INTERFACE STATES IN STRESSED SEMICONDUCTOR HETEROJUNCTION WITH ANTIFERROMAGNETIC ORDERING

Kantser V.G., Malkova N.M.,

Institute of Applied Physics, Academy of Sciences of Moldova, 277028 Kishinev, Moldova, e-mail: malkova@lises.moldova.su

Abstract

The stressed heterojunctions with antiferromagnetic ordering in which the constituents have opposite band edge symmetry and their gaps have opposite signs have been investigated. The interface states have been shown to appear in these heterojunctions and they are spin-split. As a result if the Fermi level gets into one of the interface bands then it leads to magnetic ordering in the interface plane. That is the interface magnetization effect can be observed.

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1 Introduction

The majority of semiconductor structures are known to be stressed as far as there is a lattice mismatch of their constituents. The electron energy spectrum of the stressed semiconductor structures is determined by the strains besides the widths of their layers and physical parameters of the constituents. More direct strain effect is a change of the energy spectrum which is different in each constituent and depends upon the acoustic deformation potentials of both conduction and valence bands. Last time this problem has been hard investigated in different semiconductor structures [1]. On the other hand in stressed semiconductor structures the elastic strains or their gradients due to piezoelectric or flexometric effects can lead to static polarization fields [2]. 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. The polarization is known to be conditioned by the shift of the cation and anion sublattices of the binary (or multinary) semiconductors. So it is obvious that for different crystal growth directions of the epitaxial layer structures the polarization vector is differently directed depending on the crystal lattice type. For example, for the structures based on IV-VI or II-VI semiconductors the polarization is maximum for the trigonal orientation along [111] axis and it is directed along the same axis.

In our earlier work [3] we have investigated the polarization effect on the boundary interface states of the semiconductor heterojunction, taking into account a specific character of this polarization influence on the semiconductor energy spectrum (looking like the spectrum of the semiconductor undergoing the structural phase transition with appearance of the ferroelectricity ordering). The direct genesis of such interface states by means of the inhomogeneous polarization field induced by the semiconductor layer strains has been studied in heterojunctions with both the normal bands arrangement and the inverse one [3]. In the latter structures the universal electronic interface states have been predicted to appear. These semiconductor heterojunctions have been called the inverted band contacts (or simpler inverted contacts) [4], [5]. They are characterized by the oppo-
site band edge symmetry of their constituents and so their gaps have opposite signs. As an example of the inverted contacts the heterojunctions based on some narrow-gap IV-VI or II-VI semiconductors are usually considered. It is worth noting that quite recently in the work [8] the magnetic-field dependences of the Hall coefficient in PbTe/SnTe superlattices have been interpreted assuming that in addition to the electrons in PbTe and holes in SnTe a third kind of charge carries appears, which have been connected with the above-mentioned interface states.

At doping with transition or rare-earth elements the above-mentioned semiconductors turn into dilute magnetic ones and at low temperature they might transit to the ferromagnetic or antiferromagnetic states. Last time the quantum structures based on such semimagnetic semiconductors have been intensively investigated [7],[8],[9] because of the opportunity their practical applications. As for the interface states in these quantum structures the antiferromagnetic ordering with the different signs in the initial components has been shown [10] to lead to the boundary states localized near the interface plane.

Thus the aim of this work is to study the interface states in stressed inverted contacts based on the semimagnetic narrow-gap semiconductors with antiferromagnetic ordering. It is worth noting that this situation might be realized by the static spin density wave. Its co-existence with the commensurate charge density wave in the so-called systems with electron-hole pairing results in the spin-split and under limit doping leads to the electronic spin ordering [11]. Now taking into account that the charge density wave might be induced by the structural lattices distortions which accompany the polarization one can affirm that the situation with antiferromagnetic ordering will be like the one in systems with the exciton ferromagnetism but with its specific characteristics. Firstly, the fields of the polarization and ferromagnetic ordering are considered to be settled. Secondly, the main attention in the evolution of the electron spectrum will be paid to the interface states resulting in the interface magnetic ordering.

