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Anderson impurity states in band-inverted semiconductor heterojunctions

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The development of the Anderson impurity model for the case of the symmetry-inverted band-edge heterojunction that was considered in the framework of the effective Dirac model has been suggested. The Anderson impurity due to interaction with the heterojunction and the band states is shown to give the impurity level inside the band gap for the proper model parameters, its energy being changed with the impurity-atom location relative to the interface plane.

I. INTRODUCTION

Due to the systematic and extensive investigations of the layered semiconductor structures (such as heterojunctions, quantum wells, and superlattices), the problems of the impurity states have received growing attention.[1] Considerable progress has been attained in the study of the impurity states of the semiconductor structures based on the classic semiconductors (Si and Ge) and their multiple isoelectronic analogs (III-V semiconductors);[2] the shallow hydrogenic impurity states have mainly being investigated.[1] On the one hand, the impurity states in those semiconductor structures are characterized by the disturbance of the space and translation crystal symmetry along the growth axis. As a result, the impurity-state energy depends on the impurity-atom position relative to the interface boundary. On the other hand, there is quite a strong variation of the impurity binding energy with the characteristic dimension of the structure.

The problem of the impurity states in the narrow-gap semiconductor structures has received somewhat less attention despite its obvious importance. The principal peculiarity of the narrow-gap semiconductor impurity states is that, due to small gaps and other properties, the shallow impurity states do not appear. Note that in the past ten years, for the complicated problem of the impurity states of the narrow-gap IV-VI semiconductors, a new aspect connected with the doping by the group-III elements (In, Tl, and Ga) has appeared. An unusual behavior of such doped materials is connected with the generation of the resonant energy levels localized either in the conduction band (for example, In in PbTe) or in the valence band (Tl in PbTe) as well as of deep levels (Ga in PbTe).[3,4] As a result the physical properties (for example, carrier density) dramatically change. Experimental investigations show that these impurities are of the substitutional type. Taking into account the resonant character of the impurity states in the narrow-gap semiconductors, their theoretical investigation is known to use the Anderson impurity model[5] as one of the proper models for this situation.

Besides, in contrast to the problem for the bulk semiconductors, while investigating the impurity states in the quantum structures based on the narrow-gap semiconductors it is necessary to take into account the following aspect. It has been shown[6-8] that in semiconductor heterojunctions based on some narrow-gap semiconductors such as II-VI (HgTe/CdTe) or IV-VI (PbTe/SnTe), where the constituents have opposite band-edge symmetry and overlapping gaps, the interface states seem to be localized near the boundary. These states appear independently of the interface region nature and are similar to the midgap states which arises in the presence of the solitons in one-dimensional systems.[9] Later interface states were shown[10-12] to occur also in the normal heterojunction when $E_{ga}E_{gb} > 0$ (E_{ga},E_{gb} are the band gaps of the initial compounds). However, they appear at the finite values of the in-plane (along the plane of the interface) momentum and overlap band states of the semiconductor constituents.[12] In the case of the inverted band-edge heterojunction (called the inverted contact) when $E_{ga}E_{gb} < 0$, a nondegenerate gapless state has been shown[8,13] to appear inside the band gap, being localized near the boundary and having a linear spectrum in the interface plane. When the width of the transition region is quite large, besides this zeroth mode (Weyl branch) there is a set of the doubly degenerate interface states with the finite effective masses.

As a matter of fact the interface states are Tamm states,[14] which is why they generate from the bulk states of the initial compounds. So, taking into account the strong interaction of the band and impurity states in the Anderson model, the strong interdependence between impurity and interface states in the semiconductor heterojunction should be expected. Thus the aim of this paper is to develop the Anderson model for the deep impurity in the heterojunction of the narrow-gap semiconductors with mirror symmetrical bands such as those in IV-VI semiconductors, for example. Here only the case of the heterojunction with band inversion is investigated. We shall consider the symmetry heterojunction with the mirror bands and with constituent gaps equal in absolute value, that is, $|E_{ga}| = |E_{gb}|$, their middles coinciding.

