KP-approach for non-symmetric short-range defects: resonant states and alloy bandstructure

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The short-range defect with reduced symmetry is studied in the framework of kp-approach taking into account a matrix structure of potential energy in the equations for envelope functions. The case of the narrow-gap semiconductor, with defects which are non-symmetric along the [001], [110], or [111] directions, is considered. Resonant state at a single defect is analyzed within the Koster-Slater approximation. The bandstructure modification of the alloy, formed by non-symmetric impurities, is discussed and a generalized virtual crystal approximation is introduced.

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I. INTRODUCTION

Examinations of electron states, localized at short-range defects, began with the development of the band theory (see Refs. in [1]). The approach for the calculation of the photoionization cross-section was formulated in the framework of the effective mass approximation with short-range impurity potential (Lukovsky model [2].) The short-range acceptor states were described with the use of the multi-band approach based on the matrix kp-Hamiltonian and on the scalar potential energy $U\delta(r)$ for the impurity placed at $r = 0$ [3]. The same approach was used [4] for the description of both the resonant and localized electronic states in the gapless and $p$-type materials under uniaxial stress. The multi-band considerations in [3] and [4] have demonstrated a good agreement with the experimental data for the photoionization cross-section of acceptor state and the transformation of impurity states under uniaxial stress (see discussions in [5] and [6] respectively). The considerations [2, 3, 4] were restricted by the presumption that defect does not mix different bands by itself due to the scalar character of the impurity potential used. To the best of our knowledge, a complete description of electronic states at short-range defect, taking into account a matrix structure of potential energy, has not been performed yet. This issue is also of interest in connection with the last investigations of $A_3B_5$ alloys formed by materials with distinctly different parameters (see reviews in [7]).

In the present paper, we evaluate the generalized kp-approach with the matrix potential energy described a short-range defect with reduced symmetry. We demonstrate both the appearance of resonant electron state at single defect and the significant modification of alloy bandstructure due to the non-diagonal contributions to the matrix potential of defect. The consideration is performed in the framework of $6 \times 6$ Kane model [8], corresponding to a narrow-gap semiconductor, for the cases of defect which is non-symmetric along the [001], [110], or [111] directions. The matrix Green’s function of the resonant states is obtained in the Koster-Slater approximation and the conditions for a narrow resonant peak over the conduction or valence band are discussed. The low-energy electronic states in semiconductor alloy are described by the Dyson equation with the self-energy function, written in the Born approximation. Due to the weak damping, we arrive to the effective Hamiltonian with the non-diagonal matrix of the extreme energies, i.e. we introduce the generalized virtual crystal approximation. As a result, the energy spectrum appears to be anisotropic and splitting of the degenerate hole states takes place. In addition, a zero-gap case can be realized with an increase of alloy composition.

The consideration below is organized as follows. In Sec. II we present the theoretical background including the zero-radius approach for description of the short-range defect, the Koster-Slater solution for the resonant state at a single defect, and the generalized virtual crystal approximation for the low-energy electron states. The results for the resonant states and for the alloy bandstructure are discussed in Sec. III with the use of the $6 \times 6$ Kane model. In Sec. IV we make concluding remarks and discuss the assumptions made.

II. BASIC EQUATIONS

We consider here the equations for the envelope function and for the single-particle Green’s function in the crystal with short-range defects. Further, we evaluate the contribution of the resonant states into the density of states and describe the low-energy electronic states using the Dyson equation with the second-order self-energy function.
A. Zero-radius approach

The general equation for the envelope wave function, $\Psi_{lr}$, which is introduced through the expansion of an exact wave function, $\sum_{l'} \Psi_{lr} u_{lr}$, over the Bloch amplitudes of $l$th state in the center of Brillouin zone, $u_{lr}$, is written as:

$$\sum_{l'} \left[ \hat{H}_{ll'} \Psi_{lr} + \int d\mathbf{r}' U_{ll'}(\mathbf{r}, \mathbf{r}') \Psi_{lr'} \right] = E \Psi_{lr}. \tag{1}$$

