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Interface states in stressed band-inverted heterojunctions based on semimagnetic compounds

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Abstract. The electronic states of stressed heterojunctions formed from narrow-gap semiconductors with mutually inverted bands and showing antiferromagnetic ordering have been studied. 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 leads to magnetic ordering in the interface plane. An interface magnetization effect is expected to occur. Using representative estimates of the model parameters, the value of the relative interface magnetization has been obtained.

1. Introduction

Recently, there has been considerable interest in the study of Tamm-type interface states which arise in some semiconductor structures. These interface states (in contrast to the ones traditionally considered) are not governed by the transition region structure, being generated from the bulk energy bands of the constituents. At first, Tamm's interface states were considered theoretically [1–3] in so-called inverted contacts (that is, in semiconductor heterojunctions based on semiconductors with mutually inverted bands), so the gaps of the constituents had opposite signs. It was shown in [4, 5] that such interface states could in fact appear not only at the heterojunction boundary but almost at the positions of other inhomogeneities of the electron system, such as an antiferromagnetic ordering vector inhomogeneity (realized as an antiferromagnetic domain wall) or a polarization vector inhomogeneity (realized as a ferroelectric domain wall), combinations of these inhomogeneous fields producing a variety of systems with disturbed symmetrical properties. This is an important point, providing a means for separating off the interface states under consideration into one particular group.

As an example of inverted contacts, heterojunctions based on certain narrow-gap IV–VI or II–VI semiconductors were previously considered. In such cases, in a treatment based on the simplest two-band approximation, the interface states have a gapless band spectrum, linear in the interface plane, their energy falling in the gap of the constituent semiconductors. Subsequent investigations [3, 6] showed that such interface states can also exist in heterojunctions with normal band arrangements. However, in contrast to the case for the inverted heterojunction, these states appear either inside the conduction bands or inside the valence bands of the constituents, the energy spectrum being cut off at finite transverse (along the interface plane) momentum. Later it was shown that there are interface states

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in superlattices [7, 8], quantum wells [9], and quantum dots [10]. It is worth noting that quite recently, in [11], the magnetic field dependences of the Hall coefficients of PbTe/SnTe superlattices have been interpreted by assuming that in addition to the electrons in PbTe and holes in SnTe a third kind of charge carrier connected with the above-mentioned interface states appears. A more direct investigation of the two-dimensional interface states was performed by means of magneto-tunnelling spectroscopy of the p-HgCdTe quantum well, and is described in [12].

The majority of semiconductor structures are stressed due to the lattice mismatch of their constituents. The electron energy spectrum of a stressed semiconductor structure is determined by the strains in addition to the widths of the layers and the physical parameters of the constituents. A more direct strain effect is the change of the energy spectrum, which is different for each constituent, and depends upon the acoustic deformation potentials of both the conduction and the valence bands. This problem has been thoroughly investigated for different semiconductor structures [13]. Moreover, 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 are plainly 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 turn generates energy states of either conduction or valence bands, in our earlier work [6] we investigated the strain-induced polarization effect on the boundary interface state of the semiconductor heterojunction. It has been shown [6] that the normal deformation effect on the interface-state energy spectrum is quite trivial and leads to homogeneous shifts of the energy bands.

Upon doping with transition or rare-earth elements, IV–VI and II–VI semiconductors turn into dilute magnetic ones, and at low temperature they might become ferromagnetic or antiferromagnetic. Earlier, quantum structures based on such semimagnetic semiconductors were intensively investigated because of their interesting physical properties [15–17], their non-trivial (as compared with those of 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 was previously thought 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 feature of the problems concerning the interface states is that for inverted stressed semiconductor structures with antiferromagnetic ordering we have a situation in which all three of the above-mentioned fields (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 of a stressed heterocontact, an additional space asymmetry arises due to the 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. For the structures in question, both types of degeneracy are absent. Therefore, such heterostructures must be systems with unusual microscopic electronic properties. One of them is the interface magnetization effect considered in this paper.