In Sec. II we develop the Anderson impurity model for the case of the symmetry-inverted contact that is considered in the framework of the effective Dirac model with a coordinate-dependent band gap. In this work the band gap of the considered structure is supposed to be changed by the law $E_g(z) = E_g \tanh(z/L)$ (where L defines the heterojunction width and $E_g = |E_{ga}| = |E_{gb}|$). In Sec. III the equation determining the impurity energy level is obtained by the Green function method. Two particular cases are considered: one when $E_g L = 2\hbar v$ (v is Fermi velocity) and the other when $L \to 0$. A discussion of the results obtained and some numerical estimations are given in Sec. IV.

II. MODEL

The full Hamiltonian of the system

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{imp}} \tag{1}$$

includes the heterojunction Hamiltonian $\hat{H}_0$ and the impurity Anderson Hamiltonian $\hat{H}_{\text{imp}}$. Both materials of the studied heterojunctions of IV-VI narrow-gap semiconductors are known to have a direct gap at L points of the Brillouin zone, so that near the middle of the gap there are two bands L^+ and L^-. Thus the simplest model describing their spectrum is the two-band one, which is absolutely necessary for describing the states near the band edges of the narrow-gap semiconductors. Moreover, in the inverted-band heterojunction, the band with the fixed symmetry in one semiconductor forming the structure is the conduction band and in the other one it is the valence band. Therefore the crucial material properties we invoke are that the states near the gap in the bulk materials are adequately described by the two-band model and that one of the semiconductors has inverted bands. In earlier papers it was shown that the energy spectrum of the heterojunctions based on the narrow-gap IV-VI semiconductors in the framework of the two-band $\vec{k} \cdot \hat{\vec{p}}$ model might be described by the effective Dirac Hamiltonian with a coordinate-dependent band gap[15]

$$\hat{H}_0 = \int \Psi^\dagger(\vec{r}) \left[\gamma^0 \vec{\gamma} \cdot \hat{\vec{p}} + \gamma^0 \Delta(\vec{r}) + V(\vec{r}) \right] \Psi(\vec{r}) d\vec{r}, \tag{2}$$

where the field operator $\Psi(\vec{r})$ due to the symmetry properties of the IV-VI semiconductors is a bispinor representing the the L^- and L^+ bands; $\gamma^0, \vec{\gamma} = (\gamma^1, \gamma^2, \gamma^3)$ are the Dirac matrices; $\hat{\vec{p}} = -i\hbar(v_x \nabla_x, v_y \nabla_y, v_z \nabla_z)$ is a momentum operator, with v_x, v_y, v_z the components of the Fermi velocities; $2\Delta(\vec{r}) = E_g(\vec{r})$; and $V(\vec{r})$ is the work function, which also depends on the coordinate. To simplify analytical calculations in this paper we consider only the symmetry case when $v_x = v_y = v_z = v$. Note that accounting for the Fermi surface anisotropy does not cause the principal difficulties.

The second term in (1) describes the Anderson impurity with one level E_d localized at the lth site of the lattice. Here on-site Coulomb repulsion is neglected. In the second quantum representation $\hat{H}_{\text{imp}}$ is written in the usual form

$$H_{\text{imp}} = E_d \sum_s d_s^\dagger d_s + V \sum_s (d_s^\dagger c_{ls} + c_{ls}^\dagger d_s), \tag{3}$$

where d_s is the annihilation operator of a localized electron at the impurity atom with spin s, E_d is the atomic level, V is the mixing matrix element between the impurity and band states, and c_{ls} is the annihilation operator of an electron at the lth site of the lattice with spin $s[\vec{R}_l = a(l_1, l_2, l_3)$, a being a half period of the fcc lattice of the constituents]. Here the parameters a, E_d, and V are believed to be equal in both semiconductors.

