Model of a deep impurity center in a semiconductor two-band-approximation

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The zero-radius-potential model is extended to include the case of deep impurity center interacting with two bands in a semiconductor with a narrow forbidden band. The spectral dependences of the photoionization cross sections of such a center are calculated. Some of their features due to the large difference between the effective masses of the electrons and heavy holes are discussed.

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A deep impurity center in a semiconductor is frequently described by using the Lucovsky model.[1] It describes well in a number of cases processes that are determined by the behavior of the impurity-electron wave function at distances larger than the radius of the potential of the center. The success of this model is due to the fact that it does not presuppose any concrete form of the potential of the center. All that is important for its application is that the characteristic distance over which the wave function decreases be larger than the radius R_0 of the potential well. In this case the matrix elements of the transitions are determined by the behavior of the wave function outside the well, where it depends directly only on the binding energy ε and does not depend on the concrete form of the potential:

$$\Psi = \left(\frac{\varkappa}{2\pi}\right)^{1/2} \frac{1}{r} e^{-\varkappa r}, \quad \varkappa = \frac{(2m\varepsilon)^{1/2}}{\hbar}. \tag{1}$$

The normalization of the function (1) is determined completely by its asymptotic expression if $\varkappa R_0 \ll 1$. This condition means in fact that the binding energy of the level is much less than the depth of the potential well. The Lucovsky model is in essense an application of the zero-radius-potential method[2-4] to the theory of deep centers in semiconductors.

Lucovsky used the wave function (1) to calculate the cross section for the photoionization of the deep impurity center. The value of ε was taken from experiment, and the mass was assumed equal to the effective mass of the nearest band. It is clear that this approach is good if the binding energy $\varepsilon \ll E_g$ (E_g is the width of the forbidden band) and if the nearest band is simple.

The purpose of the present paper is to generalize the zero-radius-potential method to include the case of a complicated band, as well as to the case when the binding energy ε is comparable with E_g. We assume here that we can confine ourselves to the two-band approximation in the spirit of Kane's model.[5]

In this model the masses m_c of the electrons and the light holes are equal and substantially smaller than the masses m_h of the heavy holes. At $m_c \ll m_h$, as will be shown below, we can distinguish between two types of states connected with deep centers. One type, which we shall call the $l-c$ states are characterized by a mass m_c and are constructed out of the wave functions of the conduction band and of the light-hole band. The second type are designated h states, are characterized by a mass m_h and are made up of the wave functions of the heavy holes.[1)] The h states are in fact single-band, and their analysis reduces to a generalization of the Lucovsky model to the case of a complex band.

In this reasoning we did not take into account the split-off band; this is valid in the case of large spin-orbit splitting Δ. For a narrow-gap semiconductors it can be assumed that the wave function of an electron bound on a center is a linear combination of Bloch amplitudes with coefficients (envelopes) that depend continuously on the coordinates. (This is valid, at least, outside the range of action of the potential of the center.) It is natural to expect for each of the two state types that the largest binding energy is possessed by states for which the envelopes contain s-waves. For the $l-c$ type, such a state is doubly degenerate in spin and has symmetry Γ_1. For the h type, only the four-fold degenerate state Γ_8 includes an s wave (in combination with a d wave).[7]

We obtain in this paper expressions for the wave functions of the $l-c$ and h states outside the well and use them to calculate the matrix element of the dipole moment for transitions from a deep center to a band. We also obtain expressions for the dependence of the photoionization cross section on the quantum energy.

Many recent papers are devoted to the theory of deep impurity centers (see the literature cited in Ref. 8). In these papers, principal attention is paid to the internal structure of the center. The photoionization cross sections are calculated in an energy interval which is substantially larger than the width of the forbidden band.[9] These calculations yield valuable information on the wave-function behavior near the impurity, which determines the binding energy of the carrier on the center. It is practically impossible in this case, however, to ensure the accuracy needed for a comparison of the results with the experimental data on the photoionization cross sections, which are observable in much smaller energy intervals.[9]

A number of studies has been devoted specially to photoionization of centers with d electrons.[10-12] The starting point there is the bare atomic wave function of the d electron, and its distortion in the crystal field of the lattice is obtained, i.e., in fact an attempt is also made to perform the calculations on the basis of speci-

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fic assumptions concerning the nature of the center.

