THE SPECTROSCOPIC SPLITTING FACTOR FOR ELECTRONS LOCALIZED AT SHORT-RANGE DEFECTS

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A generalized **kp**-approach to describe the g-factor of an electron localized at a short-range defect in a narrow gap semiconductor has been developed. The consideration has been carried out in the framework of the Green's function method and the Kane model for semiconductor band states, as well as the zero-potential model for a deep center. The values of the g-factor for an electron in a conduction band, at a shallow donor, and at a deep short-range center located not far from the bottom of the conduction band have been demonstrated to be large and negative and not to differ too much from each other. However, as the center becomes deeper, the g-factor of the electron localized at it decreases, so that the g-factor changes its sign and becomes positive for a center located below the middle of the gap.

The spectroscopic splitting factor of electrons bounded at shallow centers in narrow-gap semiconductors has been the subject of intensive theoretical and experimental researches for a long time (see, e.g., work [1] and the references therein). At the same time, the extensive application of these semiconductors as materials in infra-red photoelectronics (see, e.g., review [2]) makes also actual the study of the g-factor of electrons bounded at deep short-range defects. In connection with the complexity of the theoretical description of deep centers, there are only a few works on the specified topic which take into account the complicated multiband structure of the localized wave function. In particular, in works [3–5], such a consideration in the framework of the Luttinger model has been carried out for acceptors in cubic semiconductors.

The theory of deep centers with a short-range potential in the multiband approximation has been developed in work [6]. The center located at the origin of the coordinate system, $\vec{r} = 0$, was described with the help of the matrix band **kp**-Hamiltonian and the scalar potential energy $U\delta(\vec{r})$. Such a description was based on the assumption that the center does not mix different band states due to the scalar character of the impurity potential in use (which, generally speaking, is not always valid).

This approximation was used in works [3–5] when considering deep acceptor states. At the same time, we do not know works where the similar problem has been solved for deep donors in narrow-gap materials such as cadmium—mercury—tellurium ternary compounds and indium antimonide.

We have developed the generalized **kp**-approach for the description of the g-factor of an electron localized at a short-range defect in a narrow-gap semiconductor. The consideration was carried on in the framework of the Green's function method and the Kane model for semiconductor band states, as well as the zero-potential model for a deep center.

The electron density of states in a crystal with short-range defects is determined by the expression

$$\rho_E = -\frac{Im}{\pi V}\int d\vec{r}\,\mathrm{tr}\hat{G}_E(\vec{r},\vec{r}). \tag{1}$$

Here, V is the normalization volume, and tr denotes the trace of the Green's matrix, the latter being determined by the equation

$$\left[E + i\lambda - \hat{\varepsilon} - \vec{\hat{v}}\cdot\vec{\hat{\pi}} - \sum_j \Delta(\vec{r}-\vec{R}_j)\hat{U}\right]\hat{G}_E(\vec{r},\vec{r'}) =$$

$$= \delta(\vec{r}-\vec{r'})\hat{I}. \tag{2}$$

Here, $\lambda \to +0$, $\hat{\varepsilon}$ is the band edge energy, $\hat{\vec{v}}$ the matrix of interband velocities, and $\hat{\vec{\pi}} = \hat{\vec{p}} - \frac{e}{c}\vec{A}$ the kinematic momentum. The last term in the brackets in Eq. (2) describes the potential energy of the short-range defects located at points $\vec{R}_j$, $j = 1 \ldots N_{\mathrm{im}}$, with $\hat{U}$ being the matrix potential.

Let us introduce the free Green's function $\hat{g}_E(\vec{r},\vec{r'})$ using the equation

$$\left[E + i\lambda - \hat{\varepsilon} - \vec{\hat{v}}\cdot\vec{\hat{\pi}}\right]\hat{g}_E(\vec{r},\vec{r'}) = \delta(\vec{r}-\vec{r'})\hat{I}. \tag{3}$$

With the help of this equation, the Green's function for a crystal with defects is written down as

$$\hat{G}_E(\vec{r},\vec{r'}) \approx \hat{g}_E(\vec{r},\vec{r'}) + \sum_j \hat{g}_E(\vec{r},\vec{R'_j})\hat{U}\hat{G}_E(\vec{R}_j,\vec{r'}). \quad (4)$$

The approximate relationship

$$[1 - \tilde{g}_E(\vec{R}_j,\vec{R}_j)\hat{U}]\hat{G}_E(\vec{R}_j,\vec{r'}) \approx \tilde{g}_E(\vec{R}_j,\vec{r'}) \quad (5)$$

is fulfilled at the point $\vec{r} = \vec{R}_j$, where the notation $\tilde{g}(\vec{R}_j,\vec{R}_j)$ means that the singularity is "cut off" at distances about the center radius.

