^{-1/2} e^{i\mathbf{kr}} |\alpha, \mathbf{k}_0\rangle$.[5] Here, $\mathbf{k}_0$ can be any extremal point of the energy in the Brillouin zone and the wave vector $\mathbf{k}$ is measured from the point $\mathbf{k}_0$; the index α represents the band states at the point $\mathbf{k}_0$ and V is the volune of the crystal. Using the Schrödinger equation

$$(\hat{H}_c - E)\,|m\rangle = -\hat{V}\,|m\rangle, \tag{2}$$

where $\hat{H}_c$ is the Hamiltonian of an electron in a crystal and E is the energy of a level, we can readily obtain equations for the coefficients C_α^m.

$$\sum_\beta [H_{\alpha\beta}(\mathbf{k}) - E\delta_{\alpha\beta}] C_\beta^m = -I_\alpha^m(\mathbf{k}_0, \mathbf{k}). \tag{3}$$

Here, $H_{\alpha\beta}$ is the Hamiltonian of the **k·p** method in the vicinity of the point $\mathbf{k}_0$ and

$$I_\alpha^m(\mathbf{k}_0, \mathbf{k}) = \langle \alpha, \mathbf{k}|\, \hat{V}\,|m\rangle \equiv V^{-1/2} \int d\mathbf{r}\, \psi_{\alpha k_0}^{*} e^{-i\mathbf{kr}} \hat{V} \Psi^m. \tag{4}$$

Since the potential $\hat{V}$ is of the short-range type, in the case when $k \ll R_0^{-1}$ we can assume that $e^{i\mathbf{kr}} \approx 1$, and then the coefficients I are independent of $\mathbf{k}$:

$$I_\alpha^m(\mathbf{k}_0, \mathbf{k}) \approx I_\alpha^m(\mathbf{k}_0, 0) \equiv I_\alpha^m(\mathbf{k}_0),$$

and the solution of Eq. (3) can be represented in the form

$$C_\alpha^m(\mathbf{k}_0, \mathbf{k}) \approx -\sum_\beta G_{\alpha\beta}(E, \mathbf{k})\, I_\beta^m(\mathbf{k}_0), \tag{5}$$

where

$$G_{\alpha\beta} = (H - E)_{\alpha\beta}^{-1}$$

is the Green's function of the **k·p** Hamiltonian H.

If we limit our treatment to the interaction with the nearest energy bands, we can use Eq. (5) to construct the wave functions in the vicinity of extremal energy points using a small nunber of parameters.

In the case of silicon there are two special points in the Brillouin zone: the point Γ at the top of the valence band and the points Δ located on axes equivalent to [100].

We shall consider the behavior of the wave function in

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the vicinity of the point Γ. The potential of an impurity center, which is formed by replacing one of the lattice atoms with an impurity atom, has the symmetry T_d (it should be pointed out that the center has no definite parity). The selection rules ensure that out of the nearest nine bands only two bands contribute to the wave function of an impurity state and their symmetries are Γ_{25}' (valence band) and Γ_{15}, for which the wave functions have opposite parities relative to inversion. Therefore, only the following differ from zero:

$$^{+}I_{\alpha}^{m}(0)=\langle\Gamma_{25}',\ \alpha|\hat{V}|m\rangle=V^{-1/2}A_{\Gamma}^{+}\delta_{\alpha m}$$

and (6)

$$^{-}I_{\alpha}^{m}(0)=\langle\Gamma_{15},\ \alpha|\hat{V}|m\rangle=V^{-1/2}A_{\Gamma}^{-}\delta_{\alpha m}.$$

Here, the index α labels degenerate states in the Γ_{25}' and Γ_{15} bands and, as in the case of m, these states correspond to three projections of the momentum $L=1$ along a quantization axis, selected so as to be parallel to the [001] direction.