Here $l$ includes band and spin indexes, $\hat{H}_{ll'}$ is the single-electron $\mathbf{k}\mathbf{p}$-Hamiltonian described a motion in the ideal crystal. The microscopic potential of defect, $\delta U_r$, appears in the kernel:

$$U_{ll'}(\mathbf{r}, \mathbf{r}') = \int d\mathbf{r}_1 u_{lr}^* \delta(\mathbf{r} - \mathbf{r}_1) \delta U_{r_1} \delta(\mathbf{r}_1 - \mathbf{r}') u_{lr'}, \tag{2}$$

where $\Delta(\mathbf{r}) = (1/V) \sum_{\mathbf{k}} \exp(i\mathbf{k}\mathbf{r})$ is the $\delta$-like function; $V$ is the normalization volume and $\sum_{\mathbf{k}} \ldots$ is taken over the first Brillouin zone. Here we consider the short-range (localized in the elementary cell) defect placed at $\mathbf{r} = 0$. For the case of the low-energy states, with the wavelength higher than the lattice constant, $a$, we substitute $\Psi_{lr'=0}$ into the integral term of Eq.(1) and this equation takes form

$$\sum_{l'} \left[ \hat{H}_{ll'} \psi_{lr} + U_{ll'}(\mathbf{r}) \Psi_{lr=0} \right] = E \Psi_{lr}. \tag{3}$$

Thus, we have obtained the equations for the envelope wave function with the matrix potential energy $U_{ll'} \Delta(\mathbf{r})$ determined through the components

$$U_{ll'} = \int d\mathbf{r} u_{lr}^* \delta(\mathbf{r}) \delta U_{r} u_{lr'}, \tag{4}$$

moreover $U_{ll'} = U_{l'l}^*$. It is necessary to stress that there are no reasons in order to neglect the non-diagonal components of this matrix if the local symmetry of $\delta U_r$ is reduced in comparison to the crystal symmetry. This point is a main difference from the standard $\mathbf{k}\mathbf{p}$-description of the large-scale potential case and from the previous consideration of the deep impurities cited above.

Using the potential energy $\sum_j \Delta(\mathbf{r} - \mathbf{R}_j)U$ for the crystal with $N_{im}$ short-range defects in the volume $V$ placed at $\mathbf{R}_j$, $j = 1 \ldots N_{im}$, we write the equation for the retarded Green’s function in the matrix form

$$\begin{bmatrix} E + i\lambda - \hat{H} - \sum_j \Delta(\mathbf{r} - \mathbf{R}_j)U \end{bmatrix} \hat{G}_E(\mathbf{r}, \mathbf{r'}) = \delta(\mathbf{r} - \mathbf{r'}) \hat{1}, \tag{5}$$

where $\lambda \rightarrow +0$ and $\hat{1}$ is the identity matrix. Next, we transform Eq.(5) into the equation:

$$\hat{G}_E(\mathbf{r}, \mathbf{r'}) \simeq \hat{g}_E(\mathbf{r}, \mathbf{r'}) + \sum_j \hat{g}_E(\mathbf{r}, \mathbf{R}_j)U \hat{G}_E(\mathbf{R}_j, \mathbf{r'}) \tag{6}$$

where the free Green’s function, $\hat{g}_E(\mathbf{r}, \mathbf{r'})$, determined from: $(E + i\lambda - \hat{H})\hat{g}_E(\mathbf{r}, \mathbf{r'}) = \delta(\mathbf{r} - \mathbf{r'})\hat{1}$. Thus, the zero-radius approach gives us an infinite (if $N_{im} \rightarrow \infty$) set of equations for $\hat{G}_E(\mathbf{R}_j, \mathbf{r'})$.

B. Koster-Slater approximation

In order to describe a localized (or resonant) state at $j$th defect, we rewrite Eq.(6) for $\hat{G}_E(\mathbf{R}_j, \mathbf{r'})$ neglecting the neighbor defect contributions:

$$\left[ 1 - \hat{g}_E(\mathbf{R}_j, \mathbf{R}_j)U \right] \hat{G}_E(\mathbf{R}_j, \mathbf{r'}) \simeq \hat{g}_E(\mathbf{R}_j, \mathbf{r'}). \tag{7}$$