We consider a one-dimensional heterojunction with the axis along C_3 of the initial compounds directed along the z axis. The x and y axes lie in the heterojunction plane. In this case $\Delta(\vec{r}) = \Delta(z)$. Taking into account the geometry of the task, the function Ψ can be picked out in the form

$$\Psi(\vec{r}) = \Psi(z) e^{i\vec{k}_\perp \cdot \vec{r}}, \tag{4}$$

where $\vec{k}_\perp = (k_x, k_y, 0)$ and $\Psi(z)$ is the envelope of the wave function. For the symmetry heterojunction it is necessary to set $V(\vec{r}) = 0$. So instead of (2) we obtain

$$\hat{H}_0 = \int \Psi^\dagger(z) [\gamma^0 \gamma^3 \hat{p}_z + \hbar v \gamma^0 (\vec{\gamma} \cdot \vec{k_\perp}) + \gamma^0 \Delta(z)] \Psi(z) dz. \tag{5}$$

Using the results of Ref. 15, we find that in the representation in which

$$\gamma^0 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix},$$
$$\vec{\gamma} = \begin{pmatrix} i\vec{\sigma} & 0 \\ 0 & -i\vec{\sigma} \end{pmatrix}, \tag{6}$$
$$\alpha = \gamma^0 \vec{\gamma} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix},$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, $\sigma_{x,y,z}$ are the Pauli matrices, the eigenfunctions of the equation $\hat{H}_0 \Psi = E\Psi$ can be represented in the form

$$\Psi_\lambda(z) = \frac{1}{A_\lambda} \begin{pmatrix} 1 \\ i\lambda e^{i\theta} \frac{\partial_z + k(z)}{\varepsilon + \lambda k_\perp} \\ -i \frac{\partial_z + k(z)}{\varepsilon + \lambda k_\perp} \\ \lambda e^{i\theta} \end{pmatrix} \varphi(z). \tag{7}$$

The function $\Psi_\lambda(z)$ is an eigenfunction of the "pseudoparity" operator $\hat{P} = i\gamma^0 \gamma^3 (\vec{\gamma} \cdot \vec{k_\perp})/k_\perp$, its eigenstates being $\lambda = \pm 1$. In (7) the following definitions have been introduced: $\partial_z = \partial/\partial z, \varepsilon = E/\hbar v$, $k(z) = \Delta(z)/\hbar v$, $\exp(\pm i\theta) = (k_x + ik_y)/k_\perp$, $k_\perp = \sqrt{k_x^2 + k_y^2}$, A_λ is a normalized factor, and the function $\varphi(z)$ satisfies the equation

$$\{[\partial_z - k(z)][\partial_z + k(z)] + \varepsilon^2 - k_\perp^2\} \varphi(z) = 0. \tag{8}$$

In this work the band gap of the inverted contact is supposed to be changed by the law

$$\Delta(z) = \Delta_0 \tanh\left(\frac{z}{L}\right), \tag{9}$$

where L defines the heterojunction width and $2\Delta_0 = |E_{ga}| = |E_{gb}|$. In this case the solution Eq. (8) is expressed through the hypergeometric functions. For the delocalized states determining the spectrum of the quasi-two-dimensional energy bands of the heterojunction one obtains

$$\varphi_k(z) = e^{ikz} F\left(1 + k_0L, -k_0L, 1 - ikL; \frac{1}{2}\left[1 - \tanh\left(\frac{z}{L}\right)\right]\right) . \tag{10}$$

Here $k_0 = \Delta_0/\hbar v$ and $\varepsilon = \pm\sqrt{k_0^2 + k^2 + k_\perp^2}$ for any k.

