Interface states in stressed semiconductor heterojunctions with antiferromagnetic ordering

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Stressed heterojunctions with antiferromagnetic ordering, in which the constituents have opposite band-edge symmetry and their gaps have opposite signs, have been investigated. Interface states have been shown to appear in these heterojunctions, and they are spin split. If the Fermi level lies in one of the interface bands, this results in magnetic ordering in the interface plane. The interface magnetization effect is expected to take place. A breakdown of the fundamental symmetries of time and space inversions in such structures is outlined. [S0163-1829(97)05927-4]

I. INTRODUCTION

Interest in quantum structures (such as heterojunctions, quantum wells, and superlattices) is to a certain extent conditioned by interface states localized near the boundary between constituent semiconductors. The interface states appearing in semiconductor structures due to a band bending are traditionally considered. Such interface states are known to be bound up with the transitional region structure. On the other hand, there is a considerable interest in the study of Tamm's-type interface states arising in some semiconductor structures. In contrast to the first case, the latter interface states are not concerned with the transition region structure, being generated from the bulk energy bands of the constituents. At first the Tamm's interface states were theoretically considered[1–3] in the so-called inverted contacts (that is, in semiconductor heterojunctions based on semiconductors with mutually inverted bands), so that the gaps of their constituents have opposite signs. The same interface states have been shown[4,5] to appear not only on the heterojunction boundary but on other inhomogeneities of the electron system, such as an antiferromagnetic ordering vector inhomogeneity (realized as an antiferromagnetic domain wall) and a polarization vector inhomogeneity (a ferroelectric one); combinations of these inhomogeneous fields result in a variety of systems with disturbed symmetrical properties. This is an important point, giving an opportunity to separate the interface states into a separate group.

As an example of inverted contacts, heterojunctions based on some narrow-gap IV-VI or II-VI semiconductors used to be considered. In this case, a treatment of the simplest two-band approximation, the interface states have a gapless band spectrum that is linear in the interface plane, their energy reaching the gap of the constituent semiconductors. Subsequent investigations[3,6] showed that the same interface states can exist in heterojunctions with normal band arrangements. However, in contrast to the inverted heterojunction, these states appear either inside the conduction or valence bands of the constituents, the energy spectrum being cut off at a finite transverse (along the interface plane) momentum. Later it was shown that there are interface states in superlattices[7,8], quantum wells,[9] and quantum dots.[10] It is worth noting that, quite recently,[11] magnetic-field dependences of the Hall coefficient in PbTe/SnTe superlattices have been interpreted, assuming that, in addition to electrons in PbTe and holes in SnTe, a third kind of charge connected with the abovementioned interface states appears. A more direct investigation of the two-dimensional interface states has been performed by means of magnetotunneling spectroscopy of the p-$Hg_xCd_{1-x}Te$ quantum well in Ref. 12.

The majority of semiconductor structures are stressed due to a lattice mismatch of their constituents. The electron energy spectrum of the stressed semiconductor structures is determined by the strains, as well as by the widths of their layers and physical parameters of the constituents. A more direct strain effect is the change of the energy spectrum, which is different in each constituent and depends upon the acoustic deformation potentials of both conduction and valence bands. This problem has been rigorously investigated in different semiconductor structures.[13] In stressed semiconductor structures the elastic strains, or their gradients due to piezoelectric or flexometric effects, can lead to static polarization fields.[14] These fields are determined by the strain values, elastic constants, piezoelectric coefficients, and other material parameters which apparently are different in each of the alternating layers. In fact the polarization is conditioned by the mutual shifts of the cation and anion sublattices of a binary (or multinary) semiconductor. Proceeding from the fact that each of these sublattices in their turn generates the energy states of either conduction or valence bands, in our earlier work[6] we investigated the strain-induced polarization effect on the boundary interface states of the semiconductor heterojunction. As for the straight deformation effect on the interface states' energy spectrum, it was shown[6] that this effect is quite trivial, and results in homogeneous shifts of the energy bands.

At doping with transition or rare-earth elements, IV-VI or II-VI semiconductors turn into dilute magnetic ones, and at low temperature they might transit to ferromagnetic or antiferromagnetic states. Quantum structures based on such semimagnetic semiconductors have been intensively investigated in view of their interesting physical properties,[15–17] their nontrivial (as compared with bulk materials) magnetic properties being emphasized.[18–20] Moreover, it has been recognized[21] that interfaces play a key role in the magnetic properties of heterostructures based on semimagnetic semiconductors. The origin of the effects used to be connected with the structure of the interface plane, its imperfection, and

the disposition of the magnetic impurities across the interface. In this paper another model of the interface magnetization effect, based on magnetic properties of the interface states, will be developed.

A crucial point of problems concerning the interface states is that for inverted stressed semiconductor structures with antiferromagnetic ordering, we have a situation in which all three fields cited above (composition, polarization, and antiferromagnetic) are applied to the system. Such stressed semiconductor heterocontacts with antiferromagnetic ordering are quantum structures with a breakdown of the fundamental symmetries of time and space inversion. The breakdown of the T invariance is a result of the antiferromagnetic ordering, while the space inversion asymmetry is a general property of any heterostructure. In our case for a stressed heterocontact, an additional space asymmetry occurs due to strain-induced polarization. It is well known that time inversion symmetry provides the Kramers degeneracy, while space inversion symmetry gives a twofold degeneracy which is referred to as the spin degeneracy. In the structures in question, both types of degeneracy are absent. Therefore, such heterostructures must be systems with unusual microscopic electron properties. One of them is interface magnetization effect considered in this paper.