The function $\hat{g}_E(\mathbf{R}_j, \mathbf{R}_j)$ means the free Green’s function with the cut-off singularity at coinciding arguments (i.e. at distances $\sim a$). This approximation is valid if the radius of states is shorter than $n_{im}^{-1/3}$, $n_{im} = N_{im}/V$ is the
concentration of defects. Substituting \( \hat{G}_E(R_j, r') \) determined by Eq.(7) into Eq.(6) we obtain the Green’s function written in the framework of the Koster-Slater approximation:

\[
\hat{G}_E(r, r') \simeq \hat{g}_E(r, r') + \sum_j \hat{g}_E(r, R_j) \hat{U} \left( 1 - \hat{\Lambda}_E \hat{U} \right)^{-1} \hat{g}_E(R_j, r')
\]  

(8)

with \( \hat{\Lambda}_E \equiv \hat{g}_E(r, r) \).

The density of states is expressed through \( \hat{G}_E(r, r') \) according to the standard formula: \( \rho_E = -Im \text{tr} \int d\mathbf{r} \hat{G}_E(r, r')/(\pi V) \) where tr . . . means sum over diagonal matrix elements. The impurity contribution to the density of states, \( \Delta \rho_E \), is determined by the second term of (8). After the permutation of \( \hat{g}_E \) under tr , . . . , we use the equality \( \int d\mathbf{r} \hat{g}_E(R_j, r) \hat{g}_E(r, R_j) = -[d\hat{g}_E(R_j, R_j)/dE] \) and \( \Delta \rho_E \) is transformed into (see similar formulas in [3, 4]):

\[
\Delta \rho_E = \frac{n_{im}}{\pi} \text{Im} \frac{d\hat{\Lambda}_E}{dE} \left( 1 - \hat{\Lambda}_E \hat{U} \right)^{-1}, \quad \hat{\Lambda}_E = \frac{1}{V} \sum_p \hat{g}_E(p),
\]

(9)

where \( \sum_p \ldots \) means the summation over the region \( |p| < h/\alpha \). Here we have also used the free Green’s function in the momentum representation: \( \hat{g}_E(p, p') = \delta_{pp'} \hat{g}_E(p) \) with \( \hat{g}_E(p) = (E + i\lambda - \hat{\epsilon} - \hat{\mathbf{v}} \cdot \mathbf{r})^{-1} \), where the \( kp \)-Hamiltonian in \( p \)-representation, \( \hat{\epsilon} + \hat{\mathbf{v}} \cdot \mathbf{r} \), is written through the extreme energy and interband velocity matrices, \( \hat{\epsilon} \) and \( \hat{\mathbf{v}} \). It is convenient to write \( \hat{g}_E(p) \) through the dispersion laws of \( k \) th band, \( \epsilon_{kp} \), according to:

\[
\hat{\Lambda}_E = \frac{1}{V} \sum_{kp} \frac{\hat{P}_{kp}}{E - \epsilon_{kp} + i\lambda},
\]

(10)

where the projection operators onto the \( k \) th band, \( \hat{P}_{kp} \), are given by the matrix elements: \( \langle \hat{P}_{kp} \rangle_{ll'} = \sum_p \psi_p^{(k\sigma)} \psi_{l'}^{(k\sigma)} \). Here \( \sigma \) is the spin index and the column \( \psi_p^{(k\sigma)} \) is determined through the eigenstate problem: \( (\hat{\epsilon} + \hat{\mathbf{v}} \cdot \mathbf{r}) \psi_p^{(k\sigma)} = \epsilon_{kp} \psi_p^{(k\sigma)} \).

C. Generalized virtual crystal approximation

Consideration of the low-energy electronic states, with the wavelength exceeds \( n_{im}^{-1/3} \), is based on the matrix Dyson equation for the averaged Green’s function. Such equation is obtained from Eq.(6) in the form:

\[
\hat{G}_E(p) = \hat{g}_E(p) + \hat{g}_E(p) \hat{\Sigma}_E \hat{G}_E(p),
\]

(11)

\[
\hat{\Sigma}_E = \frac{n_{im}}{V} \sum_p \hat{U} \hat{G}_E(p) \hat{U} + \ldots
\]

where the self-energy function, \( \hat{\Sigma}_E \), is written in the self-consistent approximation. Using \( \hat{g}_E(p) \) in \( \hat{\Sigma}_E \) (the Born approximation) we write the self-energy function through \( \hat{\Lambda}_E \) given by Eq. (10) according to \( \hat{\Sigma}_E \simeq n_{im} \hat{U} \hat{\Lambda}_E \hat{U} \).