The interface states localized near the boundary are described by the function

$$\varphi_p(z) = \mathrm{sech}^p\left(\frac{z}{L}\right) F\left(1 + p + k_0L, p - k_0L, p + 1; \frac{1}{2}\left[1 - \tanh\left(\frac{z}{L}\right)\right]\right), \tag{11}$$

where $\varepsilon = \pm\sqrt{k_0^2 + k_\perp^2 - (\frac{p}{L})^2}$. As follows from the boundary conditions, the localized interface state spectrum is discrete, the parameter p being defined from the condition

$$p = k_0L - n \ , \tag{12}$$

where the integer n changes in the limits

$$0 \leq n < Lk_0. \tag{13}$$

At $n = 0$ the zero mode, called the Weyl branch, with a spectrum linear on $k_\perp$, has been obtained.[8] In the limit of the infinite structure dimensions the zero mode is spin nondegenarate. Note that, as it follows from (7), in the case of the finite structure, any eigenstate E of the Hamiltonian $\hat{H}_0$ is doubly degenerate on the parameter λ. This is an obvious consequence of the double Kramer's degeneracy of all energy levels of the original compounds having a center of inversion that is still preserved in the investigated symmetry-inverted contact.

Thus taking into account the dependence of the wave function $\Psi_\lambda(z)$ (7) on the parameters λ, k (or p), $k_\perp$, and the sign of ε, the field operator is written in the expansion form

$$\Psi(\vec{r}) = \frac{1}{\sqrt{L_1L_2}} \sum_i \Psi_i(z) e^{i\vec{k}_\perp \cdot \vec{r}} a_i, \tag{14}$$

where i marks the set of all the quantum numbers defining $\Psi(z)$; a_i is the annihilation operator of the particle in the ith state; and L_1, L_2, and L_3 are the system sizes along x, y, and z axes, respectively.

Using the expansion (14) for $\hat{H}_0$ and $\hat{H}_{\text{imp}}$ one obtains

$$\hat{H}_0 = \sum_i E_i a_i^\dagger a_i, \tag{15}$$

$$\hat{H}_{\text{imp}} = a^{3/2} V[d_s^\dagger \chi_l^\dagger \Psi(\vec{R}_l) + \Psi^\dagger(\vec{R}_l)\chi_l d_s] + E_d \sum_s d_s^\dagger d_s. \tag{16}$$

Here E_i is the eigenstate of the Hamiltonian $\hat{H}_0$ following from Eq. (8). Taking into account the symmetry properties of the initial compounds the operator c_l in $\hat{H}_{\text{imp}}$ has been expressed through $\Psi(\vec{R}_l)$

$$c_l = a^{3/2}\chi_l^\dagger \Psi(\vec{R}_l), \tag{17}$$

where in the representation (6) used

$$\chi_l^\dagger = \sqrt{2}\left(\cos\frac{\pi}{2}l, \cos\frac{\pi}{2}l, -i\sin\frac{\pi}{2}l, -i\sin\frac{\pi}{2}l\right), \tag{18}$$

$l = l_1 + l_2 + l_3$. In the expression (16), the supposition about the equality of the interaction matrix elements between impurity states, on the one hand, and states of the conduction and valence bands as well as localized interface states, on the other hand, has been used. Refuse from this supposition leads to the appearance of some new parameters instead of the one parameter V.

III. SOLUTION

Following the method elaborated in Ref. 16, we define the Green functions

$$\begin{aligned} G_d^s(\tau) &= -\langle T\tau d_s(\tau) d_s^\dagger(0)\rangle \ , \\ G_i(\tau) &= -\langle T\tau a_i(\tau) a_i^\dagger(0)\rangle \ , \\ G_{id}^s(\tau) &= -\langle T\tau a_i(\tau) d_s^\dagger(0)\rangle \ , \end{aligned} \tag{19}$$

where $d_s(\tau) = e^{\tilde{H}\tau} d_s e^{-\tilde{H}\tau}$, $\tilde{H} = H + \mu N_e$, μ being the chemical potential and N_e the electron number. By means of the method of the Green function motion equations in the energy representation one obtains