The aim of this work is to study interface states in stressed inverted contacts based on semimagnetic narrow-gap semiconductors with antiferromagnetic ordering. It is worth noting that a similar situation might be found in the system with electron-hole pairing. After placing commensurate waves of spin and charge density over the system, the energy spectrum of the latter turns out to be spin split. Under limit doping this leads to electron-spin ordering (that is, we have a system with exciton ferromagnetism).[22] Now, taking into account that spin- and charge-density waves might be induced by the antiferromagnetic ordering and by structural lattice distortions (which are accompanied by the polarization), respectively, one can affirm that systems with polarization and antiferromagnetic ordering will be similar to the system with the exciton ferromagnetism.

To define our calculations completely, heterojunctions based on semimagnetic narrow-gap IV-VI semiconductors will be studied. Since Tamm's interface states are generated from the bulk states of the constituent semiconductors, initially in Sec. II we develop a spectrum model of the bulk stressed narrow-gap IV-VI semiconductors with antiferromagnetic ordering. The effective Dirac Hamiltonian will be used as a model. In Sec. III the interface states of the inverted stressed contact with antiferromagnetic ordering will be considered, two cases being studied. One of these is a case in which the antiferromagnetic ordering is the same in the initial semiconductors, and the other a case when it has opposite signs in the constituents. A spin analysis of the interface states is given in Sec. IV. This is followed by a brief summary.

II. MODEL AND SPECTRUM OF THE BULK SEMICONDUCTORS

Both materials of the studied heterojunctions of narrow-gap IV-VI semiconductors are known to have a direct gap at L points of the Brillouin zone. Thus near the gap middle there are two double degenerate bands L^+ and L^- with opposite coordinate symmetries. Thus the simplest model of the narrow-gap IV-VI semiconductor spectrum is the two-band one.[23,24] In the case of mirror symmetry bands, the energy spectrum of the semiconductor heterojunction with the trigonal [111] crystal axis picked as the z axis might be described by the effective Dirac Hamiltonian

$$\hat{H}_{00}=\begin{pmatrix} \Delta & \vec{\sigma}\cdot\hat{\vec{p}} \\ \vec{\sigma}\cdot\hat{\vec{p}} & -\Delta \end{pmatrix}, \tag{1}$$

where the upper and lower blocks are related to the states φ and χ of the conduction and valence bands, respectively; $\vec{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ is the vector with the components of the Pauli matrices $\hat{\vec{p}}=-i\hbar(v_\perp\nabla_x,v_\perp\nabla_y,v_\parallel\nabla_z)$, $v_{\perp,\parallel}$ being the interband coupling matrix elements having dimensions of velocity; and $\Delta=E_g/2$, E_g is the energy gap depending on the z coordinate, if the heterojunction along z is in question. Note that this Dirac form of Hamiltonian (1) is just a first approximation of the $\vec{k}\cdot\hat{\vec{p}}$ perturbation theory, when only matrix elements between near-band states are kept. In the next approximation, the effects of more distant bands are treated in second-order perturbation theory, leading to k^2 terms in the Hamiltonian. In this work we neglect the far-band corrections, keeping in mind that this is the first approximation of the perturbation theory. This question will be discussed in some detail below.

As was emphasized in Sec. I, in stressed semiconductor heterojunctions the polarization effect is induced by the strain. Being conditioned by mutual shifts of the cation and anion sublattices of the initial semiconductors, in our model Hamiltonian this effect can be described by the following term:[25]

$$V_{\rm st}=\vec{u}\cdot\nabla_r[V_A(\vec{r})-V_B(\vec{r})]=\vec{u}\cdot\vec{O}, \tag{2}$$

where $V_A(\vec{r})$ and $V_B(\vec{r})$ are the potentials of the A and B sublattices being shifted by the vector $\vec{u}$ in opposite directions. By adding the potential $V_{\rm st}$, the symmetry of the cubic IV-VI semiconductors is reduced. If the vector $\vec{u}$ is directed along the trigonal C_3 axis, the symmetry of the L points is reduced from D_{3d} to C_{3v}. Using an explicit form of the basis functions of the conduction L_6^- and valence L_6^+ bands from Ref. 24, by direct calculation of the matrix elements of the potential $V_{\rm st}$ one obtains

$$\hat{H}_{\rm st}=\begin{pmatrix} 0 & -i\vec{\sigma}\cdot\vec{E} \\ i\vec{\sigma}\cdot\vec{E} & 0 \end{pmatrix}, \tag{3}$$

where the components of the vector $\vec{E}$ are $E_i=\langle L_6^-|u_iO_i|L_6^+\rangle$. The situation with the polarization field $\vec{u}$ directed along the trigonal C_3 axis is considered here, as it is this direction in which the polarization effect is greatest in the structure considered.

In the framework of the deformation potential approximation the direct strain effect can also be taken into account. Due to the symmetry properties the effect contributes to the diagonal blocks of the Hamiltonian (3), resulting in trivial shifts of the interface states. Apparently, this effect can be

accounted for by means of the renormalization of the gap parameters in our model Hamiltonian (1).