Our method, just as Lucovsky's method, does not yield any information on the internal structure of the center or on the energy of the deep level, but on the other hand makes it possible to obtain with good accuracy the frequency dependence of the photoionization cross section in a vital frequency interval. In addition, it makes it possible to take into account also details that are essential for this interval, such as the influence of the spin-orbit interaction and the difference between the carrier masses. This explains a number of qualitative features of the behavior of the photoionization cross sections.

1. WAVE FUNCTIONS

We seek the wave function Ψ of the electron on the center in the form of an expansion in the wave functions ψ_{nk} if the free electrons:

$$\Psi=\sum_{nk}c_n(\mathbf{k})\psi_{nk}. \tag{2}$$

Here n is the number of the band and k is the wave vector. The function ψ_{nk} satisfies the equation

$$H\psi_{nk}=E_{nk}\psi_{nk}, \tag{3}$$

where H is the Hamiltonian of the electron in the crystal-lattice field and E_{nk} is the spectrum of the free electrons in the band n. The set of coefficients $c_n(\mathbf{k})$ specifies the wave function Ψ in the k-representation, and $|c_n(\mathbf{k})|^2$ yields the distribution of the electron on the center over the bands and the quasimomenta.

The function Ψ satisfies the Schrödinger equation

$$(H+V)\Psi=E\Psi,$$

where V is the potential of the center[2)] and E is the level energy. From (2) and (3) follows an expression[13] for the coefficients $c_n(\mathbf{k})$:

$$c_n(\mathbf{k})=\frac{1}{E-E_{nk}}\int\psi_{nk}^{*}V\Psi\,d^3r. \tag{4}$$

The denominator of (4) is the energy distance between the level of the center and the band state $n\mathbf{k}$. Thus, the contribution of a given band state to the wave function Ψ is inversely proportional to this distance. It is this which makes it possible to confine ourselves in the expansion (1), in the case of semiconductors with narrow forbidden band, to the contribution of the nearest valence bands and of the conduction band.

We write down the band wave function in the form

$$\psi_{nk}=v^{-1/2}u_{nk}(\mathbf{r})e^{i\mathbf{kr}}, \tag{5}$$

where $u_{nk}(\mathbf{r})$ is the Bloch amplitude and v is the normalization volume. We assume that the potential of the impurity V is characterized by an action radius R_0, and find the coefficients $c_n(\mathbf{k})$ for values of k such that $kR_0\ll 1$. We then obtain

$$c_n(\mathbf{k})=\frac{v^{-1/2}}{E-E_{nk}}\int u_{nk}^{*}V\Psi\,d^3r. \tag{6}$$

For the calculations that follow we must know the explicit dependence of the Bloch amplitudes u_{nk} on $\mathbf{k}$. This dependence is provided, e.g., by the Kane model which makes it possible to express u_{nk} in terms of the Bloch amplitudes $u_{bm}(\mathbf{r})$ of the band edges:

$$u_{nk}(\mathbf{r})=\sum_{bm}\chi_n^{bm}(\mathbf{k})u_{bm}(\mathbf{r}). \tag{7}$$

Here b and m number respectively the edges of the bands and the corresponding degenerate states.

We confine ourselves hereafter for the sake of argument to straight-band semiconductors such as InSb, in which the band edges are located at the Γ point, and $\Delta\gg E_g$. In this case b and m run through the following values: $b=c$ and $m=\pm 1/2$ for the bottom of the conduction band, and $b=v$ and $m=\pm 3/2$ and $\pm 1/2$ for the tops of the heavy and light hole bands. We write down the functions u_{bm}, so as to fix the choice of the phase shifts:

$$\begin{gathered}u_{c,1/2}=S\uparrow,\quad u_{c,-1/2}=S\downarrow,\quad u_{v,3/2}=-2^{-1/2}(X+iY)\uparrow,\\ u_{v,-3/2}=2^{-1/2}(X-iY)\downarrow\quad u_{v,1/2}=3^{-1/2}[-2^{-1/2}(X+iY)\downarrow+2^{1/2}Z\uparrow],\\ u_{v,-1/2}=3^{-1/2}[2^{-1/2}(X-iY)\uparrow+2^{1/2}Z\downarrow].\end{gathered} \tag{8}$$