Thus, the aim of this work is to study the 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 a so-called 'system with electron–hole pairing'. After putting commensurate waves of spin and charge density on the system, the energy spectrum of the latter turns out to be spin splitting. Under limited doping this leads to electron spin ordering (that is, we have a system with exciton ferromagnetism) [22]. Now, taking into account the fact that the spin- and charge-density waves might be induced by antiferromagnetic ordering and by structural lattice distortions (which are accompanied by polarization), respectively, one can affirm that a system with polarization and antiferromagnetic ordering will be similar to one with exciton ferromagnetism.

To completely specify our calculations, 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 section 2 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 section 3 the interface states of the inverted stressed contact with antiferromagnetic ordering will be considered, two cases being studied. One of them is the case in which the antiferromagnetic ordering is the same in the initial semiconductors, and the other is one in which it has opposite signs in the constituents. A spin analysis of the interface states is given in section 4. This is followed by a brief summary.

2. The model Hamiltonian

Each of the materials making up the heterojunctions of the narrow-gap IV–VI semiconductors under study is known to have a direct gap at the L points of the Brillouin zone, there being two doubly degenerate bands, L^+ and L^-, with opposite coordinate symmetry near the middle of the gap. 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

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

where the upper and lower blocks are related to the states φ and χ of the conduction and valence bands, respectively, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector whose components are the Pauli matrices, $\hat{\boldsymbol{p}} = -\mathrm{i}\hbar(v_\perp\boldsymbol{\nabla}_x, v_\perp\boldsymbol{\nabla}_y, v_\parallel\boldsymbol{\nabla}_z)$, $v_{\perp,\parallel}$ being interband coupling matrix elements having the dimensions of velocity, and $\Delta = E_g/2$, where E_g is the energy gap, depending on the z-coordinate, if the heterojunction in question is aligned in the z-direction. Note that this Dirac form of the Hamiltonian (1) is just the first approximation of the $\boldsymbol{k}\cdot\hat{\boldsymbol{p}}$ perturbation theory in which only matrix elements connecting near-band states are retained. 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 a first approximation of the perturbation theory. The justification of this assumption will be discussed in some detail below.

As was emphasized in the introduction, in stressed semiconductor heterojunctions the polarization effect is induced by the strain. As it is governed 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]:

$$V_{st} = \boldsymbol{u}\cdot\boldsymbol{\nabla}_{\boldsymbol{r}}(V_A(\boldsymbol{r}) - V_B(\boldsymbol{r})) = \boldsymbol{u}\cdot\boldsymbol{O} \tag{2}$$

where $V_A(\boldsymbol{r})$ and $V_B(\boldsymbol{r})$ are the potentials of the A and B sublattices shifted by the vector $\boldsymbol{u}$ in opposite directions. On applying the potential V_{st}, the symmetry of the cubic IV–VI semiconductors is reduced. If the vector $\boldsymbol{u}$ 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 [24], by direct calculation of the matrix elements of the potential V_{st} one gets

$$\hat{\mathbf{H}}_{st} = \begin{pmatrix} 0 & -\mathrm{i}\boldsymbol{\sigma}\cdot\boldsymbol{E} \\ \mathrm{i}\boldsymbol{\sigma}\cdot\boldsymbol{E} & 0 \end{pmatrix} \tag{3}$$

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

Then, in the Hamiltonian describing the energy spectrum of the stressed semiconductor heterojunction with antiferromagnetic ordering, the exchange interaction between the magnetic impurity spin $\boldsymbol{S}_n$ and the bare spin of the electron $\boldsymbol{\sigma}$

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

has to be included (where $A(|\boldsymbol{r} - \boldsymbol{R}_n|)$ is an s-like coupling function centred at the magnetic impurities). We make the plausible assumption that the magnetic impurities are localized in the interstitials, their antiferromagnetic vectors being directed along the z-axis. In this case the spin density of the magnetic impurities S_n is an odd function—that is, $S_n(\boldsymbol{R}_n) = -S_n(-\boldsymbol{R}_n)$ (where $\boldsymbol{R}_n$ represents the location of the magnetic impurity). As a result, the potential V_{ex} gives rise to coupling states with opposite parity. So, the matrix form of the exchange interaction constructed again with the wave functions from [24] is