In the Hamiltonian describing the energy spectrum of the stressed semiconductor heterojunction with antiferromagnetic ordering, the exchange interaction between the magnetic impurities spin $\vec{S_n}$ and a bare spin of electron $\vec{\sigma}$,

$$V_{\rm ex}=\sum_n A(|\vec{r}-\vec{R}_n|)\vec{S}_n\vec{\sigma}, \tag{4}$$

has to be included, where $A(|\vec{r}-\vec{R}_n|)$ is an s-like coupling function centered at the magnetic impurities. We make the plausible assumption that the magnetic impurities are localized in the interstitials, and have the antiferromagnetic vector along the z axis. In this case a spin density of the magnetic impurities S_n is an odd function, that is, $S_n(\vec{R}_n)=-S_n(-\vec{R}_n)$ (where $\vec{R}_n$ locates the magnetic impurity). As a result the potential $V_{\rm ex}$ gives rise to coupling states with opposite parity. So the matrix form of the exchange interaction constructed again with the wave functions from Ref. 24 is

$$\hat{H}_{\rm ex}=\begin{pmatrix} 0 & -iL \\ iL & 0 \end{pmatrix}, \tag{5}$$

the matrix element L in the mean-field approximation being

$$\begin{aligned} L&=i\langle L_{6\beta}^{-}|V_{\rm ex}|L_{6\beta}^{+}\rangle=i\langle L_{6\alpha}^{-}|V_{ex}|L_{6\alpha}^{+}\rangle \\ &=iS_0\sum_n\ [\langle L_{6\beta}^{-}|A(|\vec{r}-\vec{R}_n|)\sigma_z|L_{6\beta}^{+}\rangle \\ &\quad -\langle L_{6\beta}^{-}|A(|\vec{r}+\vec{R}_n|)\sigma_z|L_{6\beta}^{+}\rangle], \end{aligned}$$

where S_0 is an absolute mean value of the magnetic impurity spin, and the indices α and β reflect the Kramers-conjugate states. Here the sum index n runs just over the impurity sites R_n from one side of the interface plane $z=0$ (that is, the magnetic impurities symmetry arrangement is supposed). The matrix structure of the exchange Hamiltonian $\hat{H}_{\rm ex}$, with cross-coupling matrix elements (between L^- and L^+), is a result of the antiferromagnetic ordering of the interstitial magnetic impurities. If the magnetic impurities were substitutional ones, the magnetic impurities' spin density would be an even function, and as a result we should have a standard diagonal form $\hat{H}_{\rm ex}$ with the coupling between the states of the same parity (see, for example, Ref. 26).

Being expressed in terms of Mitchell's energy spectrum parameters and overlap integrals, the matrix elements E and L will be considered as parameters of our model approach. Some numerical evaluations can be given for these. Coming from the definition of the polarization potential $V_{\rm st}$, Eq. (2), we might estimate the value E by $2Du$ (where D is a deformation potential, and u is a relative displacement). Using appropriate values for D and u, we obtain $E\sim 50-100$ meV. Thus the strain-induced polarization effect is comparable in magnitude to spontaneous polarization in weak ferroelectrics. As for the parameter L, on the basis of the data for the exchange parameters of the semimagnetic IV-VI semiconductors given in the Ref. 27, one obtains $L\sim 20-40$ meV.

So the Hamiltonian describing the energy spectrum of the stressed IV-VI semiconductor heterojunction with the antiferromagnetic ordering along the z axis is

$$\begin{aligned} \hat{H}_0&=\hat{H}_{00}+\hat{H}_{\rm st}+\hat{H}_{\rm ex} \\ &=\begin{pmatrix} \Delta & \vec{\sigma}\cdot\hat{\vec{p}}-i(\vec{\sigma}\vec{E}+L) \\ \vec{\sigma}\cdot\hat{\vec{p}}+i(\vec{\sigma}\vec{E}+L) & -\Delta \end{pmatrix}. \end{aligned} \tag{6}$$

In the general case for the semiconductor structures considered, the matrix elements E and L are functions depending on the coordinate z. Note that the Hamiltonian $\hat{H}_0$ looks like the one for the energy spectrum of the exciton ferromagnetic within the framework of the mean-field approximation.[22] It is quite clear taking into account the above-mentioned analogy between these two problems.

After the transformation

$$\hat{U}=\begin{pmatrix} i\sigma_z & 0 \\ 0 & 1 \end{pmatrix},$$

Hamiltonian (6) has the form

$$\hat{\tilde{H}}_0=\hat{U}\hat{H}_0\hat{U}^{-1}=\begin{pmatrix} \Delta & i\hat{p}_z+\hat{W}+E \\ -i\hat{p}_z+\hat{W}+E & -\Delta \end{pmatrix}, \tag{7}$$

where $\hat{W}=\vec{\sigma}[\hat{\vec{p}}\cdot\vec{n}]+\sigma_z L$, and $\vec{n}$ is a unit vector along the z axis.