Using the spectral representation of the Green's function

$$G_{\alpha\beta}=\sum_{\nu}\frac{\chi_{\alpha}^{\nu*}(\mathbf{k})\chi_{\beta}^{\nu}(\mathbf{k})}{\varepsilon_{\nu}(\mathbf{k})-E} \tag{7}$$

[χ^{ν} is the eigenfunction of the Hamiltonian in Eq. (3) corresponding to the eigenvalue of the energy $\varepsilon_{\nu}(\mathbf{k})$] and Eq. (5); we can readily see that the contribution of each band is inversely proportional to the difference between the energies of the level and of the given band. Therefore, in discussing the majority of the effects we need to consider only the contribution of one valence band. This approximation was used in Ref. 4.

If we describe the valence band using the Luttinger Hamiltonian in the spherical approximation[5] and ignore the spin–orbit interaction, we obtain from Eqs. (5)–(7)

$$C_{\alpha}^{m}(0,\mathbf{k})\approx\frac{A_{\Gamma}^{+}}{V^{1/2}}\sum_{\nu}\frac{D_{\alpha\nu}^{(1)*}(\mathbf{k})D_{m\nu}^{(1)}(\mathbf{k})}{E_{v}+\varepsilon_{\nu}(\mathbf{k})}. \tag{8}$$

Here, E_v is the difference between the energies of the level and the top of the valence band (Fig. 1) and $D^{(1)}$ represents the matrices of finite rotations of the momentum $L=1$ (Ref. 6), which ensure that the quantization axis is parallel to the quasimomentum. The index ν labels the valence subbands: $\nu=\pm$ represents the doubly degenerate heavy-hole subband, whereas $\nu=0$ corresponds to the light-hole subband. In our approximation the energy spectrum of the subbands is isotropic: $\varepsilon_{+}(\mathbf{k})=\hbar^2k^2/2m_h$; $\varepsilon_0(\mathbf{k})=\hbar^2k^2/2m_l$; m_h and m_l are the effective masses of the heavy and light holes.

In discussing the wave function in the vicinity of the point Δ we shall consider only the contribution made by the conduction band (symmetry Δ_1) to the impurity state. Six $|c,\mathbf{k}_{\Delta,l}\rangle$ wave functions are characterized by the directions of the vector $\mathbf{k}_{\Delta,l}$ (l is the index of a valley). Only one of the $I^m(\mathbf{k}_{\Delta,l})\equiv I_l^m(\mathbf{k}_{\Delta})$ constants is independent, so that these constants can be represented conveniently in the form

$$I_l^m(\mathbf{k}_{\Delta})=A_{\Delta}V^{-1/2}D_{0m}^{(1)}(\mathbf{k}_{\Delta,l}). \tag{9}$$

The matrix $D_{0m}^{(1)}$ describes the rotation which ensures that the axis of the l th valley coincides with the quantization axis. In the case of the wave function in the vicinity of the point Δ, we find from Eqs. (5)–(7) that

$$C^m(\mathbf{k}_{\Delta,l},\mathbf{k})\equiv C_l^m(\mathbf{k}_{\Delta},\mathbf{k})=\frac{A_{\Delta}\ D_{0m}^{(1)}(\mathbf{k}_{\Delta,l})}{V^{1/2}\ E_c+\varepsilon_c(\mathbf{k})}. \tag{10}$$

Here, E_c is the difference between the energies of the level and the bottom of the conduction band (Fig. 1); $\varepsilon_c(\mathbf{k})=\hbar^2k_{\parallel}^2/2m_{\parallel}+\hbar^2k_{\perp}^2/2m_{\perp}$; $K_{\parallel}$, $k_{\perp}$, $m_{\parallel}$, and $m_{\perp}$ are the components of the wave vector and of the effective masses along directions parallel or perpendicular to the axis of a valley (oriented along the vector $\mathbf{k}_{\Delta,l}$).