$$\hat{\mathbf{H}}_{ex} = \begin{pmatrix} 0 & -\mathrm{i}L \\ \mathrm{i}L & 0 \end{pmatrix} \tag{5}$$

in which the matrix element L in the mean-field approximation is

$$\begin{aligned} L &= \mathrm{i}\langle L_{6\beta}^-|V_{ex}|L_{6\beta}^+\rangle = \mathrm{i}\langle L_{6\alpha}^-|V_{ex}|L_{6\alpha}^+\rangle \\ &= \mathrm{i}S_0 \sum_n [\langle L_{6\beta}^-|A(|\boldsymbol{r} - \boldsymbol{R}_n|)\sigma_z|L_{6\beta}^+\rangle - \langle L_{6\beta}^-|A(|\boldsymbol{r} + \boldsymbol{R}_n|)\sigma_z|L_{6\beta}^+\rangle] \end{aligned}$$

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 on one side of the interface plane $z = 0$ (that is, a symmetric arrangement of the magnetic impurities is assumed). The matrix structure of the exchange Hamiltonian $\hat{\mathbf{H}}_{ex}$ with the cross coupling matrix elements (connecting L^- and L^+) is a result of the antiferromagnetic ordering of the interstitial magnetic impurity. If the magnetic impurities were substitutional ones, the magnetic impurity spin density would be an even function, and we would have a standard diagonal form for $\hat{\mathbf{H}}_{ex}$ with coupling between states of the same parity (see for example [26]).

Expressed in terms of Mitchell's energy spectrum parameters and the overlap integrals, the matrix elements E and L will be considered as parameters of our model approach. Some numerical evaluations can be made. On the basis of the definition of the polarization potential V_{st}, equation (2), we might estimate the value E as $2Du$ (where D is a deformation potential, and u is a relative displacement). Using the appropriate values for D and u, we obtain $E \sim$ 50–100 meV. Thus, the strain-induced polarization effect is comparable in magnitude to the spontaneous polarization in weak ferroelectrics. For the parameter L, on

the basis of the data for the exchange parameters of semimagnetic IV–VI semiconductors given in [27], one obtains $L \sim 20$–40 meV.

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

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

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 $\hat{\mathbf{H}}_0$ looks like the one for the energy spectrum of the exciton, which is ferromagnetic within the framework of the mean-field approximation [22]. This is quite in order, taking into account the above-mentioned analogy between these two problems.

After applying the transformation

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

the Hamiltonian (6) has the form

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

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

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

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

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

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

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

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

Here $\varphi_0^{\pm}$ is a normalized factor and $p_{\perp}$ is the length of the vector $\boldsymbol{p}_{\perp} = (p_x, p_y, 0)$—that is, $p_{\perp}^2 = p_x^2 + p_y^2$. After simple calculations, we obtain that the energy spectrum consists of 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. Using the wave functions in the form (9) for the average value of the spin after normalization, one obtains

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

So 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 opposite directions of the average spin value $\boldsymbol{S}$. As follows from (11), $\boldsymbol{S}$ is directed along the vector

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

3. The interface energy spectrum

Now let us consider a non-symmetry-inverted contact, with its axis along z, as an inhomogeneous semiconductor structure, for which, 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 the same for the two types of semiconductor. Since the gap-centre 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 $V(z)$ in terms of a single function $f(z)$:

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

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

So the Hamiltonian of the system is

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

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

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

where the angle Θ is determined by the condition

$$\Delta_0 \cos 2\Theta - E_0 \sin 2\Theta + V_0 = 0 \tag{16}$$

the Hamiltonian $\hat{\mathbf{H}}$ is transformed into

$$\hat{\tilde{\mathbf{H}}} = \hat{\mathbf{V}}^{-1}\hat{\mathbf{H}}\hat{\mathbf{V}} = \begin{pmatrix} -W_{\pm}\sin 2\Theta & -\sqrt{E^2 + \Delta^2 - V^2} + W_{\pm}\cos 2\Theta + \mathrm{i}\hat{p}_z \\ \mathrm{HC} & 2V + W_{\pm}\sin 2\Theta \end{pmatrix}. \tag{17}$$

It immediately follows from (17) that the Schrödinger equation

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

where

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

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 [1, 2, 6] by means of supersymmetry quantum mechanics, and in the terminology of this field they were called Weyl states.