Since Eq.(11) is transformed into \( \hat{G}_E(p) = [\hat{g}_E(p)^{-1} - \hat{\Sigma}_E]^{-1} \), we obtain the averaged density of states in the form:

\[
\bar{\rho}_E = -\frac{1}{\pi V} \sum_p \text{tr} \left( E - \hat{\epsilon} - \hat{\mathbf{v}} \cdot \mathbf{r} - \hat{\Sigma}_E \right)^{-1}
\]

(12)

and matrix \( \hat{\Sigma}_E \) reduces the symmetry at \( p = 0 \). According to the consideration below (see Eqs.(16)-(20)), the self-energy matrix appears to be weakly dependent on \( E \) and the damping contributions to \( \hat{\Sigma} \) are also small. Thus, we arrive to the effective Hamiltonian:

\[
\hat{H}^{(eff)}_p = \hat{\epsilon} + \hat{\Sigma} + \hat{\mathbf{v}} \cdot \mathbf{r}, \quad \hat{\Sigma} \simeq n_{im} \hat{U} \hat{\Lambda}_E \hat{U}
\]

(13)

with the non-digonal matrix \((\hat{\epsilon} + \hat{\Sigma})\) which determines the energies of the band extremes. This Hamiltonian corresponds to the generalized virtual crystal approximation for the alloy formed by low-symmetric defects: not only the energies of the band extremes are shifted with the alloy composition (see [11]; note, that \( \hat{\Sigma} \propto n_{im} \) in the Born approximation), but also the symmetry of \( \hat{H}^{(eff)}_p \) is reduced due to the non-diagonal contributions from \( \hat{\Sigma} \). The characteristic equation correspondent to the effective Hamiltonian (13) is written in the form:

\[
\text{det}[\hat{\epsilon} + \hat{\Sigma} + \hat{\mathbf{v}} \cdot \mathbf{r} - E] = 0
\]

(14)

and the dispersion laws appear to be anisotropic, with splitted valence bands, like for the case of stressed semiconductors.
III. RESULTS

Let us turn to Eqs. (9) and (14) for the narrow-gap semiconductor described in the framework of the isotropic 6 × 6 Kane model. For the sake of simplicity, we restrict our consideration to the model of defect with the microscopic potential, δUr, which is only non-symmetric along the [001] (case A), [110] (case B), or [111] (case C) directions.

A. 6 × 6 Kane model

The matrices ̂U and ̂ΛE are determined below using the set of Bloch functions which are expressed according to [1] in terms of the periodic basis |S⟩, |X⟩, |Y⟩, and |Z⟩. Within the above approximations, the potential matrix (4) is written in the form:

\[
\hat{U} = \begin{pmatrix}
\hat{u}_c & \hat{u}^+ & \hat{u}_A & 0 \\
\hat{u}^+ & \hat{u}_c & 0 & 0 \\
\hat{u}_A & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix},
\]

(15)

where ̂uA is proportional to \(|\lambda⟩\), so that ̂uv with \(\langle \lambda | u \rangle = 0\) (case B), \(\langle \lambda | v \rangle = 0\) (case C), and ̂uv|c⟩ is determined as follows:

Here ̂uc and ̂uc are proportional to the 2 × 2 and 4 × 4 identity matrices: ̂uc = 1(|S⟩⟨S|) = 1uc and ̂uc = 1(|X⟩⟨X|) = 1uc; the non-diagonal part of ̂U is expressed through the 4 × 2 matrix, ̂u, where \(\epsilon_{\pm} = (1 \pm i)/\sqrt{2}\). The matrices ̂uA,B,C are proportional to \(u_\pm = \langle S|\delta U|Z⟩ \neq 0\) with \(u_{\pm} = \langle S|\delta U|X⟩ = 0\) (case A), or \(u_d = \langle S|\delta U|X⟩ = 0\) (case B), or \(u_\pm = \langle S|\delta U|X⟩ = 0\) (case C).