$$(i\omega_n + \mu - E_d)G^s_d(\omega_n) = 1 - \sqrt{\frac{a^3}{L_1L_2}} V\chi_l^\dagger \sum_i e^{-i\vec{k}\cdot\vec{R}_l}\Psi_i(\vec{R}_l)G^s_{id}(\omega_n)\ , \tag{20}$$

$$(i\omega_n + \mu - E_i)G^s_{id}(\omega_n) = -\sqrt{\frac{a^3}{L_1L_2}} V e^{i\vec{k}\cdot\vec{R}_l}\Psi_i^\dagger(\vec{R}_l)\chi_l G^s_d(\omega_n). \tag{21}$$

Then we have

$$G^s_d(\omega) = \left[i\omega_n+\mu-E_d-\frac{V^2a^3}{L_1L_2}\sum_i \chi_l^\dagger\frac{\Psi_i(\vec{R}_l)\Psi_i^\dagger(\vec{R}_l)}{i\omega_n+\mu-E_i}\chi_l\right]^{-1}. \tag{22}$$

Here the summation over i is implied to be carried out over all the quantum numbers defining the function Ψ_i, that is, over $\vec{k}_\perp, k$ for delocalized states and over p for localized states as well as over states with $E_i > 0$ and $E_i < 0$. Substituting the evident expression of the function $\Psi_i(\vec{R}_l)$ (7) for the sum from (22) we find

$$\begin{aligned}\sum \equiv \chi_l^\dagger \sum_i \frac{\Psi_i(\vec{R}_l)\Psi_i^+(\vec{R}_l)}{\omega - E_i}\chi_l = \sum_{\vec{k}_\perp, k(p)} \frac{2\omega}{\omega^2 - E_i^2}\Bigg\{ &\frac{1}{A_i^\dagger}\left[\varphi^2(z_l) + \left(\frac{\partial_z + k(z)}{\varepsilon_i + k_\perp}\varphi(z)\,|_{z=z_l}\right)^2\right] \\ &+ \frac{1}{A_i^-}\left[\varphi^2(z_l) + \left(\frac{\partial_z + k(z)}{\varepsilon_i - k_\perp}\varphi(z)\,|_{z=z_l}\right)^2\right]\Bigg\},\end{aligned} \tag{23}$$

where $\omega = i\omega_n + \mu$, the normalized multiplier being expressed in the form

$$A_i^\pm = 2\int_{-L_3/2}^{L_3/2}\left[\varphi^2(z) + \left(\frac{\partial_z + k(z)}{\varepsilon_i \pm k_\perp}\varphi(z)\right)^2\right]dz. \tag{24}$$

Now we shall consider two particular cases: one when $k_0L = 1$ and the other when $L \to 0$. Note that in both cases only the zeroth mode with $n = 0$ appears. All calculations are performed analytically. So when $k_0L = 1$, the sum from (22) is written in the form

$$\frac{V^2a^3}{L_1L_2}\sum = -\frac{V^2a^3\hbar v}{8\pi L^2}\int_0^\infty \frac{\omega\,\mathrm{sech}^2(\frac{z_l}{L})dk_\perp^2}{(\hbar^2v^2k_\perp^2 - \omega^2)\sqrt{\Delta_0^2 + \hbar^2v^2k_\perp^2 - \omega^2}} + 2\omega\frac{V^2a^3}{(2\pi)^3}\int\frac{d\vec{k}}{\omega^2 - \Delta_0^2 - \hbar^2v^2k^2}. \tag{25}$$

Here it is supposed to be $\Delta_0^2 - \omega^2 \geq 0$, that is, only the states lying inside the band gap are considered.

When integrating over $\vec{k}$ the second term in (25) is divergent. This divergence is conditioned by the approximation of the effective mass method and is common for a task such as this. The problem of the divergent integral calculation can be formally solved by introducing the additional parameter K to limit the integration region over k. In its essence K describes the bandwidth.