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

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

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

$$(\mathrm{i}p_z + W^{\pm}(z))\tilde{\varphi}^{\pm} = 0 \tag{20}$$

where

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

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

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

So the 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 same expressions, (19)–(21), on making the replacements $\Delta_0 \to -\Delta_0$ and $p_z \to -p_z$.

It is useful to consider a situation in which the parameter of the antiferromagnetic ordering is not the same for the two types of semiconductor, but is determined by the same function $f(z)$ as is used above, so that $L(z) = L + L_0 f(z)$ (where L, 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. Here we omit all analytical calculations and just give the final result for the interface-state energy spectrum:

$$\epsilon_i^{\pm} = \mp L \sin 2\omega^{\pm} \mp \frac{p_\perp^2 \sin^2(\omega^+ + \omega^-)}{L(\sin 2\omega^+ + \sin 2\omega^-)} \tag{22}$$

where the $\omega^{\pm}$ are determined by the equation

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

(To simplify the analytical calculations, we have put the work-function $V(z)$ equal to 0 here.) The wave functions $\varphi^{\pm}$ are spin-up ones for the energy states ϵ_i^+ and spin-down ones for the ϵ_i^-, satisfying the equation

$$\left(-\mathrm{i}\hat{p}_z + f(z)A^{\pm} \pm L \cos 2\omega^{\pm} \mp \frac{p_\perp^2 \cos^2(\omega^+ + \omega^-)}{f(z)(A^- - A^+) - L(\cos 2\omega^+ + \cos 2\omega^-)} \right) \varphi^{\pm} = 0 \tag{23}$$

where $A^{\pm} = \sqrt{\Delta_0^2 + (E_0 \pm L_0)^2}$. At the given asymptotes of the 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 restricted again. It is obvious that at $L_0 = 0$ the interface-state energy spectrum obtained for the inverted contact with variable antiferromagnetic ordering tends to the one for the contact with constant antiferromagnetic ordering.

4. A spin analysis of the interface states

Each interface state of the inverted contact with constant antiferromagnetic ordering

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

is non-degenerate, and the average spin value $\boldsymbol{S}_i^{\pm}$ is

$$\boldsymbol{S}_i^{\pm}(z) = C \exp\left(-\frac{2}{\hbar v_{\parallel}} \int_0^z W^{\pm}(z)\, \mathrm{d}z\right) \frac{2}{L \pm \sqrt{p_{\perp}^2 + L^2}} (p_y, -p_x, L) \qquad (24)$$

where C is a constant determined by a normalizing condition. Here the first type of $f(z)$ asymptote has been used. After integrating (24) (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

$$\langle \boldsymbol{S}_i^{\pm}(0) \rangle = \pm \frac{\sqrt{E_0^2 + \Delta_0^2 - V_0^2}}{2\pi\hbar^3 v_{\parallel} v_{\perp}^2} \left(\sqrt{L^2 + p_{\perp max}^2} - L\right) \times \left(1 - \frac{B^2}{3}(2L^2 + p_{\perp max}^2 + L\sqrt{L^2 + p_{\perp max}^2})\right)(0, 0, L) \qquad (25)$$

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

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

So, we see that the average spins of the interface Ψ^+ and Ψ^- states are oppositely directed along the z-axis.

As follows from (19), when $f(+\infty) > 0$, $f(-\infty) < 0$ 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 exchange their relative positions. So the state with the average spin down is higher than the state with the average spin up. For the asymptotes $f(+\infty) < 0$, $f(-\infty) > 0$, the state ϵ_i^- with the spin down is higher than the state ϵ_i^+ with the spin up for all cases considered. Figures 1 and 2 show rough sketches of the interface energy spectrum of the stressed inverted contact with constant antiferromagnetic ordering for both types of the asymptotes of the function $f(z)$ (where for the relations between the parameters Δ_0, E_0 and L_0 the above-mentioned estimates 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 directions relative to the z-axis. From the figures we can see that for the values of the model parameters used there is an actual region of the transverse momentum where the condition (21) is fulfilled and so the 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.