Since the dispersion laws \(\varepsilon_{kp}\) are isotropic, we use in Eq.(10) the projection operators which are averaged over the angle, so that \(P_{kp}\) are proportional to \(\delta_{ll}\). Thus, the diagonal matrix \(\Lambda_E\) is determined by the matrix elements

(16)

where \(\lambda_{kk}\) are weakly dependent on \(E\) due to the dominant contribution from \(|p| \sim h/a\). Because of this, we use the expansion \(\lambda_{kk} \simeq \lambda_k - l_k(E + \epsilon_g/2)\) where the energy \(-\epsilon_g/2\) corresponds the middle of gap and the coefficients \(\lambda_k\) and \(l_k\) are given by

(17)

Here \(\sum_q\) means summation over the electron (c-) and light-hole (lh-) state while the heavy hole (hh-) state, with the dispersion law \(\varepsilon_{hp}\), appears in \(\lambda_v\) and \(l_v\). Note also, that the coefficients \(l_k\) have no divergence at \(|p| \rightarrow \infty\). Eqs. (17) are written through the coefficient, \(a_{qp}\), and the normalization factor, \(C_{qp}\), which are determined as follows:

(18)

where \(P\) is the Kane velocity. The broadening factors in Eq.(16), \(\eta_{kk}\), are expressed through the \(k\)th band density of states, \(\rho_k(E) = \langle 2/V \rangle \sum_p \delta(E - \varepsilon_{kp})\), according to

(19)
Thus, the model under consideration involves five phenomenological parameters: the potentials \( u_{c,v} \) and \( u_z \) (case A), or \( u_d \) (case B), or \( u_e \) (case C) in Eq.(15) and the factors \( \lambda_{c,v} \) determined by Eq.(17). Another values \( l_{c,v} \) in Eq.(17) and the functions \( \eta_{c,v,E} \) given by Eq. (19)) are expressed through the parameters of the ideal crystal determined in kp-approach.

B. Resonant states

We consider here \( \Delta \rho_E \) determined by Eq.(9) taking into account both diagonal and non-diagonal contributions to Eq.(15). Below we use \( 6 \times 6 \) matrix \( \hat{\Lambda}_E \hat{U} \) and we introduce \((1 - \hat{\Lambda}_E \hat{U})^{-1}\) in the matrix form:

\[
\hat{\Lambda}_E \hat{U} = \begin{bmatrix}
\lambda_{cE} u_c & \lambda_{cE} \tilde{u} \\
\lambda_{vE} \tilde{u}^+ & \lambda_{vE} u_v \\
\end{bmatrix},
(1 - \hat{\Lambda}_E \hat{U})^{-1} = \begin{bmatrix}
\hat{x}_c & \hat{x}_{cv} \\
\hat{x}_{vc} & \hat{x}_v \\
\end{bmatrix},
\]

where the \( 4 \times 2 \) matrices \( \tilde{u}_{A,B,C} \) are given by the Eq.(15). The components of the reciprocal matrix in (20) are determined from the \( 6 \times 6 \) matrix equation:

\[
\begin{bmatrix}
\lambda_{cE} u_c & \lambda_{cE} \tilde{u} \\
\lambda_{vE} \tilde{u}^+ & \lambda_{vE} u_v \\
\end{bmatrix} \begin{bmatrix}
\hat{x}_c \\
\hat{x}_{cv} \\
\hat{x}_{vc} \\
\hat{x}_v \\
\end{bmatrix} = 1.
\]