The band states are characterized by the number of the branch and by the index μ that distinguishes between the degenerate subbands. We shall therefore use in place of the symbol n the two symbols η and μ, with $\eta=c$ and $\mu=\pm 1/2$ for the conduction band, $\eta=l$ and $\mu=\pm 1/2$ for the light-hole band, and $\eta=h$ and $\mu=\pm 3/2$ for the heavy-hole band. We use the so called spherical approximation, so that μ denotes a projection of the angular momentum on the direction of the wave vector (helicity).

We assume that the potential V of the center has the point symmetry of the crystal, and consider two types of states on the center.

1. *Symmetry state* Γ_6 (*l–c state*). After substituting the expansion (7) in (6), only the integral containing the Bloch amplitudes of the bottom of the conduction band will differ from zero, and we obtain

$$c_n^{m}(k)=\frac{A}{v^{1/2}}\frac{\chi_n^{cm}(k)}{E-E_{nk}},\quad A=\int u_{cm}^{*}V\Psi^{m}\,d^3r, \tag{9}$$

where $m=\pm 1/2$ numbers the two degenerate c-center states with different spins.

Thus, the different band states contribute to a wave function of the l–c type of an electron on a center only to the extent to which the Bloch amplitude of the bottom of the conduction band has been admixed to the given state. According to the Kane model[5], the heavy-hole band does not have such an admixture and therefore makes no contribution to the l–c state.

In the case of a large spin-orbit splitting, $\Delta\gg E_g$, we have according to Ref. 5 for the electrons (c) and the light holes (l)

$$\chi_{c\mu}^{cm}(\mathbf{k})=\left(\frac{\varepsilon_k+E_g}{2\varepsilon_k+E_g}\right)^{1/2}D_{m\mu}^{1/2}(\mathbf{k}),\quad \chi_{l\mu}^{cm}(\mathbf{k})=-\left(\frac{\varepsilon_k}{2\varepsilon_k+E_g}\right)^{1/2}D_{m\mu}^{1/2}(\mathbf{k}), \tag{10}$$

where

$$\varepsilon_k=(E_g/2+\gamma^2k^2)^{1/2}-E_g/2 \tag{11}$$

is the Kane spectrum of the electrons and light holes, $D_{m\mu}^{J}$ are the finite-rotation matrices that align the co-

ordinate system containing the fixed quantization axis z with the coordinate system in which the quantization is directed along k. In (11), γ is a parameter connected with the effective mass of the electrons at the bottom of the conduction band:

$$\gamma^2=\hbar^2E_g/2m_c. \tag{12}$$

Equations (9)–(12) determine the wave function of the $l-c$ state accurate to a normalization constant A. This constant should be determined from the condition

$$v\sum_n \int \frac{d^3\mathbf{k}}{(2\pi)^3}|c_n(\mathbf{k})|^2=1. \tag{13}$$

However, the integral in (13) diverges at large k, since the Kane spectrum is linear in k at large k. This means that the main contribution to the normalization integral is made by the region of k for which one cannot assume that $kR_0\ll 1$. An estimate of the normalization constant A will be presented below.

An explicit expression for the function Ψ can be obtained in the coordinate representation from Eqs. (2), (5), and (9) in the form of an expansion in the Bloch amplitudes of the band edges. This calls for knowledge of the coefficients χ_n^{bm} not only for $b=c$, which have already been written down [Eqs. (10)], but also for $b=v$. At $\Delta\gg E_g$ they are given by

$$\chi_{c\mu}^{vm}=-i\left(\frac{\varepsilon_k}{2\varepsilon_k+E_g}\right)^{1/2}D_{m\mu}^{1/2}(\mathbf{k}),\quad \chi_{l\mu}^{vm}=-i\left(\frac{\varepsilon_k+E_g}{2\varepsilon_k+E_g}\right)^{1/2}D_{m\mu}^{1/2}(\mathbf{k}). \tag{14}$$