We shall normalize the wave function of the bound state following the BIP method.[7,8] We shall do this by splitting the Brillouin zone into regions centered at the critical points Γ and Δ. Inside each of the regions Ω_{Γ} and $\Omega_{\Delta,l}$ we shall consider only the contributions made to the impurity state by the nearest of the bands, which gives

$$\frac{V}{(2\pi)^3}\left\{\sum_{\nu}\int_{\Omega_{\Gamma}}|C_{\nu}^{m}(0,\mathbf{k})|^2\,d^3k+\sum_{l}\int_{\Omega_{\Delta,l}}|C_l^m(\mathbf{k}_{\Delta},\mathbf{k})|^2\,d^3k\right\}\approx 1. \tag{11}$$

Substituting here Eqs. (8) and (10) for the coefficients C, we obtain the following approximate relationship between the constants A_{Γ}^{+} and A_{Δ}:

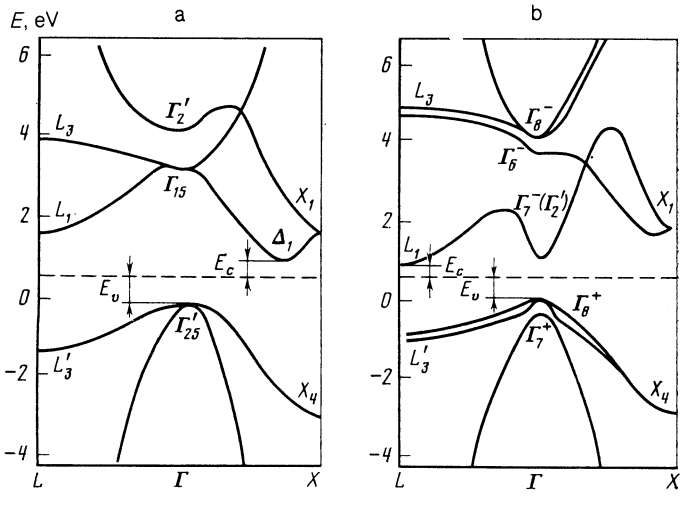

FIG. 1. Energy band structure of silicon (a) and germanium (b).[12] The dashed line represents the position of an impurity level in the band gap.

$$\frac{(A_\Gamma^+)^2}{12\pi}\frac{(2m_h)^{3/2}}{\hbar^3}\frac{1}{E_v^{1/2}}+\frac{(A_\Delta)^2}{4\pi}\frac{(2\mu_c)^{3/2}}{\hbar^3}\frac{1}{E_c^{1/2}}\approx 1. \qquad (12)$$

Here, $\mu_c=(m_\perp^2 m_\parallel)^{1/3}$ is the density-of-states mass in the Δ valley of the conduction band. The radius of convergence of the first integral in Eq. (11) is of the order of $\hbar^{-1}(2m_hE_v)^{1/2}$, which in the case of a level lying in the middle of the band gap ($E_v\approx 0.6$ eV) is about $0.3k_\Delta$. Such a value of the wave vector is clearly at the boundary between the range of validity of the effective mass approximation and that of the BIP method. Nevertheless, in this range of energies we can regard Eq. (12) as an interpolation formula bearing in mind that its contribution, in accordance with Eq. (12), decreases as we move away from one of the bands.

We shall now consider deep centers with t_2 symmetry in germanium. The spin–orbit splitting of the valence band of Ge is $\Delta_{so}\approx 0.28$ eV, which is comparable with the energy of a level, so that we can naturally expect the spin–orbit interaction in the Ge lattice to split the sixfold-degenerate level of the symmetry t_2 (when spin is allowed for) into a fourfold-degenerate state γ_{8t} and a doubly degenerate state γ_{7t}. We shall consider only the state γ_{8t}. It should be pointed out that, in contrast to a shallow acceptor, this state does not have a definite parity. We shall label the states of a center by the index M which has four values $M=\pm 3/2, \pm 1/2$, corresponding to the projection of the "angular momentum" $J=3/2$ along the quantization axis. We shall construct the wave function in the vicinity of the point Γ (where the top of the valence band is located) and of the point L (where the conduction band minima are situated). We can readily show that, by analogy with Eq. (6), the state γ_{8t} includes contributions only of the states Γ_8^+ (valence band) and Γ_8^- (Fig. 2) in the vicinity of the point Γ. Therefore,