So after simple calculations we obtain

$$G_d(\omega) = \left\{\omega - E_d - \frac{\omega\alpha\Delta_0}{8\pi}\mathrm{sech}^2\left(\frac{z_l}{L}\right) \times \left[\ln\left|\frac{\Delta_0 - \sqrt{\Delta_0^2 - \omega^2}}{\Delta_0 + \sqrt{\Delta_0^2 - \omega^2}}\right| - i\pi\right] + \frac{\alpha\omega}{\pi^2}\left(\hbar vK - \frac{\pi}{2}\sqrt{\Delta_0^2 - \omega^2}\right)\right\}^{-1}, \tag{26}$$

where $\alpha = V^2a^3/(\hbar^3v^3)$. From here the local density of the impurity states is found

$$\rho_{dd}(\omega) = -\frac{1}{\pi}\mathrm{sgn}\omega\,\mathrm{Im}G_{dd}(\omega) = \frac{\frac{1}{\pi}\mathrm{sgn}\omega f_2(\omega)}{f_1^2(\omega) + f_2^2(\omega)}, \tag{27}$$

where

$$f_1(\omega) = \omega - E_d + \frac{\alpha\omega}{\pi^2}\left(\hbar vK - \frac{\pi}{2}\sqrt{\Delta_0^2 - \omega^2}\right) - \frac{\alpha\Delta_0}{8\pi}\omega\,\mathrm{sech}^2\left(\frac{z_l}{L}\right)\ln\left|\frac{\Delta_0 - \sqrt{\Delta_0^2 - \omega^2}}{\Delta_0 + \sqrt{\Delta_0^2 - \omega^2}}\right|, \tag{28}$$

$$f_2(\omega) = \frac{\omega\alpha\Delta_0}{8}\mathrm{sech}\left(\frac{z_l}{L}\right). \tag{29}$$

In the quasiparticle approximation the equation

$$f_1(\omega) = 0 \tag{30}$$

defines the energy of the impurity level in the system of the symmetry-inverted contact when $k_0L = 1$.

The finite quantity of the impurity state density is bound up with the interaction between the impurity and interface states. While the impurity atom is removed from the heterojunction boundary, the peak of the density of states abruptly increases. When $z_l \to \infty$, $\rho_{dd}(\omega) \sim \delta(\tilde{E}_d)$, $\tilde{E}_d$ satisfying Eq. (30) at $z_l \to \infty$ and determining the impurity level position renormalized due to an interaction with the band states in the homogeneous semiconductor. From (27) we get $\rho_{dd}(0) = 0$. It is conditioned by the linear dependence of the interface state density on the energy.

In the case $\omega^2 > \Delta_0^2$, after simple calculations for the impurity Green function we obtain

$$G_d(\omega) = \left(\omega - E_d + \frac{\omega\alpha\hbar v K}{\pi^2} + i\frac{\alpha\omega}{2\pi}\left\{\operatorname{sech}^2\left(\frac{z_l}{L}\right) \times\frac{\Delta_0}{2}\left[\frac{\pi}{2} + \arctan\left(\frac{\sqrt{\omega^2-\Delta_0^2}}{\Delta_0}\right)\right] + \sqrt{\omega^2-\Delta_0^2}[\Theta(\omega-\Delta_0) - \Theta(-\omega-\Delta_0)]\right\}\right)^{-1} . \tag{31}$$

The local density of impurity states is defined by Eq. (21) with

$$f_1(\omega) = \omega - E_d + \frac{\alpha\omega\hbar v K}{\pi^2}, \tag{32}$$

$$f_2(\omega) = \frac{\omega\alpha}{2\pi}\left[\sqrt{\omega^2-\Delta_0^2} + \operatorname{sech}^2\left(\frac{z_l}{L}\right) \times\frac{\Delta_0}{2}\left(\frac{\pi}{2} + \arctan\frac{\sqrt{\omega^2-\Delta_0^2}}{\Delta_0}\right)\right] . \tag{33}$$

Then Eq. (30) again defines the energy of the impurity states.