We now write down the expression for the wave function Ψ^m of the electron in the center in the $l-c$ state in the coordinate representation at $m=\frac{1}{2}$:

$$\Psi^{1/2}=-\frac{A}{4\pi\gamma^2}\left\{\varepsilon_- u_{c,1/2}\frac{e^{-\varkappa r}}{r}-\left[\frac{1}{2}(x+iy)u_{v,-1/2}+zu_{v,1/2}\right.\right.$$
$$\left.\left.-\frac{\sqrt{3}}{2}(x-iy)u_{v,1/2}\right]\frac{\gamma}{r}\frac{\partial}{\partial r}\frac{e^{-\varkappa r}}{r}\right\}. \tag{15}$$

Here $\varkappa$ is defined by

$$\varkappa^2=\varepsilon_+\varepsilon_-/\gamma^2, \tag{16}$$

where ε_+ and ε_- are respectively the energy distances from the level center to the edges of the conduction and valence bands.

The parameter γ is connected with the effective mass m_c by Eq. (12). On the other hand, γ is expressed in terms of a matrix element of the Bloch amplitudes of the band edges for $\Delta\gg E_g$ in the form

$$\gamma=\left(\frac{2}{3}\right)^{1/2}\frac{\hbar^2}{m_0v_0}\int S\frac{\partial}{\partial z}Z\,d\Omega. \tag{17}$$

An equation for $\Psi^{-1/2}$ is obtained from (15) by reversing the signs of subscripts $(\frac{1}{2},-\frac{1}{2})$ of the Bloch amplitudes.

An estimate of the normalization constant A is obtained by solving the problem for a rectangular spherical well in the two-band approximation

$$A^2=2\pi\gamma^2R_0\left(1+\frac{\varkappa R_0}{4}\frac{\varepsilon_-}{\varepsilon_+}\right)^{-1}. \tag{18}$$

2. *Symmetry state* Γ_8 (*h-state*). When the expansion (7) is substituted in (6) in this case, the only nonzero contributions are made by the integrals containing the Bloch amplitudes u_{vm} of the top of the valence band, and we obtain

$$c_n^m(\mathbf{k})=\frac{A_h}{v}\frac{\chi_n^{vm*}(\mathbf{k})}{E-E_{n\mathbf{k}}}. \tag{19}$$

Here $m=\pm 3/2$ and $\pm\frac{1}{2}$ number the four degenerate states of the h center. The coefficients $\chi_n^{vm}(\mathbf{k})$ that determine the contribution of the top of the valence band to the various states are written out for the conduction and light-hole bands in Eqs. (14). For the heavy-hole band they take the form

$$\chi_{h\mu}^{vm}=D_{m\mu}^{3/2}(\mathbf{k}). \tag{20}$$

At $m_h\gg m_c$ we can neglect the contributions of the conduction and light-hole bands to the wave function of the h state, since the energy denominator in $c_{l\mu}^m$ and $c_{c\mu}^m$ is much larger than in $c_{h\mu}^m$. In the limit $m_c\ll m_h$ it can therefore be assumed that the h state on the center is made up exclusively of heavy-hole wave functions[3)]:

$$\Psi^m=\sum_{\substack{\mu=\pm 3/2\\ m'=\pm 3/2,\pm 1/2}}\int\frac{d^3k}{(2\pi)^3}D_{m\mu}^{3/2}(\mathbf{k})D_{m'\mu}^{3/2}(\mathbf{k})\frac{u_{vm'}}{\varepsilon_-+\varepsilon_{hk}}e^{i\mathbf{kr}}, \tag{21}$$

where

$$\varepsilon_{hk}=\hbar^2k^2/2m_h \tag{22}$$

determines the energy spectrum of the heavy holes.

For the h state, the normalized integral (13) converges and we have

$$A_h=16\pi\varepsilon_-^{3/2}(\hbar^2/2m_h)^{3/2}. \tag{23}$$

Integrating with respect to k in (21), we obtain the electron wave function in the h-state in the coordinate representation.