$$\begin{aligned} {}^+I_\alpha^M(0)&=\langle\Gamma_8^+,\alpha|\hat V|M\rangle=B_\Gamma{}^+V^{-1/2}\delta_{M\alpha},\\ {}^-I_\alpha^M(0)&=\langle\Gamma_8^-,\alpha|\hat V|M\rangle=B_\Gamma{}^-V^{-1/2}\delta_{M\alpha}. \end{aligned} \qquad (13)$$

The index α labels excited states in the bands Γ_8^+ and Γ_8^- ($\alpha=\pm 3/2, \pm 1/2$). If, by analogy with the case of silicon, we consider only the contribution of the valence band, then using the Luttinger Hamiltonian in the spherical approximation, we find that

$$C_\alpha^M(0,\mathbf{k})\approx\frac{B_\Gamma{}^+}{V^{1/2}}\sum_\nu\frac{D_{\alpha\nu}^{(3/2)*}(\mathbf{k})D_{M\nu}^{(3/2)}(\mathbf{k})}{E_v+\varepsilon_\nu(\mathbf{k})}. \qquad (14)$$

Here, $\varepsilon_{\pm 1/2}(\mathbf{k})=\hbar^2k^2/2m_l$, $\varepsilon_{\pm 3/2}(\mathbf{k})=\hbar^2k^2/2m_h$; m_h and m_l are the effective masses of the heavy and light holes.

In discussing the behavior of the wave function in the vicinity of the point L we shall allow for the contributions made to the impurity state both by the conduction band (of symmetry L_1) and of the doubly degenerate valence band (symmetry L_3'). This is necessary because the separations from the level to the valence and conduction bands are comparable, at least for those levels which are in the lower half of the band gap (Fig. 2). We shall ignore the spin–orbit splitting of the valence band at the point L, because it is small compared with the depth of the level. The basis functions of the **k·p** method for this valley are six wave functions $|\alpha,s,\mathbf{k}_{\Delta,l}\rangle$:

$$\begin{aligned} |0,s,l\rangle&=|S,s,l\rangle,\\ |\pm,s,l\rangle&=\mp 2^{-1/2}(|X,s,l\rangle\pm i|Y,s,l\rangle). \end{aligned}$$

Here, l is the valley index; $\alpha=0$ corresponds to the bottom of the conduction band; $\alpha=\pm$ represents the states in the valence band; $s=\pm 1/2$ is the spin index.[2)] We shall assume that the effective Hamiltonian in the vicinity of the point L is a two-band Hamiltonian of the Kane type:

$$H-E=\begin{matrix}0\\+\\-\end{matrix}\begin{pmatrix}\varepsilon_+ & ik_+P & ik_-P\\ ik_-P & -\varepsilon_- & 0\\ ik_+P & 0 & -\varepsilon_-\end{pmatrix}. \qquad (15)$$

Here, ε_+ and ε_- are the separations from the investigated level to the conduction and valence bands at the point L (Fig. 2); $k_\pm=\mp 2^{-1/2}(k_x\pm ik_y)$; P is the Kane parameter; $P^2=\hbar^2E_{g,L}/2m_\perp$; $E_{g,L}$ is the width of the band gap at the point L. The Green's function corresponding to the Hamiltonian of Eq. (15) is

$$G=\frac{1}{D}\begin{pmatrix}\varepsilon_- & ik_+P & ik_-P\\ ik_-P & -(\varepsilon_+ + P^2k_\perp^2/2\varepsilon_-) & -k_-^2P^2/\varepsilon_-\\ ik_+P & -k_+^2P^2/\varepsilon_- & -(\varepsilon_+ + P^2k_\perp^2/2\varepsilon_-)\end{pmatrix}, \qquad (16)$$

where $D=\varepsilon_+\varepsilon_- + P^2k_\perp^2$, $k_\perp^2=k_x^2+k_y^2$.