At last, in the Koster–Slater approximation, we obtain

$$\hat{G}_E(\vec{r},\vec{r'}) \approx \hat{g}_E(\vec{r},\vec{r'}) +$$

$$+\sum_j \hat{g}_E(\vec{r},\vec{R}_j)\hat{U}(1 - \hat{\Lambda}_E\hat{U})^{-1}\hat{G}_E(\vec{R}_j,\vec{r'}), \quad (6)$$

where the matrix $\hat{\Lambda}_E \equiv \hat{g}_E(\vec{r},\vec{r})$.

The contribution of a short-range impurity to the electron density of states $\Delta\rho_E$ is defined by the second term on the right-hand side of Eq. (6). Substituting Eq. (6) into Eq. (1), we obtain

$$\Delta\rho_E = -\frac{\mathrm{Im}}{\pi V}\times$$

$$\times \int d\vec{r}\,\mathrm{tr}\sum_j \hat{g}_E(\vec{R}_j,\vec{r})\hat{g}_E(\vec{r},\vec{R}_j)\hat{U}(1 - \hat{\Lambda}_E\hat{U})^{-1}. \quad (7)$$

Using the equality

$$\int d\vec{r}\,\hat{g}_E(\vec{R}_j,\vec{r})\hat{g}_E(\vec{r},\vec{R}_j) = -\frac{d\Lambda_E}{dE}$$

and summing up in expression (7) over all the centers with the concentration $n_{\mathrm{im}} = N_{\mathrm{im}}/V$, let us rewrite Eq. (7) as follows:

$$\Delta\rho_E = \frac{n_{\mathrm{im}}}{\pi}\mathrm{Im}\,\mathrm{tr}\frac{d\Delta_E}{dE}\hat{U}(1 - \hat{\Lambda}_E\hat{U})^{-1}. \quad (8)$$

In the general case, the analysis of even such an expression represents significant difficulties. Therefore, let us consider the elementary case which includes the three-band Kane model (i.e. when the value of the spin-orbit splitting is much greater than the energy gap width) and the scalar potential $\hat{U} = u\hat{I}$. The 6×6-matrix Λ_E is diagonal in this approximation, and the relationships $(\hat{\Lambda}_E)_{kk} = \Lambda_{Ek}$, $\Lambda_{E1} = \Lambda_{E2}$, and $\Lambda_{E3} = \Lambda_{E4} = \Lambda_{E5} = \Lambda_{E6}$ hold true for it in the absence of a magnetic field [7]. In this case, the first two diagonal components in Eq. (2) correspond to the so-called l—c-centers with the Γ_6 symmetry, and the last four to the h-centers with the Γ_8 symmetry [6, 7]. In what follows, we confine the consideration to the l—c-centers which correspond, as a rule, to deep donor states in narrow-gap semiconductors.

Applying the technique developed in work [7], one can show that, in the case of a weak magnetic field,

$$\begin{pmatrix} \Lambda_{E1} \\ \Lambda_{E2} \end{pmatrix} = \Lambda^{(c)}_{E_0} - h\begin{pmatrix} a_{E1} \\ a_{E2} \end{pmatrix}. \quad (9)$$

Here, E_0 is the energy of the l—c-level provided the absence of the magnetic field, the dimensionless parameter h is proportional to the intensity of the magnetic field H:

$$h = \left(\frac{Pp_0}{E_g}\right)^2; \quad p_0^2 = \frac{2\hbar|e|H}{c}, \quad (10)$$

and P is the parameter of the three-band Kane model.