2. OPTICAL TRANSITIONS

Optical transitions between a deep center and a band are characterized by the transition matrix element $\langle\eta,\mu,\mathbf{k}|\hat{\mathbf{d}}\cdot\mathbf{e}|m\rangle$, where $\hat{d}$ is the dipole-moment operator and $\mathbf{e}$ is the polarization vector. The matrix element is taken between the states of the electron in the band, $\langle\eta,\mu,\mathbf{k}|$, and the state $|m\rangle$ on the center. The transition probability is proportional to the squared modulus of this matrix element, summed over the degenerate subbands and the degenerate states on the center. We introduce therefore the symbol

$$D_\eta(\mathbf{k})=\sum_{\mu m}|\langle\eta,\mu,\mathbf{k}|\hat{\mathbf{d}}\mathbf{e}|m\rangle|^2. \tag{24}$$

In the calculation of D_η we encounter the expression

$$\Phi_{\eta'\mu',\eta''\mu''}=\sum_m c_{\eta'\mu'}^m(\mathbf{k})c_{\eta''\mu''}^{m*}(\mathbf{k}). \tag{25}$$

The quantity Φ characterizes the composition of the state on the center. Using the equation for $c_{\eta\mu}^m$, it is easy to verify that the matrix Φ is diagonal in the symbols μ' and μ'':

$$\Phi_{\eta'\mu',\eta''\mu''}=\Phi_{\eta'\eta'',\mu'\mu''}\delta_{\mu'\mu''}. \tag{26}$$

We then obtain

$$D_\eta(\mathbf{k})=\sum_{\eta'\eta''}\Phi_{\eta'\eta''}(\mathbf{k})g_{\eta'\eta'',\eta}(\mathbf{k}), \tag{27}$$

where $g_{\eta'\eta'',\eta}(\mathbf{k})$ is expressed in terms of the matrix elements of the optical transitions between the band states:

$$g_{\eta'\eta'',\eta}=\sum_{\mu\mu'}\langle\eta,\mu,\mathbf{k}|\hat{\mathbf{de}}|\eta',\mu',\mathbf{k}\rangle\langle\eta,\mu,k|\hat{\mathbf{de}}|\eta'',\mu',k\rangle. \tag{28}$$

The state of $l-c$ type is made up only of functions of the conduction band and the heavy-hole band. We have for it

$$\Phi_{cc}=\frac{A^2}{v(\varepsilon_++\varepsilon_k)^2}\frac{(\varepsilon_k+E_g)}{(2\varepsilon_k+E_g)},$$
$$\Phi_{ll}=\frac{A^2}{v(\varepsilon_-+\varepsilon_k)^2}\frac{\varepsilon_k}{(2\varepsilon_k+E_g)}$$
$$\Phi_{lc}=\Phi_{cl}=\frac{A^2}{v(\varepsilon_++\varepsilon_k)(\varepsilon_-+\varepsilon_k)}\frac{[\varepsilon_k(\varepsilon_k+E_g)]^{1/2}}{(2\varepsilon_k+E_g)}. \tag{29}$$

The h-type state is made up exclusively of functions of the heavy hole band (in the $m_h\gg m_c$ approximation), and its only nonzero element is

$$\Phi_{hh}=A_h^2/v(\varepsilon_-+\varepsilon_{hk})^2. \tag{30}$$

To calculate the quantities $g_{\eta'\eta'',\eta}$, which are determined by the band functions, it is convenient to express these functions in the form (we use the spherical approximation)

$$\Psi_{c\mu k}=\left[\left(\frac{\varepsilon_k+E_g}{2\varepsilon_k+E_g}\right)^{1/2}u_{c\mu}+\left(\frac{\varepsilon_k}{2\varepsilon_k+E_g}\right)^{1/2}u_{l\mu}\right]\frac{e^{ikr}}{v^{1/2}};$$
$$\Psi_{l\mu k}=\left[\left(\frac{\varepsilon_k+E_g}{2\varepsilon_k+E_g}\right)^{1/2}u_{l\mu}-\left(\frac{\varepsilon_k}{2\varepsilon_k+E_g}\right)^{1/2}u_{c\mu}\right]\frac{e^{ikr}}{v^{1/2}}, \tag{31}$$
$$\Psi_{h\mu k}=u_{h\mu}\frac{e^{ikr}}{v^{1/2}}.$$

In (31), $u_{\eta\mu}$ are the Bloch amplitudes of the band edges in a coordinate system in which the z axis is directed along k, and the symbol μ identifies the projection of the angular momentum on the k axis.