Comparing expression (10) for the energy levels of the homogeneous semiconductors and (19) for the 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, as a result of doping—falls in one of the two-dimensional interface bands, then it leads to magnetic ordering in the interface plane. Being proportional to the value $\langle \boldsymbol{S}_i^+ \rangle$ or $\langle \boldsymbol{S}_i^- \rangle$, equation (25)—according to which of the interface states, ϵ_i^+ or ϵ_i^- respectively, is occupied—the interface magnetization will be directed

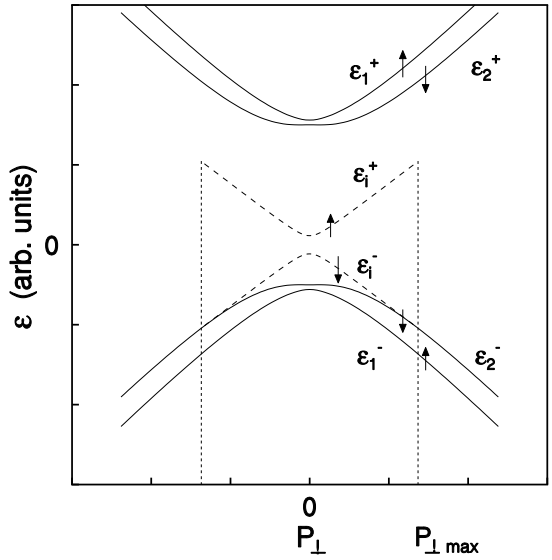

Figure 1. A rough sketch of the interface energy spectrum in the stressed inverted contact with constant antiferromagnetic ordering for the asymptotes $f(+\infty) > 0$, $f(-\infty) < 0$ ($\Delta_0^2 > V_0^2$). The solid lines show the energy branches of the constituents and the dashed lines show the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

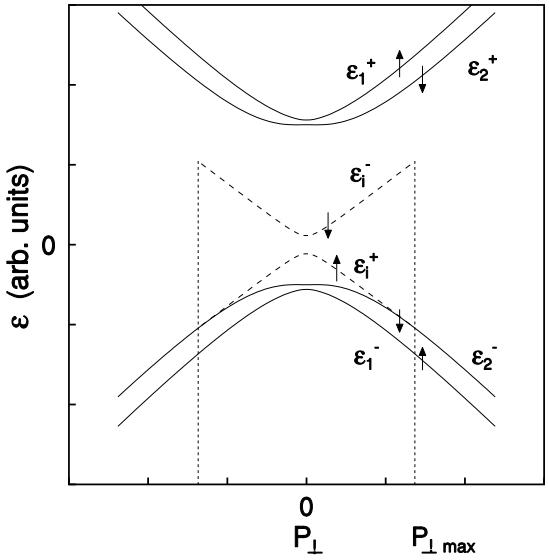

Figure 2. As figure 1, but for the asymptotes $f(+\infty) < 0$, $f(-\infty) > 0$.

along the z-axis or in the opposite direction, the magnetization value being exponentially attenuated moving away from the interface plane. Clearly the interface magnetization is maximal 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 directed oppositely. In the intermediate case, where 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 governed 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 $S^{\pm}_{1,2}$, equation (11), over the occupied states, we have

$$M = \frac{\langle S_i^{\pm}(0)\rangle}{\langle S^{\pm}_{1,2}\rangle} = \frac{\pi\sqrt{E_0^2 + \Delta_0^2}}{p_F v_{\parallel}} \frac{(1-\delta)(\delta+2)}{3} \tag{26}$$

where $\delta = \epsilon_i^{\pm}/\epsilon_i^{\pm}(p_{\perp max}) = E_0 L/(\Delta_0^2 + E_0^2)$. Here we have put $V_0 = 0$ and determined the Fermi energy from the value of $p_{\perp max}$, equation (21), i.e. the ideal situation in which the interface magnetization is a maximum is considered. It is obvious that the relationship of the interface magnetization to the band one is governed by the ratio of the energies of the occupied interface states and band states (i.e. ϵ_F).