Using the rule for the addition of angular momenta, we find that the constants $I_{l\alpha s}^M(\mathbf{k}_L)$ can be represented in the form

$$I_{l\alpha s}^M(\mathbf{k}_L)=(-1)^{M+1/2}B_L{}^\alpha\sum_m\begin{pmatrix}1 & 1/2 & 3/2\\ m & s & -M\end{pmatrix}D_{\alpha m}^{(1)}(\mathbf{k}_{L,l}). \qquad (17)$$

Here the parentheses contain the Wigner $3j$ symbol[6] and D is a matrix which, as in the case of silicon, ensures that the axis of the lth valley coincides with the [001] quantization axis.

Equations (16) and (17) describe the wave function in the vicinity of the point L and in this case the constants $B_L^+=B_L^-\equiv B_L^v$ are related to the contribution of the valence band, whereas $B_L^0\equiv B_L^c$ is related to the conduction band.

In general, it is not possible to find the relationship between the parameters B at the points Γ and L, because the corresponding normalization integral diverges. If an energy level is closer to the conduction band ($\varepsilon_+\ll\varepsilon_-$) we can use

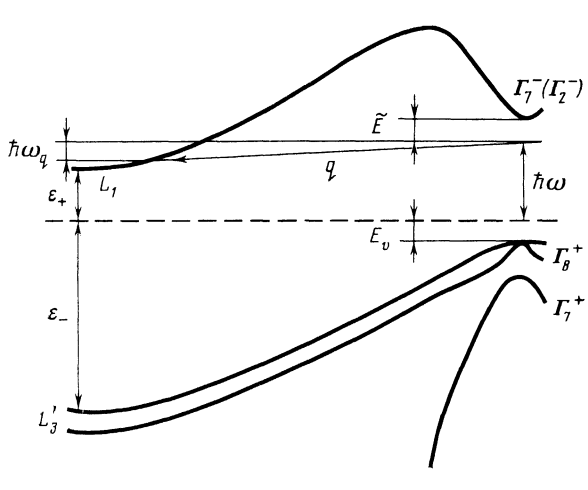

FIG. 2. Parameters of direct and indirect optical transitions from a deep impurity center in Ge.

the one-band approximation. Then, the normalization condition subject to the comments made in the derivation of Eq. (12), yields

$$\frac{(B_\Gamma^+)^2}{16\pi}\left(\frac{2m_h}{\hbar^2}\right)^{3/2}\frac{1}{E_v^{1/2}}+\frac{(B_L^0)^2}{6\pi}\left(\frac{2\mu_c}{\hbar^2}\right)^{3/2}\frac{1}{E_c^{1/2}}\approx 1. \quad (18)$$

Here, μ_c is the density-of-states effective mass of the L valley of the conduction band of Ge.

2. CROSS SECTION FOR A DIRECT OPTICAL TRANSITION BETWEEN AN ACCEPTOR CENTER AND THE CONDUCTION BAND OF Ge

It is known that band states with any value of the quasimomentum right up to the reciprocal lattice vector can contribute to a state localized in **r** space. Consequently, direct optical transitions from an acceptor center to the conduction band of Ge are possible. Naturally, the probability of a transition of this kind is governed by the asymptotic form of the wave function of a deep center corresponding to $k\sim k_L$. We shall calculate the photoionization cross section for a transition which is accompanied by the formation of an electron in the conduction band and of a hole in an acceptor state. For γ_{8t} center of symmetry this cross section for direct allowed transitions is given by

$$\sigma_d(\hbar\omega)=\left(\frac{2\pi e}{m_0}\right)^2\frac{1}{n_0\omega c}\cdot\sum_{M,s,l,\mathbf{k}}|\langle\gamma_{8t},M|pe|ls\mathbf{k}\rangle|^2\delta[\hbar\omega-\varepsilon_+-\varepsilon_c(\mathbf{k})]. \quad (19)$$

Here, k is the quasimomentum of the final state of the conduction band; s is the spin symbol; l is the valley index; $\hat{\mathbf{p}}$ is the momentum operator; **e** is a unit vector of the polarization of light; e and m_0 are the charge and mass of a free electron; n_0 is the refractive index; $\hbar\omega$ is the photon energy; c is the velocity of light.