Thus, it is evident from Eqs. (8) and (9) that the l—c-level undergoes splitting in the magnetic field, the splitting energy being

$$\Delta_{12} = h\frac{a_{E_01} - a_{E_02}}{(d\Lambda^{(c)}_E/dE)_{E_0}}. \quad (11)$$

Taking into account the explicit form of the wave functions which are the solutions of the equation with the three-band Kane Hamiltonian in the presence of the magnetic field, substituting the summation over all the Landau levels N by the integration over the variable $t = hN$, and using the Euler formula, the difference $a_{E1} - a_{E2}$ in Eq. (11) reads

$$a_{E1} - a_{E2} = \frac{1}{3}\left(\frac{E_g}{\hbar P}\right)^2 \int\limits_{-\infty}^{\infty} \frac{dx}{(2\pi)^2}\times$$

$$\times \sum_{j=\pm 1}\left\{\int\limits_0^{\infty} dt\left[\frac{j}{2\eta_t^3\left[E + \frac{E_g}{2}(1 - j\eta_t)\right]} + \right.\right.$$

$$\left.\left. + \frac{E_g}{2}\frac{j(\eta_t + j)}{2\eta_t^2\left[E + \frac{E_g}{2}(1 - j\eta_t)\right]^2}\right]\right\}. \quad (12)$$

In this expression, $\eta_t = \sqrt{1 + \frac{8}{3}(x^2 + t)}$.

It should be noted that both the denominator and the numerator of Eq. (11) involve the identical linear singularity at large momenta, which is caused by the

linear character of the Kane spectrum of high-energy electrons. Nevertheless, both the "cut off" parameter $\rho_{\max} \sim \frac{P\hbar}{aE_g}$, where a is the lattice constant, and the explicit form of the short-range potential U are reduced in Eq. (11) and do not enter the final expression for the splitting energy.

The effective spectroscopic splitting factor of the l—c-level is introduced by the relationship

$$\Delta_{12} = g_{l-c}^{\text{eff}} \mu_{\text{B}} H, \tag{13}$$

where $\mu_{\text{B}} = \frac{|e|\hbar}{2m_0 c}$ is the Bohr magneton and m_0 the free electron mass.

Taking into account the value of the Kane parameter $P^2 = \frac{3E_g}{4m_c}$, where m_c is the effective mass of an electron near the bottom of the conduction band, we obtain the ultimate expression for the g-factor of the short-range l—c-center as

$$g_{l-c}^{\text{eff}} = -\frac{m_0}{m_c}(1 + \frac{2E_0}{E_g}). \tag{14}$$

Expression (14) turns into the known expression for the g-factor of Kane electrons near the bottom of the conduction band [8] (as well as into the expression for the spectroscopic splitting factor of the electrons bounded at shallow donors [1]). In the narrow-gap semiconductors described by the three-band Kane model, the relationship $\frac{m_0}{m_c} \gg 1$ holds true. Therefore, the values of the spectroscopic splitting factor for electrons in the conduction band, at a shallow donor, and at a deep short-range center located not too far from the bottom of the conduction band are large and negative and do not differ substantially from each other.

Nevertheless, as follows from Eq. (14), as the center becomes deeper (the energy E_0 reckoned from the bottom of the conduction band is negative!), the g-factor of the electrons localized at this center decreases, so that it changes its sign and becomes positive for a center located below the middle of the energy gap.

The proposed method allows the g-factor to be also calculated for an arbitrary form of the matrix impurity potential $\hat{U}$ [9]. Such a problem represents a significant interest, which is connected to the enhancement of researches dealing with the behavior of the isoelectron nitric impurity in A^3B^5 semiconductors [10] during last years. In those systems, there are significant differences between the characteristics of a light N atom (with the atomic mass 14) and those of substantially heavier ones P (31), As (75), or Sb (122), which the former substitutes for in the crystal lattice. Therefore, the scalar approach to the description of the impurity potential that was developed in work [6] is obviously inapplicable here.

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ФАКТОР СПЕКТРОСКОПІЧНОГО РОЗЩЕПЛЕННЯ ЕЛЕКТРОНІВ, ЗВ'ЯЗАНИХ НА КОРОТКОДІЙНИХ ДЕФЕКТАХ

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Р е з ю м е

Розвинуто узагальнений **kp**-підхід для опису g-фактора електрона, зв'язаного на короткодійному дефекті в вузькощілинному напівпровіднику. Розгляд проведено в рамках методу функцій Ґріна й моделі Кейна для зонних станів напівпровідника, а також моделі потенціалу нульового радіуса для глибокого центра. Показано, що значення g-фактора для електронів у зоні провідності, на мілкому донорі й на глибокому короткодійному центрі (розташованому не надто далеко від дна зони провідності) є великими, від'ємними і відрізняються не надто сильно. Проте по мірі заглиблення центра g-фактор локалізованих на цьому центрі електронів зменшується і для центра, розташованого нижче від середини забороненої зони, змінює знак і стає додатним.