Using these notations, we write Eq.(9) as follows:

\[
\Delta \rho_E = \frac{\eta_{im}}{\pi} \text{Im} \left[ \lambda'_{cE} \text{tr} \left( u_c \hat{x}_c + \tilde{u} \hat{x}_{vc} \right) + \lambda'_{vE} \text{tr} \left( u_v \hat{x}_v + \tilde{u}^+ \hat{x}_{cv} \right) \right].
\]

where \( \lambda'_{cE} = d\lambda_{cE}/dE \). Further calculations reduce Eq.(21) to the \( 2 \times 2 \) linear equations and result for \( \Delta \rho_E \) takes standard form:

\[
\Delta \rho_E = \frac{2n_{im}}{\pi} \text{Im} \left[ \frac{(dL'_E/dE)}{L_E} + \frac{\lambda'_{vE} u_v}{1 - \lambda_{vE} u_v} \right],
\]

where the last term is due to the heavy hole contribution. The function \( L_E \) is written as:

\[
L_E = (1 - \lambda_{cE} u_c)(1 - \lambda_{vE} u_v) - w\lambda_{cE} \lambda_{vE}, \quad w = \begin{cases} 
2u^2_0/3, & A \\
4u^2_0/3, & B \\
2u^2_0, & C 
\end{cases}
\]

with the different factors \( w \) for the cases A-C under consideration.

According to Eqs.(16)-(19), \( L_E \) depends on \( E \) weakly and has the small imaginary part. It is convenient to introduce the level energy \( E_o \), which is given by a root of the linear equation: \( \text{Re} L_{E_o} = 0 \). Thus, the function \( L_E \) is transformed into \( L'_0(E - E_o - i\Gamma_o) \) where the coefficient, \( L'_0 \), and the broadening energy, \( \Gamma_o \), are introduced as follows:

\[
L'_0 = l_c u_c (1 - \lambda_{cE} u_v) + l_v u_v (1 - \lambda_{vE} u_c) + w(l_c \lambda_{cE} \lambda_{vE} + l_v \lambda_{cE} \lambda_{vE}),
\]

\[
\Gamma_o = \left[ \eta_{cE} u_c + \eta_{vE} u_v + w(\eta_{cE} \lambda_{cE} \lambda_{vE} + \eta_{vE} \lambda_{cE} \lambda_{vE}) \right]/L'_0
\]

Note that \( \eta_{cE} \) and \( \Gamma_o \) are proportional to the density of states in c- or v-band, if \( E_o > 0 \) or \( E_o < -\varepsilon_g \). It follows that the broadening energy for the v-band resonant state, with \( E_o < -\varepsilon_g \), exceeds \( \Gamma_o \) for the c-band resonant state, with \( E_o > 0 \). The same transformation can be performed for the last term of Eq.(23), so that the level, \( E_v \), is determined from the equation \( 1 - \lambda_{cE} u_v = 0 \) and the broadening energy is equal to \( \eta_{cE}/l_v \).

If a deep local level appears in the gap, \( 0 > E_{o,n} > -\varepsilon_g \), then the broadening energy is replaced by +0 and the contribution to \( \Delta \rho_E \) takes form: \( 2n_{im}\delta(E - E_{o,n}) \). The cases \( E_{o,v} > 0 \) or \( E_{o,v} < -\varepsilon_g \) are corresponded to a resonant state over c- or v-band and \( \Delta \rho_E \) has the Lorentzian shape with the broadening energy \( \Gamma_o \):

\[
\Delta \rho_E = \frac{2n_{im}}{\pi} \frac{\Gamma_o}{(E - E_o)^2 + \Gamma_o^2}.
\]

The same result with the level energy \( E_o \) and the broadening energy \( \eta_{cE}/l_v \) is valid for the hh-contribution. Here and in Eq.(24) we have supposed that \( E_{o,v} \) or \( |E_{o,v} - \varepsilon_g| \) exceed the broadening energies for the resonant states over c- or v-bands respectively. Both \( E_o \) and \( \Gamma_o \) in Eq.(26) are determined by the short-range contributions to the factors \( \lambda_{c,v} \), so that neither an absolute value of broadening energy nor a sign of \( \Gamma_o \), which determines peak- or dip-modification in the density of states, are not fixed in the consideration performed. The only dependence on \( \varepsilon_g \) (i.e. on hydrostatic pressure) can be evaluated from these results within a few fitting parameters.
The diagonal matrices $\hat{\Delta}$ are determined by the components presented in the Table. The spin-degenerate dispersion equations are obtained from the Eqs.(14), (27) and (28) as follows:

$$
\frac{(Pp_z)^2}{2}(E-E_3) + \left[ \frac{(Pp_x)^2}{6} + \frac{2}{3}(Pp_z)^2 \right] (E-E_5) = (E-E_1) \times \begin{cases} 
(E-E_3)(E-E_5), \\
(E-E_3)(E-E_5) - \delta^2, 
\end{cases}
$$