From (26) we note that the interface magnetization is equal to zero at $\delta = 1$, i.e., as follows from (21), at $p_{\perp max} = 0$. This is a quite trivial result, because there are no interface states in this case. In the interval $0 \leqslant \delta \leqslant 1$ the value of the relative interface magnetization M is a monotonically decreasing function of the parameter δ; this is obviously caused by the decrease of the interface-state fraction with δ increasing from 0 to 1. The value of M is a maximum at $\delta = 0$, i.e. at E_0 or $L = 0$. However, it is quite apparent from (25) and (11) that at $L = 0$ there is neither any interface nor any band magnetization, so M takes an indeterminate value. As for the case where $E_0 = 0$, from (10) we find the energy branches $\epsilon_1^{\pm}$ to be superimposed on $\epsilon_2^{\pm}$ (for $E_0 = 0$), so the energy states $\epsilon^{\pm}$ become doubly degenerate with the net spin equal to zero. So relation (26) holds just over the interval $0 < \delta \leqslant 1$, where the point $\delta = 0$ is ignored.

Now, using representative estimates for the model parameters, we find the value of the relative interface magnetization M, equation (26), to be of the order of 1—that is, the interface magnetization may be a real effect for the structures under consideration. For the inverted contact with variable antiferromagnetic ordering, we guess that the perturbation solutions in the limit of small $p_{\perp}$ will show the same peculiarities as for the contact with constant antiferromagnetic ordering. Again, each interface state is non-degenerate. The spin of one of them is up relative to the z-axis but the spin of the other is down.

5. Summary

We have discussed in some detail the spectra for the 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 stressed semiconductor heterojunctions without antiferromagnetic ordering [6] (which correspond to $L = 0$ in our model) or with interface states arising in a 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 electron- and hole-like 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. So, if in the semiconductor heterostructures the Fermi level—for example, as a result of doping—falls

into one of the interface bands, then this leads to magnetic ordering in the interface plane. In view of this, the interface magnetization effect has been discussed. This effect can occur even in normal semiconductor heterojunctions if the gaps of the initial semiconductors have the same signs. However, as emphasized in the introduction, for a stressed semiconductor heterojunction with a normal band arrangement, the interface states appear inside either the bulk valence or conduction bands of the original semiconductors, and they exist for 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 interface magnetization might be found under more rigorous conditions.

In this work, an idealized system in the framework of certain approximations has been studied. Correlation problems treated in the self-consistent approach have been excluded from our consideration. However, the specific physical properties of the IV–VI narrow-gap semimagnetic semiconductors (used as model materials), such as the small values of the effective masses, and the very high dielectric constants (resulting in strong screening of the electromagnetic fields), lead us to believe the electron correlation effect to be of no importance for the problems discussed.

Another question arises concerning the neglect of the terms $\sim k^2$ in the 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 cut-off, but the quantitative changes are 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 for

$$p_\perp^2 < 4\Delta_0^2\left(\frac{mv^2}{\Delta_0}\right). \tag{27}$$

So, in the second approximation of perturbation theory, the condition restricting the range of transverse momentum for the interface states in stressed semiconductor heterojunctions with antiferromagnetic ordering will not be as simple as (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 of the order of 5, after a trivial estimation we find the relation (21) to be more rigorous than (27). Thus we have good reasons to assume that upon including the far-band corrections our main results would not change.

In concluding, we would like to note that there have been experimental studies [18, 19] showing some new magnetic effects in EuTe/PbTe superlattices which can be connected with interface magnetization, but a direct observation of the effect under consideration would be more likely to be achieved by means of magneto-optical experiments. From the theoretical point of view, at this moment, as a first step, the simple model developed fits the problem in question quite adequately, providing an opportunity to achieve an understanding of the physics of the phenomenon. Clearly, in order to make further progress, the interface magnetization effect discussed in this work needs to be considered by means of a self-consistent approach, treating some of the correlation effects.

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