By analogy with the foregoing calculations, in the case of the stepped heterojunction, when $L \to 0$ the impurity Green function is written in the form

$$G_d(\omega) = \left(\omega - E_d - \omega\alpha\left\{\operatorname{sech}^2\left(\frac{z_l}{L}\right)\ln\left|\frac{\Delta_0 - \sqrt{\Delta_0^2-\omega^2}}{\Delta_0 + \sqrt{\Delta_0^2-\omega^2}}\right| - \left[2\operatorname{sech}^{2k_0L}\left(\frac{z_l}{L}\right) - \operatorname{sech}^2\left(\frac{z_l}{L}\right)\right]\ln\left|\frac{\omega^2 - \hbar^2v^2K_\perp^2}{\omega^2}\right| - \frac{4}{\Delta_0}\left(\sqrt{\Delta_0^2-\omega^2+\hbar^2v^2K_\perp^2} - \sqrt{\Delta_0^2-\omega^2}\right)\right\} + i2\pi\alpha\omega\operatorname{sech}^{2k_0L}\left(\frac{z_l}{L}\right)\right)^{-1} . \tag{34}$$

Here, instead of the parameter K, another parameter $K_\perp$ has been introduced. It limits the integration region over $k_\perp$. Equation (34) is obviously written for $\Delta_0^2 - \omega^2 > 0$. Expressions such as (27)–(30) can be obtained in this case as well.

IV. DISCUSSION AND CONCLUSIONS

First let us discuss the case $k_0L = 1$. While $z_l \to \infty$, Eq. (30) determines the energy of the impurity state $\tilde{E}_d$ in the homogeneous semiconductor. Under the condition

$$E_d \leq \Delta_0\left(1 + \frac{\hbar v\alpha K}{\pi^2}\right) , \tag{35}$$

the solution of Eq. (30) is that inside the band gap, the impurity level appears. As it follows from the definition of the parameter K, the condition (35) is broken when the initial impurity state E_d lies very high inside the band. So due to the interaction with the band electrons, the impurity states fall into the band gap. Using this result the expression for $f_1(\omega)$ (28) can be simplified by substituting the second and third terms for the renormalized impurity state $\tilde{E}_d$. Then there is the single parameter $\tilde{E}_d$ in our task instead of two, E_d and K.

Equation (30) defines the impurity state in the system of the inverted contact. Under the condition (35) inside the band gap the impurity state appears. Due to the interaction between the impurity and interface localized states, there is a dependence of the impurity energy on the local position of the impurity atom relative to the interface boundary. Figure 1 shows the impurity-state energy versus the impurity-atom location on the z axis. For the calculation we used the following parameters: $V = 1$ eV, $V = 10^7$ cm/s, $E_d = 1$ eV, $a = 3.3$ Å, $K = 3$ eV, and $\Delta_0 = 0.1$ eV.

As it follows from the figure, at the heterojunction boundary the impurity level is driven into the middle of the band gap. While leaving from the interface, the impurity state goes to the limit value $\tilde{E}_d$ for the homo-