Since the interface states are of Tamm's type, and are generated from the bulk states of the initial semiconductors, first of all we consider the energy spectrum of the homogeneous semiconductor with polarization and antiferromagnetic ordering. We note that Hamiltonian (7) commutes with the operator

$$\hat{\tilde{W}}=\begin{pmatrix} \hat{W} & 0 \\ 0 & \hat{W} \end{pmatrix}, \tag{8}$$

so φ and χ wave-function components of the Hamiltonian $\hat{\tilde{H}}_0$ can be selected in the form of the eigenfunctions of the $\hat{W}$ operator

$$\hat{W}\varphi^{\pm}=W_{\pm}\varphi^{\pm},$$

where $W_{\pm}=\pm\sqrt{L^2+p_{\perp}^2}$, and

$$\varphi^{\pm}=\begin{pmatrix} 1 \\ \dfrac{p_y-ip_x}{L+W_{\pm}} \end{pmatrix}\varphi_0^{\pm}. \tag{9}$$

Here $\varphi_0^{\pm}$ is a normalized factor, and $p_{\perp}$ is a length of the vector $\vec{p}_{\perp}=(p_x,p_y,0)$, that is, $p_{\perp}^2=p_x^2+p_y^2$. After simple calculations we obtain that the energy spectrum consists of the four spin-split energy branches

$$\begin{aligned} \epsilon_{1,2}^{+}&=\sqrt{(E+W_{\pm})^2+\Delta^2+p_z^2}, \\ \epsilon_{1,2}^{-}&=-\sqrt{(E+W_{\pm})^2+\Delta^2+p_z^2}. \end{aligned} \tag{10}$$

The branches $\epsilon^{+}_{1,2}$ and $\epsilon^{-}_{1,2}$ describe two spin-split conduction and valence bands, respectively. Putting the wave functions in the form of (9) for the average value of the spin,

$$\vec{S}^{\pm}=(\varphi^{\pm\star}\chi^{\pm\star})\begin{pmatrix}\vec{\sigma} & 0\\ 0 & \vec{\sigma}\end{pmatrix}\begin{pmatrix}\varphi^{\pm}\\ \chi^{\pm}\end{pmatrix},$$

after the normalization of the wave functions one obtains

$$\vec{S}^{\pm}_{1,2}=\pm\frac{1}{\sqrt{L^2+p_\perp^2}}(p_y,-p_x,L). \tag{11}$$

Thus one can see that the polarization and antiferromagnetic ordering split the Kramers spin degeneracy. Each of the branches of the conduction $\epsilon^{+}_{1,2}$ or the valence $\epsilon^{-}_{1,2}$ bands is characterized by the opposite directions of the average spin value $\vec{S}$. As follows from Eq. (11), $\vec{S}$ is directed along the vector

$$\vec{I}=L\vec{n}+[\vec{n}\cdot\vec{p}_\perp]. \tag{12}$$

III. INTERFACE STATES OF THE STRESSED INVERTED CONTACT

Now let us consider the non-symmetry-inverted contact with the axis along the z axis as an inhomogeneous semiconductor structure, when, besides the coordinate dependence of the band gap, there is a coordinate dependence of the polarization field. At first the antiferromagnetic ordering parameter will be taken as a constant in both semiconductors. Since the gap center positions of the constituents are different in the non-symmetry-inverted contact, the Hamiltonian must include a coordinate-dependent work function $V(z)$. To simplify the analytical calculation, we determine the gap function $\Delta(z)$, the polarization function $E(z)$, and the work function $V(z)$ by a single function $f(z)$, so that

$$\Delta(z)=\Delta_0 f(z), E(z)=E_0 f(z), V(z)=V_0 f(z), \tag{13}$$

where apparently the signs of the asymptotes $f(z\to\pm\infty)$ are opposite in the inverted contact, and Δ_0, E_0, and V_0 are constants. Two different cases may be considered: (1) $f(+\infty)>0$, and $f(-\infty)<0$, and (2) $f(+\infty)<0$, and $f(-\infty)>0$.

The Hamiltonian of the system is

$$\hat{H}=\begin{pmatrix}\Delta+V & i\hat{p}_z+\hat{W}+E\\ \text{H.c.} & -\Delta+V\end{pmatrix}. \tag{14}$$

Noting again that the Hamiltonian $\hat{H}$ commutes with the operator $\hat{\tilde{W}}$, Eq. (8), we select the wave functions in the form of the eigenfunctions of $\hat{W}$ operator. Then by means of the unitary transformation

$$\hat{V}=\begin{pmatrix}\cos\Theta & -\sin\Theta\\ \sin\Theta & \cos\Theta\end{pmatrix}, \tag{15}$$

where the angle Θ is determined by the condition

$$\Delta_0\cos2\Theta-E_0\sin2\Theta+V_0=0, \tag{16}$$

the Hamiltonian $\hat{H}$ is transformed to

$$\hat{\tilde{H}}=\hat{V}^{-1}\hat{H}\hat{V}=\begin{pmatrix}-W_\pm\sin2\Theta & -\sqrt{E^2+\Delta^2-V^2}+W_\pm\cos2\Theta+i\hat{p}_z\\ \text{H.c.} & 2V+W_\pm\sin2\Theta\end{pmatrix}. \tag{17}$$

It immediately follows from Eq. (17) that the Schrödinger equation

$$(\hat{\tilde{H}}-\epsilon)\begin{pmatrix}\tilde{\varphi}^{\pm}\\ \tilde{\chi}^{\pm}\end{pmatrix}=0, \tag{18}$$

where

$$\begin{pmatrix}\tilde{\varphi}^{\pm}\\ \tilde{\chi}^{\pm}\end{pmatrix}=\hat{V}^{-1}\begin{pmatrix}\varphi^{\pm}\\ \chi^{\pm}\end{pmatrix}$$

has a solution with $\tilde{\chi}^{\pm}=0$. This is a zero mode. It is worth noting that the same states for different particular cases have been obtained in the Refs. 1, 2, and 6 by means of supersymmetry quantum mechanics, and in terms of this they have been called Weyl states.