We shall calculate the matrix element of an optical transition in the vicinity of the point L using Eqs. (16) and (17). Applying the conditions of unitarity for the $3j$ symbols and D matrices,[6] we find that the expression for the sum of the squares of the matrix elements of an optical transition to a valley with the index characterized by the quantum numbers M and s can be represented in the form

$$T_{l\mathbf{k}}(\mathbf{e})\equiv\sum_{Ms}|\langle M|\hat{\mathbf{p}}\mathbf{e}|ls\mathbf{k}\rangle|^2=\frac{1}{3V}\sum_\gamma\left|B_L^\gamma\sum_{\alpha\beta}G_{\alpha\gamma}^*P_{\alpha\beta}(\mathbf{e})\chi_\beta^c\right|^2, \quad (20)$$

where $G_{\alpha\gamma}$ and B_L^γ are given by Eqs. (16) and (17); $P_{\alpha\beta}(\mathbf{e})=\langle\alpha,k_L|\mathbf{pe}|\beta,k_L\rangle$ is the matrix element of an optical transition between the band-edge states at the point L; χ_β^2 are the coefficients which determine how the Bloch amplitudes of the conduction band depend on the wave vector in the Kane model. Using the Hamiltonian of Eq. (15), we obtain

$$\chi_0^c=\varepsilon_c(\varepsilon_c+k_\perp^2P^2)^{-1/2},\quad \chi_\pm^c=iPk_\mp(\varepsilon_c+k_\perp^2P^2)^{-1/2},$$

where ε_c is the electron energy of the conduction band measured from the valley band edge at the point L. The final expressions for the cross section will be obtained for the case of small photon energies above the threshold; $(\hbar\omega-\varepsilon_+)\ll\varepsilon_+,\varepsilon_-$. Retaining only the terms quadratic in k in Eq. (20), we find that

$$T_{l\mathbf{k}}(\mathbf{e})\approx\frac{1}{3V}\left(\frac{m_0P}{\hbar\varepsilon_-}\right)^2\left\{|B_L^c|^2\left(1+\frac{\varepsilon_-}{E_{g,L}}\right)^2\frac{P^2(\mathbf{ke})_\perp^2}{\varepsilon_+^2}+2|B_L^v|^2\left[\left(1-P^2k_\perp^2\left(\frac{2}{\varepsilon_+\varepsilon_-}+\frac{1}{E_{g,L}^2}\right)\right)\frac{e_{\perp,l}^2}{2}-\frac{2P^2}{\varepsilon_+\varepsilon_-}k_xk_ye_x^{(l)}e_y^{(l)}-\frac{P^2(\mathbf{ke})_\perp^2}{E_{g,L}\varepsilon_-}\right]\right\},$$

where $e_x^{(l)}$ and $e_y^{(l)}$ are the components of the polarization vector perpendicular to the axis of the l th valley,

$$e_{\perp,l}^2=(e_x^{(l)})^2+(e_y^{(l)})^2,\qquad (\mathbf{ke})_\perp=k_xe_x^{(l)}+k_ye_y^{(l)}.$$