For a concrete definition of our calculations the heterojunctions based on the semimagnetic narrow-gap IV-VI semiconductors will be studied.
2 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. So that near the gap middle there are two double degenerated bands $L^+$ and $L^-$ with opposite coordinate symmetry. Thus the simplest model describing the spectrum of the narrow-gap IV-VI semiconductors is the two-band one [12], [13]. In the paper [10] it has been shown that in the case of the mirror symmetry bands the energy spectrum of the stressed semiconductor heterojunction with polarization and antiferromagnetic ordering along the trigonal [111] crystal axis picked out as z-axis might be described by the effective Dirac Hamiltonian

\[ \hat{H}_0 = \begin{pmatrix} \Delta & \vec{\sigma}\vec{p} - i(\vec{\sigma}\vec{E} + L) \\ \vec{\sigma}\vec{p} + i(\vec{\sigma}\vec{E} + L) & -\Delta \end{pmatrix}, \]

(1)

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector with the components of the Pauli matrices, $\vec{p} = -i\hbar(\nu_\perp \nabla_x, \nu_\perp \nabla_y, \nu_\parallel \nabla_z)$, $\nu_\perp, \nu_\parallel$ being the electron Fermi velocities, $\Delta = E_g/2$, $E_g$ is the energy gap, the vector $\vec{E}$ describes the polarization. Following the results of the work [10] we introduced the scalar $L$ to describe the antiferromagnetic ordering with the antiferromagnetic vector along z-axis. The form of this term can be obtained using the Heisenberg like exchange Hamiltonian in the frames of the molecular field approximations and assuming that antiferromagnetic order can be described as a particular spin density wave [14]. Note that the Hamiltonian $\hat{H}_0$ looks like the one which describes the energy spectrum of the exciton ferromagnetic within the framework of the mean field approximation [11]. It is quite in order taking into account the above mentioned analogy between these two tasks. In the Hamiltonian (1) the upper and lower blocks are connected with the double degenerated states $\varphi$ and $\chi$ of the conduction and valence bands, respectively. In this work the situation with the polarization field $\vec{E}$ directed along the triagonal axis [111] is considered.

After the transformation

\[ \hat{U} = \begin{pmatrix} i\sigma_z & 0 \\ 0 & 1 \end{pmatrix} \]

(2)
the Hamiltonian (1) has the form
\[ \hat{H}_0 = U^{-1} \hat{H}_0 U = \begin{pmatrix} \Delta & ip_z + \hat{W} + E \\ -ip_z + \hat{W} + E & -\Delta \end{pmatrix}, \] (3)
where the operator \( \hat{W} = \hat{\sigma}[\hat{p}\hat{E}] + \sigma_z L \).

First of all let us consider the energy spectrum of the homogeneous semiconductor with polarization and antiferromagnetic ordering. After simple calculations we obtain that the energy spectrum consists of the four spin-split energy branches:
\[ \epsilon_{1,2}^+ = \sqrt{(E + W_\pm)^2 + \Delta^2 + p_z^2}, \]
\[ \epsilon_{1,2}^- = -\sqrt{(E + W_\pm)^2 + \Delta^2 + p_z^2}. \] (4)

Here \( W_\pm = \pm \sqrt{L^2 + p_\perp^2} \) are the eigenvalues of the operator \( \hat{W}_\pm \), which correspond to the eigenvectors
\[ \varphi^\pm = \begin{pmatrix} 1 \\ \frac{p_y - ip_x}{L \pm W_\pm} \end{pmatrix} \varphi_0^\pm, \] (5)
where \( \varphi_0^\pm \) is a normalized factor. The branches \( \epsilon_{1,2}^+ \) and \( \epsilon_{1,2}^- \) describe two spin-split conduction and valence bands, respectively. Taking into account the form of the wave functions for the average value of the spin one gets
\[ \bar{S}_{1,2}^+ = \frac{4|\epsilon_{1,2}^+|}{|E \pm \sqrt{p_\perp^2 + L^2 - \epsilon_{1,2}^+}|} \frac{1}{L \pm \sqrt{L^2 + p_\perp^2}} (p_y, -p_x, L), \]
\[ \bar{S}_{1,2}^- = \frac{4|\epsilon_{1,2}^-|}{|E \pm \sqrt{p_\perp^2 + L^2 - \epsilon_{1,2}^-}|} \frac{1}{L \pm \sqrt{L^2 + p_\perp^2}} (p_y, -p_x, L). \] (6)

So one can see that polarization and antiferromagnetic ordering split the Kramer’s spin degeneracy. Each of the branches of the conduction \( \epsilon_{1,2}^+ \) or the valence \( \epsilon_{1,2}^- \) bands are characterized by the opposite directions of the average spin value \( \bar{S} \). As it follows from (6) \( \bar{S} \) is directed along the vector
\[ \bar{I} = L \bar{n} + [\bar{n} \bar{p}_\perp], \] (7)
where \( \bar{n} \) is an unit vector along z-axis, \( \bar{p}_\perp = (p_x, p_y, 0) \).
3 Interface states of the stressed inverted contact