Simple calculations yield a set of expressions for $g_{\eta'\eta'',\eta}$ and make it possible to calculate $D_\eta(\mathbf{k})$ with the aid of (27), (29), and (30). We present the results for the products $D_\eta(\mathbf{k})\rho_\eta(k)$, to which the probabilities of the optical transitions are proportional.[4)] For the $l-c$ center we can write

$$D_\eta\rho_\eta=B\Phi_\eta(\omega), \tag{32}$$
$$B=\frac{A^2}{v}\cdot\frac{1}{3}\frac{d^2(\hbar\omega)}{\pi^2\gamma^3E_g}, \tag{33}$$
$$d=\langle S|\hat{d}_x|X\rangle\frac{1}{v_0}=\left(\frac{3}{2}\right)^{1/2}\frac{e\gamma}{\hbar\omega}. \tag{34}$$

The expression $\Phi_\eta(\omega)$ for the transitions into various bands are given by (v is the angle between $\mathbf{k}$ and $\mathbf{e}$)

$$\Phi_c(\omega)=\frac{(\hbar\omega-\varepsilon_+)^{1/2}E_g(\hbar\omega+2\varepsilon_-)^2(\hbar\omega+\varepsilon_-)^{1/2}}{(\hbar\omega)^3(\hbar\omega-\varepsilon_++\varepsilon_-)^2}\theta_c, \tag{35}$$
$$\Phi_l(\omega)=\frac{(\hbar\omega-\varepsilon_-)^{1/2}E_g(\hbar\omega+\varepsilon_+)^{1/2}}{\hbar\omega(\hbar\omega-\varepsilon_-+\varepsilon_+)^2}\theta_l, \tag{36}$$
$$\rho_c=\rho_l=(4\pi^4\gamma^3)^{-1}(2\varepsilon_k+E_g)[\varepsilon_k(\varepsilon_k+E_g)]^{1/2},$$
$$\rho_h=(2m_h/\hbar^2)^{3/2}(\varepsilon_{hk})^{1/2}/4\pi^2.$$
$$\Phi_h(\omega)=\left(\frac{m_c}{m_h}\right)^{1/2}(\hbar\omega-\varepsilon_-)^{1/2}E_g^{1/2}\varepsilon_-^2\theta_h/\hbar\omega\left[\hbar\omega-\varepsilon_-+\frac{m_c}{m_h}\frac{\varepsilon_-\varepsilon_+}{E_g}\right]^2, \tag{37}$$
$$\theta_c=\cos^2\vartheta+\frac{\sin^2\vartheta}{4}\frac{(\hbar\omega)^2}{(2\varepsilon_-+\hbar\omega)^2},\quad \theta_l=\frac{\sin^2\vartheta}{4}+\cos^2\vartheta\frac{(\hbar\omega-2\varepsilon_-)^2}{(\hbar\omega)^2},$$
$$\theta_h=\frac{3}{4}\sin^2\vartheta. \tag{38}$$

For the h-center, Eq. (32) retains the same form but B and Φ are now defined by the expressions