The partial cross section for a phototransition to a valley with the index l is readily described by the expression

$$\sigma_{d,l}=\sigma_0\Phi e_{\perp,l}^2, \quad (21)$$

where

$$\sigma_0=\frac{4\pi e^2}{m_\perp n_0\omega c}\frac{E_{g,L}}{\varepsilon_-^2}[\varepsilon_+(\hbar\omega-\varepsilon_+)]^{1/2}, \quad (22)$$

and

$$\Phi=b_v+\frac{1}{3}\frac{\hbar\omega-\varepsilon_+}{E_{g,L}}\left[b_c\left(\frac{E_{g,L}+\varepsilon_-}{\varepsilon_+}\right)^2-2b_v\left(1+\frac{E_{g,L}}{\varepsilon_+}+2\frac{E_{g,L}^2}{\varepsilon_+\varepsilon_-}\right)\right], \quad (23)$$

and the dimensionless parameters $b_{c,v}$ are defined by

$$b_{c,v}=\frac{(B_L^{c,v})^2}{6\pi}\left(\frac{2\mu_c}{\hbar^2}\right)^{3/2}\frac{1}{\varepsilon_+^{1/2}}. \quad (24)$$

The polarization dependence of the partial cross sections can be determined if we express the projections $e_{\perp,l}$ in terms of the components of the polarization vector along the [100] principal crystal axes e_x, e_y, and e_z:

$$\begin{aligned}\sigma[111]&=2/3\sigma_0\Phi[1-e_xe_y-e_z(e_x+e_y)],\\ \sigma[\bar{1}11]&=2/3\sigma_0\Phi[1+e_xe_y+e_z(e_x-e_y)],\\ \sigma[\bar{1}\bar{1}1]&=2/3\sigma_0\Phi[1-e_xe_y+e_z(e_x+e_y)],\\ \sigma[1\bar{1}1]&=2/3\sigma_0\Phi[1+e_xe_y-e_z(e_x-e_y)].\end{aligned} \quad (25)$$

Summing the contributions of four valleys, we obtain the following expression for the total photoionization cross section: $\sigma_d^{\text{tot}}=(8/3)\sigma_0\Phi$.

3. CROSS SECTION FOR AN INDIRECT OPTICAL TRANSITION TO THE CONDUCTION BAND OF Ge

The cross section for an indirect optical transition accompanied by phonon emission is

$$\sigma_i=\left(\frac{2\pi e}{m_0}\right)^2\frac{1}{n_0\omega c}\sum_{M,\mu,\mathbf{k},\mathbf{k}',s,l}\frac{|\langle\gamma_{8t},M|\mathbf{pe}|\mu\mathbf{k}\rangle|^2|M_{\mu,sl}|^2}{[E+\hbar\omega-\varepsilon_\mu(\mathbf{k})]^2}\cdot\delta[E+\hbar\omega-\hbar\omega_{\mathbf{q}}-\varepsilon_c(\mathbf{k}')]. \quad (26)$$

Here, the indices μ and **k** describe intermediate (virtual) band states of energy $\varepsilon_\mu(\mathbf{k})$; $\mathbf{k}'$, s, and l are the final states of an electron in the conduction band; $M_{\mu,sl}$ is the matrix element of the electron–phonon interaction operator; $\hbar\omega_{\mathbf{q}}$ is the

phonon energy. The rest of the notation is the same as in Sec. 2.

We shall consider only the transitions which are accompanied by phonon emission, because this indirect transition channel predominates[9] in the case of Ge. We shall assume that the only intermediate states in Eq. (25) are the Γ_2' states, so that the index μ represents double (spin) degeneracy of these states. The selection rules for a transition accompanied by the emission of an LA phonon[9] give $M_{\mu,sl}=M\delta_{\mu,-s}$. Since the phonon energy spectrum near the boundary of the Brillouin zone depends weakly on the phonon wave vector, we shall assume that $M(\mathbf{k}-\mathbf{k}')\approx M(\mathbf{q}_L)\equiv M_0$ and, moreover, we shall consider only the spontaneous process of phonon emission.