Next, we examine modifications of the alloy bandstructure due to contributions into Eq.(14) from the matrix self-energy function determined by the Eqs.(15), (20). Using $2 \times 2$ matrix notations, we write $\hat{\epsilon} + \hat{\Sigma}$ in the form:

$$
\begin{pmatrix} 
\hat{E}_1 & 0 & 0 \\
0 & \hat{E}_3 & \hat{\Delta} \\
0 & \hat{\Delta}^+ & \hat{E}_5 
\end{pmatrix},
$$

where the non-diagonal component, $\hat{\Delta}$, is determined for the cases A-C through the characteristic energies $\delta = n_{im} u^2 \lambda_c/\sqrt{3}$ and $\hat{\Delta} = n_{im} u^2 \lambda_c/\sqrt{3}$ according to:

$$
\hat{\Delta}_A = 0, \quad \hat{\Delta}_B = i\delta, \quad \hat{\Delta}_C = \delta \begin{vmatrix} 
i & -(1+i) \\
-1-i & i 
\end{vmatrix}.
$$

The diagonal matrices $\hat{E}_{1,3,5}$ are determined by the components presented in the Table.

$\begin{array}{|c|c|c|}
\hline
 & E_{1,2} & E_{3,4} \\
\hline
A & n_{im} (u^2 \lambda_c + u^2 \lambda_o) & -\varepsilon_3 + n_{im} (u^2 \lambda_v + u^2 \lambda_c) \\
\hline
B & n_{im} (u^2 \lambda_c + 4u^2 \lambda_o/3) & -\varepsilon_3 + n_{im} (u^2 \lambda_v + u^2 \lambda_c/3) \\
\hline
C & n_{im} (u^2 \lambda_c + 2u^2 \lambda_o) & -\varepsilon_3 + n_{im} (u^2 \lambda_v + u^2 \lambda_c) \\
\hline
\end{array}$

FIG. 1: The dispersion laws along $p \perp OZ$ ($p_x$, solid curves) and $p \parallel OZ$ ($p_z$, dotted curves) directions for the case A, if $E_3 > E_5$ (a) and $E_3 < E_5$ (b).

C. Alloy bandstructure

According to Eq.(29) the extreme energies, $E_{3,5}$, in the case $A$ and $E_{3} = E_3 \pm |\delta|$ in the case $B$, appear to be linear dependent on the alloy composition [12]. A bowing of $\nu$-band extreme energies with increase in alloy composition takes place for the case $B$.

$$
E_\pm = \frac{E_3 + E_5}{2} \pm \sqrt{\left(\frac{E_3 + E_5}{2}\right)^2 + \delta^2}
$$
FIG. 3: The dispersion laws along the cubic diagonal \( p \) and if \( E \) cases 

The anisotropy of energy spectrum takes place if \( E_3 \neq E_5 \) in the cases A and B, or if \( \delta \neq 0 \) in the case C. These dispersion laws are shown in Figs.1-3 for the narrow-gap alloy with 

\[ 2m_0 \Omega^2 = 25 \text{ eV}, m_0 \text{ is the free electron mass, and with } \varepsilon_g = 0.25 \text{ eV}. \]

Here we suppose the negative shift of \( c \)-extremum, \( E_1 = -0.1 \text{ eV} \), for the all cases A-C and the energies \( \delta, \bar{\delta} \) are chosen as 0.05 eV. We consider a different order of \( v \)-bands: \( E_3 = -0.2 \text{ eV}, E_5 = -0.3 \text{ eV} \) (a) and \( E_3 = -0.3 \text{ eV}, E_5 = -0.2 \text{ eV} \) (b) for the cases A, B in Figs.1,2, and we suppose \( E_{3-6} = -0.3 \text{ eV} \) and \( E_{3-6} = -0.2 \text{ eV} \) in Figs. 3a and 3b respectively. One can see that the dispersion laws appear to be weakly anisotropic in the cases A and B while a visible anisotropy takes place for the case C. We note also a substantial modification of the \( v \)-band extrema if the splitting energy, \( |E_3 - E_5| \), is comparable with \( \varepsilon_g \).