$$B=\frac{3}{\pi}\frac{e^2\hbar}{\varepsilon_-m_h\omega v}, \tag{39}$$
$$\Phi_c(\omega)=\frac{1}{2}\left(\frac{m_c}{m_h}\right)^{1/2}(\hbar\omega-\varepsilon_+)^{1/2}\varepsilon_-^{-1/2}(\varepsilon_-+\hbar\omega)^{1/2}\theta_c$$
$$/\hbar\omega E_g^{1/2}\left[\varepsilon_-+\frac{m_c}{m_h}\frac{(\hbar\omega-\varepsilon_+)(\hbar\omega+\varepsilon_-)}{E_g}\right]^2, \tag{40}$$
$$\Phi_l(\omega)=\frac{1}{2}\left(\frac{m_c}{m_h}\right)^{1/2}(\hbar\omega-\varepsilon_-)^{1/2}(\hbar\omega+\varepsilon_+)^{1/2}\varepsilon_-^{-1/2}\theta_l$$
$$/\hbar\omega\left[\varepsilon_-+\frac{m_c}{m_h}\frac{(\hbar\omega-\varepsilon_-)(\hbar\omega+\varepsilon_+)}{E_g}\right]^2E_g^{1/2}, \tag{41}$$
$$\Phi_h(\omega)=4\frac{(\hbar\omega-\varepsilon_-)^{1/2}\varepsilon_-^{1/2}}{(\hbar\omega)^3}\theta_h, \tag{42}$$
$$\theta_c=\theta_l=2\sin^2\vartheta,\quad \theta_h=\cos^2\vartheta. \tag{43}$$

3. PHOTOIONIZATION

The differential cross section for the photoionization of an impurity center, i.e., the effective cross section of the center for light absorption accompanied by emission of a carrier into the band η, per unit solid angle, is given by

$$\frac{d\sigma_\eta}{d\Omega}=\frac{1}{g}\frac{\pi D_\eta(\mathbf{k})\rho_\eta(k)v\omega}{c\varepsilon_0^{1/2}}. \tag{44}$$

Here g is the degree of the degeneracy of the state on the center ($g=2$ for the $l-c$ center and $g=4$ for the h center). The wave vector k is determined by the energy conservation law ($\hbar\omega=\varepsilon_++\varepsilon_k$ at $\eta=c$, $\hbar\omega=\varepsilon_-+\varepsilon_k$ at $\eta=l$, $\hbar\omega=\varepsilon_-+\varepsilon_{hk}$ at $\eta=h$).

For transitions from the $l-c$ state into various bands we obtain

$$d\sigma_\eta/d\Omega=\sigma_0\Phi_\eta(\omega), \tag{45}$$
$$\sigma_0=\frac{2e^2R_0}{(2\varepsilon_0m_cc^2E_g)^{1/2}}\left[1+\varkappa R_0\frac{\varepsilon_-}{4\varepsilon_+}\right]^{-1}. \tag{46}$$

Here R_0 is the characteristic scale over which the center potential falls off, and $\varkappa$ is given according to (16) and (21) by

$$\hbar^2\varkappa^2/2m_c=\varepsilon_+\varepsilon_-/E_g \tag{47}$$

and determines the scale of the fall-off of the $l-c$ state wave function, while $\Phi_\eta(\omega)$ is given by (35)–(38).

The differential cross section for the photoionization of the h-state on the center can again be written in the form (45), but now

$$\sigma_0=e^2\hbar/\varepsilon_0^{1/2}m_hc\varepsilon_-, \tag{48}$$

and $\Phi_\eta(\omega)$ is determined by Eqs. (40)–(43). The total photoionization cross section σ is obtained by integrating over the angles, and $\sigma=\sigma_0\bar{\Phi}_\eta$, where $\bar{\Phi}_\eta$ is obtained from the corresponding Φ_η by substituting $8\pi/3$ and $4\pi/3$ for $\sin^2\vartheta$ and $\cos^2\vartheta$, respectively.

Deep impurity states can be of either donor or acceptor type. Strictly speaking, the equations obtained here pertain only to the single-particle states of the center, The expressions obtained are directly applicable to electron transition from a donor into the conduction

band or to hole transition from an acceptor into the valence band.

If in the course of the photoionization an electron goes from the valence band to an empty donor or a transition takes place accompanied by formation of an electron in the conduction band and of a hole in an acceptor state, then the factor $1/g$ does not appear in (44). In these cases it is necessary to use for the phototransition cross sections equations in which σ_0 is g times larger than given by (46) and (48).

We discuss now the main features of the frequency dependences of the obtained photoionization cross sections.