Substituting in Eq. (25) the wave functions of the state γ_{8t}, which are governed by Eq. (13), we readily find the cross section for an indirect transition:

$$\sigma_i=\sigma_{0,i}\Phi_i,$$

where

$$\sigma_{0i}=\frac{4}{3}\frac{e^2b_\Gamma{}^v}{m_2n_0\omega c}\left(\frac{m_2}{m_l}\right)^{3/2}\left(\frac{2\mu_c}{\hbar^2}\right)^{3/2}\cdot\frac{E_{g,\Gamma}(\hbar\omega-\hbar\omega_{\mathbf{q}_L}-\varepsilon_+)^{1/2}}{\tilde{E}^{1/2}E_v^{3/2}}M_0{}^2V, \tag{27}$$

$$\Phi_i=1+\left[1+\left(\frac{m_2}{m_l}\frac{\tilde{E}}{E_v}\right)^{1/2}\right]^{-3},\qquad b_\Gamma{}^v=\frac{(B_\Gamma{}^+)^2}{16\pi}\left(\frac{2m_h}{\hbar^2}\right)^{3/2}\frac{1}{E_v^{1/2}}.$$

Here m_2 is the effective mass of the band Γ_2'; $E_{g,\Gamma}$ is the width of the band gap at the point Γ; $\tilde{E}$ is the energy deficit for a direct optical transition (Fig. 2). Equation (27) is derived using an approximate expression from the two-band Kane model for the matrix element of an optical transition at the point Γ: $P_{cv}^2\approx m_0^2E_{g,\Gamma}/2m_2$. We can estimate the matrix element M_0 using the data on the interband absorption of light in Ge. Such an estimate was obtained by Kane,[10] who found $M_0^2V\approx 4.3\times10^{-49}$ eV$^2\cdot$cm^3.

4. DISCUSSION OF RESULTS

Using the final expressions in Secs. 2 and 3 and the actual values of the band parameters of Ge we shall now estimate the ratio of the photoionization cross sections for a deep acceptor level γ_{8t} in the case of direct and indirect transitions:

$$\frac{\sigma_d}{\sigma_i}\sim 10^4\left(\frac{B_L{}^v}{B_\Gamma{}^+}\right)^2\left(\frac{E_v}{\varepsilon_-}\right)^2 \tag{28}$$

Hence, it follows that in the case of the centers whose wave functions are governed by a short-range potential, the direct optical transitions to the side minima of the conduction band should predominate over indirect transitions, because an estimate obtained by the strong-coupling method gives $B_L{}^v\sim B_\Gamma{}^+$.

It follows from the relationships of Eq. (25) in Sec. 2 that the partial cross sections of direct optical transitions in the vicinity of the point L depend on the orientation of the polarization vector of light relative to the axes of the valleys and this should give rise to selective optical pumping of different valleys when a sample is illuminated with polarized light. This effect can be investigated by determination of the relaxation characteristics of the cyclotron resonance signal[11] or by a study of the polarization of the luminescence under uniaxial deformation conditions.

Transitions from a deep acceptor center to the valence band have been investigated by various authors[4] allowing for the contribution of one valence band. Inclusion of a higher band Γ_8^- (Γ_{15}) opens up, in principle, a channel of allowed optical transitions from acceptor states with t_2 symmetry to the valence band, but since the band Γ_8^- is remote, this contribution can be significant only near the absorption edge.

Investigations of optical transitions in the impurity absorption region by modulation spectroscopy methods[12] makes it possible, in principle, to determine the contributions of the band states in the vicinity of various critical points in the Brillouin zone (which means we can find the constants $B_\Gamma^\pm$, B_L^γ, etc.). Investigations of the polarization dependences which then apply may prove particularly fruitful. The constants found in this way together with Eqs. (8), (10), (14), (16), and (17) would give uniquely the wave function of a deep impurity center, which could be used to calculate various effects associated with deep impurities (tunneling, radiationless recombination, etc.).

It should be pointed out that these calculations of the photoionization cross sections have been carried out ignoring impurity charge states and can be used directly in the case of centers which become neutral after the photoionization event. The charge of the centers can be considered by introducing an appropriate Sommerfeld factor.[4]

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[1)] For example, in the case of the valence band at the point Γ we have $\Delta_{so}\approx 0.05$ eV.

[2)] Here, as usual, S is a function which is invariant under transformations of the group C_{3v}; X and Y are functions which transform as the corresponding coordinates.

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