At $f(+\infty)>0$ and $f(-\infty)<0$ there is the following solution of Eq. (18):

$$\epsilon_i^{\pm}=\mp\frac{E_0V_0-\Delta_0\sqrt{E_0^2+\Delta_0^2-V_0^2}}{\Delta_0^2+E_0^2}\sqrt{p_\perp^2+L^2}, \tag{19}$$

the function $\tilde{\varphi}^{\pm}$ satisfying the equation

$$[ip_z+W^{\pm}(z)]\tilde{\varphi}^{\pm}=0, \tag{20}$$

where

$$W^{\pm}(z)=\sqrt{E_0^2+\Delta_0^2-V_0^2}\times\left(f(z)\pm\sqrt{p_\perp^2+L^2}\frac{\Delta_0V_0+E_0\sqrt{E_0^2+\Delta_0^2-V_0^2}}{(\Delta_0^2+E_0^2)\sqrt{E_0^2+\Delta_0^2-V_0^2}}\right).$$

This function plays the same role as the superpotential in the supersymmetry quantum mechanics method.[2,6] Being a solution of the first order differential equation (20), the functions $\tilde{\varphi}^{\pm}$ are

$$\tilde{\varphi}^{\pm}(z)=\varphi_0^{\pm}\exp\left(-\frac{1}{\hbar v_\parallel}\int_0^z W^{\pm}(z)dz\right),$$

where $\varphi_0^{\pm}$ are constants. These functions are localized at the interface boundary, but at given asymptotes of the $f(z)$ function they are normalized just under the conditions $W^{\pm}(+\infty)>0$ and $W^{\pm}(-\infty)<0$. At $|f(\pm\infty)|=1$ this leads to

$$\sqrt{p_\perp^2+L^2}<\frac{(\Delta_0^2+E_0^2)\sqrt{E_0^2+\Delta_0^2-V_0^2}}{\Delta_0V_0+E_0\sqrt{E_0^2+\Delta_0^2-V_0^2}}. \tag{21}$$

So states $\epsilon_i^{\pm}$ are of the interface type, but the interface state spectrum cuts off at finite transverse momentum.

At the opposite asymptotes of the function $f(z)$ the interface solutions are described by the expressions (19)–(21) by replacing $\Delta_0\to-\Delta_0$ and $p_z\to-p_z$.

It is useful to consider a situation when the parameter of the antiferromagnetic ordering is not constant in both semiconductors, this being determined by the same function $f(z)$, so that $L(z)=L+L_0 f(z)$ (where L and L_0 are constants). There is no way of finding an invariant of Hamiltonian (14) and of solving the problem analytically in this case, but we can obtain a perturbative solution. To simplify analytical calculations, we set the work function $V(z)$ equal to 0 (or a constant). After a unitary transformation

$$\hat{V}=\begin{pmatrix} \hat{C}(\omega) & \hat{S}(\omega) \\ -\hat{S}(\omega) & \hat{C}(\omega) \end{pmatrix}, \tag{22}$$

where

$$\hat{C}(\omega)=\begin{pmatrix} \cos\omega^+ & 0 \\ 0 & \cos\omega^- \end{pmatrix}, \quad \hat{S}(\omega)=\begin{pmatrix} \sin\omega^+ & 0 \\ 0 & \sin\omega^- \end{pmatrix},$$

$\omega^{\pm}$ being determined by the equation

$$\tan 2\omega^{\pm}=\frac{\Delta_0}{E_0 \pm L_0},$$

we obtain

$$\hat{\tilde{H}}=\begin{pmatrix} -L\sigma_z\hat{S}(2\omega)-\sin(\omega^+ +\omega^-)\hat{W} & i\hat{p}_z+f(z)\hat{A}+L\sigma_z\hat{C}(2\omega)+\cos(\omega^+ +\omega^-)\hat{W} \\ \text{H.c.} & L\sigma_z\hat{S}(2\omega)+\sin(\omega^+ +\omega^-)\hat{W} \end{pmatrix}. \tag{23}$$

Here

$$\hat{A}=\begin{pmatrix} \sqrt{\Delta_0^2+(E_0+L_0)^2} & 0 \\ 0 & \sqrt{\Delta_0^2+(E_0-L_0)^2} \end{pmatrix}.$$

In the framework of perturbation theory with energy corrections to order $p_\perp^2$, we again obtain two solutions with $\chi=0$. Thus, the interface states are

$$\epsilon_i^{\pm}=\mp L\sin 2\omega^{\pm}\mp\frac{p_\perp^2\sin^2(\omega^+ +\omega^-)}{L(\sin 2\omega^+ +\sin 2\omega^-)}. \tag{24}$$