1. *Transition from l–c center to conduction band.* The frequency dependence is similar to the one that follows from the Lucovsky formula,[1] but the position of the maximum is somewhat closer to the threshold. When ε_+ changes from a value $\varepsilon_+ \ll E_g$ to a value $\varepsilon_+ = E_g/2$ the position of the maximum shifts from $\hbar\omega_m = 2\varepsilon_+$ to $\hbar\omega_m = 1.7\varepsilon_+$.

2. *Transitions from l–c center to valence band.* These transitions are allowed and are therefore proportional to $(\hbar\omega - \varepsilon_-)^{1/2}$ near the threshold. A characteristic feature of the photoionization cross section in this case is the presence of a sharp peak near the threshold, due to the transition into the heavy-hole band. The width of this peak is of the order of $m_c\varepsilon_-\varepsilon_+/E_g m_h$, and is consequently smaller the smaller m_c/m_h. The cause of this peak is easily understandable. With rise above the threshold, the wave vector k of the particle that takes part in the transition increases rapidly (owing to the large mass of the heavy holes. On the other hand, the contribution of such values of k to the l–c state decreases, since the distance from the center of the level to the energy ε_k of the corresponding state in the conduction band decreases just as rapidly (because of the small electron mass). Observation of such peaks would be of interest for the identification of l–c states.

3. *Transitions from h center to valence band.* Transitions into the heavy-hole band correspond exactly to the Lucovsky formula. Transitions to the light-hole band, however, lead at $m_c \ll m_h$ to a cross section that increases with increasing quantum energy in practically the entire measurable energy range ($\hbar\omega < E_g$). As a result the total cross section may not have a maximum at all. A similar frequency dependence of the cross section was observed in a number of studies.[14,15] There is no maximum because in h-center–band transitions k increases very slowly with increasing ω (owing to the small mass of the light holes), and the contribution of these values of k to the h-center state barely decreases at all. We recall that this contribution is inversely proportional to the distance from the level of the center to the corresponding state in the heavy-hole band.

4. *Transitions from h center to conduction band.* The character of the spectral dependence of the cross section is close to the Lucovsky formula for allowed transitions.

In concluding this section, we examine the influence of the charge of the center. If the ionized center attracts a photoexcited carrier (a positively charged ionized donor or a negatively charged ionized acceptor), this charge influences strongly the wave function of the carrier and increases the probability of its being located near the center. This circumstance can be taken into account by introducing into the formula for the photoionization the Sommerfeld factor

$$S_+(\omega) = \frac{2\pi E_B^{1/2}}{(\hbar\omega-\varepsilon)^{1/2}[1-\exp(-2\pi(E_B/(\hbar\omega-\varepsilon))^{1/2})]}. \qquad (49)$$

Here E_B is the Bohr energy of the shallow donor (acveptor), and $\hbar\omega - \varepsilon$ is the distance from the photoionization threshold. This factor increases the cross section for photoionization near the threshold. In the case of a repelling center we must introduce into the formula a factor S_- that takes into account the decrease of the free-electron wave function near the center:

$$S_-(\omega) = \frac{2\pi E_B^{1/2}}{(\hbar\omega-\varepsilon)^{1/2}[\exp(2\pi(E_B/(\hbar\omega-\varepsilon))^{1/2})-1]}. \qquad (50)$$

[1)] The existence of two types of deep-center states was pointed out by Keldysh.[6]

[2)] Strictly speaking, the center cannot be characterized by a single-electron potential; we shall use, however, this concept in the spirit of the self-consistent-field approximation.

[3)] An exception is the region of very small k, namely $k \lesssim (2m_c\varepsilon_\pm/\hbar^2)^{1/2}$, as well as the case when the level lies very close to the conduction band.

[4)] The state density $\rho_\eta(k)$ in the band η is defined by the equations

$$\rho_c = \rho_l = (4\pi^4\gamma^3)^{-1}(2\varepsilon_k + E_g)[\varepsilon_k(\varepsilon_k + E_g)]^{1/2},$$
$$\rho_h = (2m_h/\hbar^2)^{3/2}(\varepsilon_{hk})^{1/2}/4\pi^2.$$

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