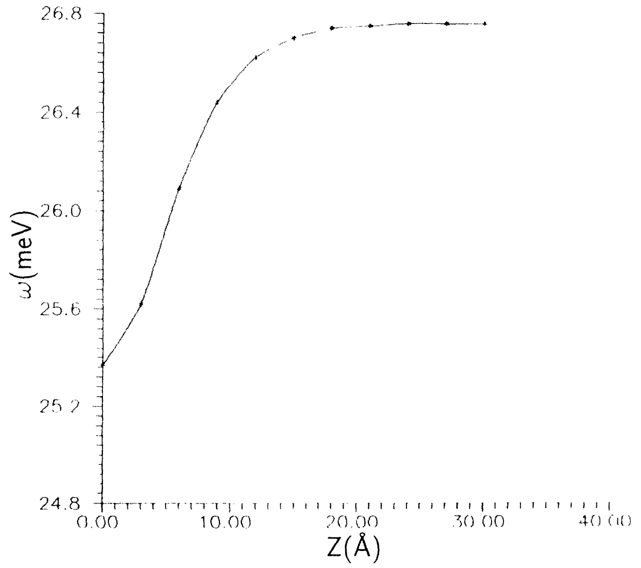

FIG. 1. The impurity state energy versus the impurity atom location on the axis z. (The origin of the energy scale is μ.)

geneous semiconductor. Decreasing the interaction between the interface and impurity states, that is, decreasing the parameter V and increasing the Fermi velocity v, this effect certainly becomes less marked.

Figure 2 shows the impurity-state density ρ_{dd} versus the energy for two positions of the impurity atoms: $z_l = 0$ when the impurity atom is located at the boundary (dashed line) and $z_l = 6$ Å (solid line). It is clear from Fig. 2 that while removing the impurity atom from the boundary, the impurity level half-width noticeably decreases. The peak of the impurity states approach the larger energy going to its limit value $\tilde{E}_d$.

While increasing the atomic impurity level E_d, the inverted contact impurity state goes to the band edge. When the condition (35) is broken the impurity level leaves the band gap and falls within the band, and as it appears from (34) its value does not depend on the impurity location. Note that from the essence of the parameter K, the condition (35) seems to be broken when the supposition about the two-band model used in this work is incorrect.

All the conclusions obtained above also apply in the case of the stepped interface when $L \to 0$. Note that the condition (35) is fulfilled for the typical parameters for the narrow-gap IV-VI semiconductors and for the initial impurity energies characteristic of them. Thus the Anderson impurity due to the interaction with the band and interface states of the inverted contact gives the energy level within the band gap, its energy being changed with the location of the impurity atom. The supposition about the symmetry of the inverted contact is obviously not principal; it only gives an opportunity to simplify the calculations. So all the conclusions are kept and for any inverted contact with any relations between band gaps of the initial compounds. Besides, as noted above, the impurity states appear both in the inverted contact and in the normal heterojunction when $E_{ga}E_{gb} > 0$. So it may be supposed that the peculiarities of the impurity states obtained in this paper have to be observed and in the normal heterojunction in which the interface states appear.

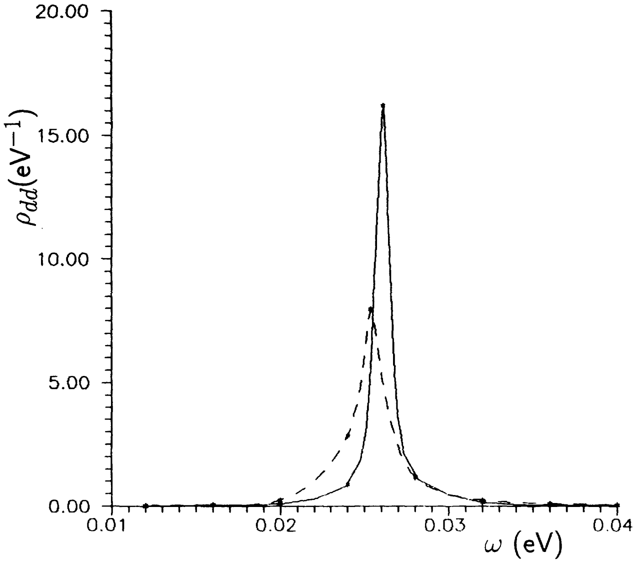

FIG. 2. The impurity state density ρ_{dd} versus the energy for two positions of the impurity atoms: $z_l = 0$ Å (dashed line) and $z_l = 6$ Å (solid line). (The origin of the energy scale is μ.)

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