The wave functions $\varphi^{\pm}$ are spin-up for the energy state ϵ_i^+, and spin-down for ϵ_i^-, satisfying the equation

$$\left(-i\hat{p}_z+f(z)A^{\pm}\pm L\cos 2\omega^{\pm} \mp\frac{p_\perp^2\cos^2(\omega^+ +\omega^-)}{f(z)(A^- -A^+)-L(\cos 2\omega^+ +\cos 2\omega^-)}\right)\varphi^{\pm}=0, \tag{25}$$

where A^+ and A^- are the upper and lower diagonal matrix elements of the matrix $\hat{A}$. At the assumed asymptotes of function $f(z)$, one can quite easily obtain conditions normalizing the wave functions $\varphi^{\pm}$. So the spectrum of the interface states $\epsilon_i^{\pm}$ is again restricted. For the opposite asymptotes $f(z)$ the same interface states appear, but to normalize the wave function one has to assume that $\varphi=0$. It is obvious that at $L_0=0$ the interface state energy spectrum obtained for the inverted contact with the variable antiferromagnetic ordering tends to the one for the contact with the constant antiferromagnetic ordering.

IV. A SPIN ANALYSIS OF THE INTERFACE STATES

Each interface state of the inverted contact with the constant antiferromagnetic ordering

$$\Psi^{\pm}=\begin{pmatrix} \tilde{\varphi}^{\pm} \\ 0 \end{pmatrix}$$

is nondegenerate, and the average spin value $\vec{S}_i^{\pm}$ [being obtained in the same way as Eq. (11)] is

$$\vec{S}_i^{\pm}(z)=C\exp\left(-\frac{2}{\hbar v_\parallel}\int_0^z W^{\pm}(z)dz\right)\frac{2}{L\pm\sqrt{p_\perp^2+L^2}} \times(p_y,-p_x,L), \tag{26}$$

where C is a constant determined by a normalizing condition. Here the first type of $f(z)$ asymptotes has been used. After integrating Eq. (26) [taken for the step function $f(z)$ and at $z=0$] over the electron momentum $p_\perp$ for the given symmetrical spectrum model, one obtains

$$\langle\vec{S}_i^{\pm}(0)\rangle=\pm\frac{\sqrt{E_0^2+\Delta_0^2-V_0^2}}{2\pi\hbar^3 v_\parallel v_\perp^2}\left(\sqrt{L^2+p_{\perp\max}^2}-L\right)\left(1-\frac{B^2}{3}(2L^2 +p_{\perp\max}^2+L\sqrt{L^2+p_{\perp\max}^2})\right)(0,0,L), \tag{27}$$

where $p_{\perp\max}$ is set by Eq. (21), and

$$B=\frac{\Delta_0 V_0+E_0\sqrt{E_0^2+\Delta_0^2-V_0^2}}{(\Delta_0^2+E_0^2)\sqrt{E_0^2+\Delta_0^2-V_0^2}}.$$

The average spins of the interface Ψ^+ and Ψ^- states are oppositely directed along the z axis.

As follows from Eq. (19), when $f(+\infty)>0$ and $f(-\infty)<0$ under the condition $\Delta_0^2>V_0^2$, the energy level ϵ_i^+ is situated higher than ϵ_i^-, while under the condition $V_0^2>\Delta_0^2$ they change their positions. So the state with the average spin-down is higher than the state with the spin-up. For the asymptotes $f(+\infty)<0$ and $f(-\infty)>0$, the state ϵ_i^- with the spin down is higher than the state ϵ_i^+ with the spin up in any case in point. Figures 1 and 2 show rough sketches of the interface energy spectrum of the stressed inverted con-

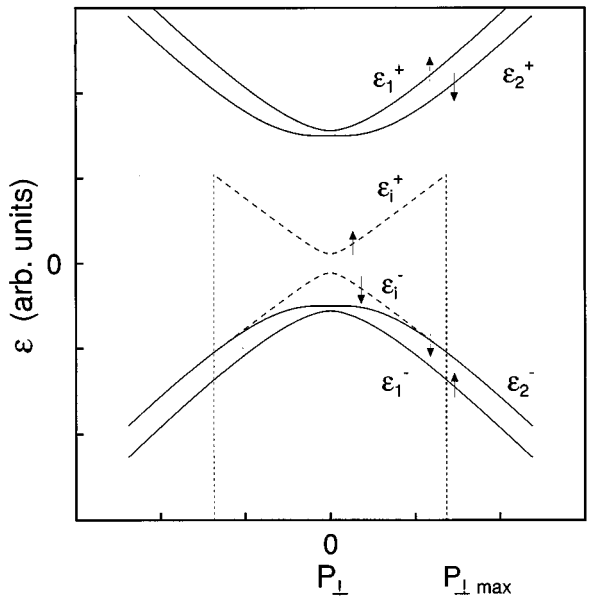

FIG. 1. Rough sketch of the interface energy spectrum in stressed inverted contact with the constant antiferromagnetic ordering for the asymptotes $f(+\infty)>0$ and $f(-\infty)<0$ ($\Delta_0^2>V_0^2$). The solid lines show the energy branches of the constituents, and the dashed lines show the interface states. The arrows show the average spin direction.