The zero-gap bandstructure can be realized if \( E_1 = E_3 \) or if \( E_1 = E_5 \) for the case A and if \( E_1 = E_+ \) for the case B and if \( E_1 = E_3 + \delta \) for the case C. In the vicinity of the cross-point energy, if \( |E - E_1|, |P| \) are less than the energy spacing to the lower \( v \)-band, the dispersion laws are given by:

\[
E_{\pm p} \simeq E_1 \pm \begin{cases} \sqrt{(P_{p_\perp})^2 + (2/3)(P_{p_\parallel})^2}, & E_1 = E_3 \\ \pm P_{p_\perp}/\sqrt{2}, & E_1 = E_5 \end{cases} \tag{A}
\]

\[
E_{\pm p} \simeq E_1 \pm \sqrt{\frac{E_1 - E_5}{E_1 - E_-} \left( \frac{p_\perp^2}{6} + \frac{2p_\parallel^2}{3} \right) + \frac{E_1 - E_3}{E_1 - E_-} \frac{p_\parallel^2}{2}}, \tag{B}
\]

\( p_\parallel, p_\perp \) are the wavevector components along and perpendicular to the bandaxis, respectively. 

\( P_{p_\perp} = p_\perp m_0 \Omega^2 \), and \( P_{p_\parallel} = m_0 \Omega^2 \).
\[ E_{\pm p} \simeq E_1 \pm \frac{\mathcal{P}}{\sqrt{3}} \sqrt{p^2 + \text{sign}(\delta)(p_x p_y + p_x p_z + p_y p_z)}, \quad (C). \]

Thus, we have obtained a linear dispersion laws which demonstrate an essential anisotropic behavior in the vicinity of the cross-point energy.

IV. CONCLUDING REMARKS

In this paper, we have developed the generalized kp-approach for the description of the short-range defects with reduced symmetry. We have considered the peculiarities of the density of states due to the resonant state contributions as well as those of the alloy bandstructure. In contrast to the previous considerations, here we have used the matrix form of the potential energy in kp-equations which leads to the additional interband mixing. In spite of the simplified model including a few phenomenological parameters, we have demonstrated an essential modification of the results due to the non-diagonal part of matrix potential.

Next, we discuss the main assumptions used. The above approach is based on the single-particle description of the electron states which is valid for many kinds of defects in A\_3B\_5 semiconductors. Although the general equations (3)-(12) are based on the presumption of low energy of electrons only, the concrete results are restricted due to the specific microscopic potentials used and due to the narrow-gap approximation based on the isotropic 6\times6 Kane model. The last approximation supposes that far-band contributions do not change the results qualitatively. We have also used the low-concentration approximation, supposing that the electronic states at different impurities do not overlap in Sec. IIB, and we have used the Born approximation in Sec. IIC. In order to include an often-discussed effect of resonant states on an alloy bandstructure, one needs to use a more complicate self-energy function, e.g. employing the coherent potential approximation, see Ref.9. Last but not least, we note that the potential \( \delta U_r \) in Eq.(2) is assumed to be spin-independent, i.e. we have neglected the spin-flip processes induced by the short-range defect. All these assumptions restrict the quantitative description of the phenomena resulting from short-range defects therefor the results obtained do not related to any concrete case. What this paper does, however, it demonstrates clearly that the matrix character of the short-range potential energy in Eq.(3) may change the results essentially.

Finally, we suppose that the consideration performed will stimulate a reexamination the later obtained results both for defects with reduced symmetry in A\_3B\_5 semiconductors (see discussion in [12]) and for bandstructure of A\_3B\_5-based alloys. Application of such kind of approach for another materials (e.g. A\_4B\_4-based alloys, see [13]) requires a special consideration. In spite of the fact that the obtained results demonstrate some peculiarities of A\_3B\_5-based alloys, a more detail comparison is restricted due to lack of experimental data for the narrow-gap case under consideration (see recent papers [14]). Since the components of the matrix potential can not be fixed in the framework of the kp-approach developed, a comparison of such type results with numerical calculations is also of interest.

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