tact with constant antiferromagnetic ordering for both types of function $f(z)$ asymptotes (where for the relations between the parameters Δ_0, E_0, and L_0 the real above-mentioned estimations have been used). The solid lines correspond to the bulk semiconductor bands of the constituents, while the dashed lines correspond to the interface states. The arrows show the average spin direction relative to the z axis. From

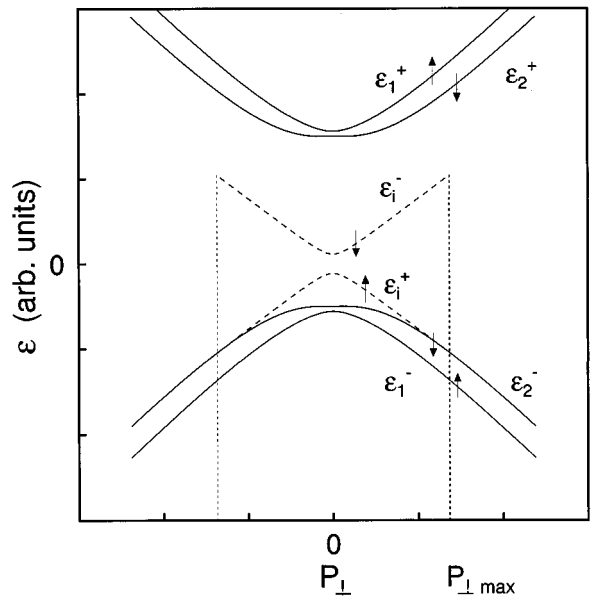

FIG. 2. The same as in Fig. 1, but for the asymptotes $f(+\infty)<0$ and $f(-\infty)>0$.

the figures we can see, that for the values of the model parameters used, there is a quite real region of transverse momentum where condition (21) is fulfilled, and so interface states exist. Note that in line with the assumed heterojunction geometry, the energy branches of the constituents are the same, but their spin directions are opposite. In contrast to the case of an unstressed inverted contact without antiferromagnetic ordering (see Fig. 3 from Ref. 2), the interface state spectrum of the stressed inverted contact with antiferromagnetic ordering is not linear in $p_\perp$, there being a gap between the electronlike and holelike states.

Comparing expression (10) for the energy levels of homogeneous semiconductors, and Eq. (19) for interface heterojunction states, we note that the interface states are situated nearer to the middle of the gap of the constituents. Thus if in the semiconductor heterojunctions the Fermi level (for example by means of doping) lies in one of the two-dimensional interface bands, then this leads to magnetic ordering in the interface plane. Being proportional to the value $\langle \vec{S}_i^+ \rangle$ or $\langle \vec{S}_i^- \rangle$ [Eq. (27)] in accord with which of the interface states ϵ_i^+ or ϵ_i^-, respectively, is occupied, the interface magnetization will be directed along the z axis or opposite to it, the one that is exponentially attenuated moving away from the interface plane. Apparently the interface magnetization is at a maximum if one of the interface bands is occupied but the other is empty, and it is equal to zero if both interface bands are completely occupied as the magnetization of one of them is directed along the z axis and the magnetization of the other is opposite to it. In the intermediate case, when one of the interface bands is completely occupied and the other is not, there is some uncompensated magnetization determined by the difference between $p_{\perp\max}$ and the Fermi momentum p_F, conditioned by relation (21) and by the Fermi energy ϵ_F, respectively.

In the framework of our model we can obtain the value of the interface magnetization (calculated for simplicity at $z=0$) relative to the magnetization determined by the band states. After integrating $S_{1,2}^\pm$, Eq. (11), over the occupied states, one obtains

$$M=\frac{\langle S_i^\pm(0)\rangle}{\langle S_{1,2}^\pm\rangle}=\frac{\pi\sqrt{E_0^2+\Delta_0^2}}{p_F v_\parallel}\,\frac{(1-\delta)(\delta+2)}{3}, \qquad (28)$$

where $\delta=\epsilon_i^\pm/\epsilon_i^\pm(p_{\perp\max})=E_0L/(\Delta_0^2+E_0^2)$. Here we set $V_0=0$, and the Fermi energy is determined by the value $p_{\perp\max}$, Eq. (21); i.e., the ideal situation is considered when the interface magnetization is at a maximum. It is obvious that the relation of the interface magnetization to the band magnetization is conditioned by the ratio between the energies of the occupied interface states and band states (i.e., ϵ_F).

From Eq. (28) we note that the interface magnetization is equal to zero at $\delta=1$, i.e., as follows from Eq. (21) at $p_{\perp\max}=0$. This is a quite trivial result because there are no interface states in this case. In the interval $0\leqslant\delta\leqslant1$ the value of the relative interface magnetization M is a monotonically decreasing function of the parameter δ, that is obviously caused by a decrease of the interface state fraction with δ increasing from 0 up to 1. The value M is at a maximum at $\delta=0$, i.e., at E_0 or $L=0$. However, it is quite apparent from

Eqs. (27) and (11) that at $L=0$ there is neither any interface nor band magnetization, so that M is an indeterminate value. For the case $E_0=0$, from Eq. (10) we find the energy branches $\epsilon_1^{\pm}$ to be superimposed on $\epsilon_2^{\pm}$ (for $E_0=0$), so that the energy states $\epsilon^{\pm}$ become doubly degenerate with the summary spin equal to zero. So relation (28) is true just in the interval $0<\delta\leqslant 1$, where the point $\delta=0$ is ignored.

Now, using characteristic estimations for model parameters, we find the value of the relative interface magnetization M, Eq. (28), to be on the order of 1; that is, the interface magnetization may be a real effect for the structures in point. Concerning the inverted contact with the variable antiferromagnetic ordering, we estimate the perturbation solutions in the limit small $p_\perp$ to show the same peculiarities as in the contact with constant antiferromagnetic ordering. Again each interface state is nondegenerate. The spin of one of them is up relative to the z axis, but the spin of the other is down. Analytical calculations can be performed in the other limit when the variation of the antiferromagnetic ordering is small (that is, the parameter L_0 is small). However, this does not give any nontrivial results, and the main peculiarities of the interface state spectrum remain the same.

The interface magnetization effect can occur even in the normal semiconductor heterojunction when the gaps of the initial semiconductors have the same signs. However, as emphasized in Sec. I, for the stressed semiconductor heterojunction with normal band arrangement the interface states appear inside either the bulk valence or conduction bands of the original semiconductors, and they exist in at most a restricted range of values of the transverse momentum. So in the case of the normal stressed semiconductor heterojunction with antiferromagnetic ordering, the effect of the interface magnetization might take place under more rigorous conditions.

V. SUMMARY

We discussed in some detail the spectra for midgap states bound to interfaces in stressed heterostructures made from materials with inverted bands and showing antiferromagnetic ordering. Comparing these interface states with those of the stressed semiconductor heterojunction without antiferromagnetic ordering[6] (that corresponds to $L=0$ in our model) or with interface states arising in the simple inverted contact[1,2] ($E_0, L=0$), one can see that in the case of the stressed inverted contact with antiferromagnetic ordering there is a gap between the electronlike and holelike states (determined by the parameter of the antiferromagnetic ordering L). Moreover, the spectrum of the interface states is not linear in $p_\perp$.

The spin analysis of the interface states showed them to be spin split. Thus, if in semiconductor heterostructures the Fermi level (for example by means of doping) falls into one of the interface bands, this then leads to magnetic ordering in the interface plane. In view of this the interface magnetization effect was discussed.

In this work the idealized system in the framework of some above approximations has been studied. Any correlation problems treated in the self-consistent approach have been beyond our consideration. However, the specific physical properties of the IV-VI narrow-gap semimagnetic semiconductors (used as model materials) such as small values of the effective masses, very high dielectric constants, and so on (resulting in strong screening of the electromagnetic fields), make us believe the electron correlation effect to be of no importance for the problems discussed. It is of special interest to consider another correlation effect caused by the exchange interaction between the interface state spins and ion spins of the magnetic layers. Due to a renormalization of the interface states resulting from this interaction, the interface magnetization can be increased or decreased. A similar effect was studied in our previous work,[28] where the Anderson impurity state renormalization induced by interaction with interface states in band-inverted semiconductor heterojunction was considered. The interface states being localized at the interface boundary, the renormalization effect was shown to be of some consequence just when the impurity atom is spaced a distance less than 1–2 lattice constants apart from the interface plane. So, analogously, as the distance between magnetic layers in narrow-gap semimagnetic semiconductors used to be larger than the above value, the overlap of these interface states with the magnetic ions will have a rather negligible effect on our results.

Another question arises about the neglecting of the terms $\sim k^2$ in Hamiltonian (1). They are diagonal terms of the Dimmock model[23] resulting from far-band corrections, and are written as $k^2/2m$ (where m is a far-band mass). A detailed investigation of interface states in band-inverted semiconductor heterojunctions[3] showed these far-band corrections to provide a modest curvature of the energy spectrum, and to give an additional spectral cutoff, but showed the quantitative changes to be not very significant. In fact these higher-order terms become important for large $p_\perp$ such that $p_\perp > \Delta_0$, the interface states existing just at

$$p_\perp^2 < 4\Delta_0^2\left(\frac{mv^2}{\Delta_0}\right). \tag{29}$$

Thus, in the second approximation of the perturbation theory, the condition restricting the range of the transverse momentum for the interface states in the stressed semiconductor heterojunctions with the antiferromagnetic ordering will be not so simple as Eq. (21). However, taking into account the real relations between the parameters Δ_0, E_0, and L used for our model materials, and the fact that for IV-VI narrow-gap semiconductors the value of mv^2/Δ_0 is on the order of 5, after a trivial estimation we find relation (21) to be more rigorous than Eq. (29). Thus we can assume the including of the far-band corrections should not change the essence of the matter for the problems under consideration.

In conclusion, we should like to note that, while there have been experimental works[18,19] showing some interesting magnetic effects in EuTe/PbTe superlattices which can be connected with interface magnetization, a direct observation of the effect in point may be performed by means of certain magneto-optical experiments. From the theoretical point of view at this moment, as a first step the simple model developed by us fits the problem in question quite adequately, providing an opportunity to understand the physical sense of the phenomenon. Apparently for further progress the interface magnetization effect discussed in this work needs to be considered by means of the self-consistent approach, treating some correlation effects.

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