Now let us consider as inhomogeneous semiconductor structure the non-symmetry inverted contact with the axis along $z$-axis when besides the coordinate dependence of the band gap there is a coordinate dependence of the polarization field, the parameter of the antiferromagnetic ordering being constant in both semiconductors. The positions of gap centres of the constituents are different in non-symmetry inverted contact, so the Hamiltonian must include a coordinate depending work-function $V(z)$. To simplify analytical calculation we put that the gap-function $\Delta(z)$, the polarization function $E(z)$ and the work-function $V(z)$ all are determined by a single function of $z$ so that

$$\Delta(z) = \Delta_0 f(z), E(z) = E_0 f(z), V(z) = V_0 f(z),$$

(8)

where apparently in the inverted contact the signs of the asymptotics $f(z \to \pm \infty)$ are opposite, $\Delta_0, E_0, V_0$ are constants. Two different cases may be considered: 1. $f(\infty) > 0, f(-\infty) < 0$; and 2. $f(\infty) < 0, f(-\infty) > 0$.

So the Hamiltonian of the system is

$$\hat{H} = \begin{pmatrix} \Delta - V & i p_z + \hat{W} + E \\ -i p_z + \hat{W} + E & -\Delta + V \end{pmatrix}.$$  

(9)

By means of the unitary transformation

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

(10)

where the angle $\Theta$ satisfies the condition

$$\Delta_0 \cos 2\Theta - E_0 \sin 2\Theta + V_0 = 0,$$

(11)

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

$$\hat{\tilde{H}} = \hat{V}^{-1} \hat{H} \hat{V} =$$

$$\begin{pmatrix} -W^\pm \sin 2\Theta & -\sqrt{E^2 + \Delta^2 - V^2} + W^\pm \cos 2\Theta + i p_z \\ -\sqrt{E^2 + \Delta^2 - V^2} + W^\pm \cos 2\Theta - i p_z & 2V + W^\pm \sin 2\Theta \end{pmatrix}.$$ 

(12)
From (12) we immediately obtain that the Schrödinger equation

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

where

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

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 papers [3], [4], [5] by means of a supersymmetry quantum mechanics and they in its term have been called Weyl states.

In the case when \(f(+\infty) > 0\) and \(f(-\infty) < 0\) there is the following solution of the equation (12)

$$\epsilon^\pm = \pm \frac{E_0 V_0 - \Delta_0 \sqrt{E_0^2 + \Delta_0^2 - V_0^2}}{\Delta_0^2 + E_0^2} \sqrt{p_{\perp}^2 + L^2}. \quad (14)$$

The function \(\tilde{\varphi}^\pm\) satisfies the equation

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

where

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

This function plays the same role as the superpotential in the supersymmetry quantum mechanics method [3], [5]. From (15) one can see that the states \(\epsilon_i^\pm\) are of the interface type because the function \(\tilde{\varphi}^\pm\) is localized at the interface boundary. At the given asymptotics of the \(f(z)\) function the wave functions \(\tilde{\varphi}^\pm\) are normalized under the conditions

$$\sqrt{p_{\perp}^2 + L^2} < \frac{(\Delta_0^2 + E_0^2) \sqrt{E_0^2 + \Delta_0^2 - V_0^2}}{\Delta_0 V_0 + E_0 \sqrt{E_0^2 + \Delta_0^2 - V_0^2}}. \quad (16)$$

So the interface states (14) are restricted both in the energy space and in the momentum space.

In the case of the opposite asymptotics the interface solutions are described by the same expressions (14)-(16) by replacing \(\Delta_0 \to -\Delta_0\), \(p_z \to -p_z\).
4 Conclusions

Comparing these interface states with those of the stressed semiconductor heterojunction without the antiferromagnetic ordering \[\text{[3]}\] one can see that in this situation the spectrum of the interface states is not linear in \(p_\perp\). Moreover in contrast to the interface states arising in the simple inverted contact \[\text{[4]}\] or in the homogeneous semiconductor with antiferromagnetic domain wall \[\text{[5]}\] in the case of the stressed inverted contact with antiferromagnetic ordering there is a gap between the electron-like and the hole-like states, which is determined by the parameter of the antiferromagnetic ordering \(L\).

Each interface state
\[
\Psi^\pm = \begin{pmatrix} \varphi^\pm \\ 0 \end{pmatrix}
\]
is nondegenerated and the average spin value, for example for the first type of the asymptotics, is

\[
<\Psi^\pm|\Sigma|\Psi^\pm> = C\exp\left(-\frac{2}{h\nu_\parallel} \int W^\pm(z)dz \right) \frac{2}{L \pm \sqrt{p_\perp^2 + L^2}} (p_y, -p_x, L),
\]
where \(C\) is a constant which is determined by a normalize condition. After averaging over the electron momentum \(p_\perp\) for the taken symmetrical spectrum model one gets

\[
<\vec{S}^\pm > \sim \pm (\sqrt{L^2 + p^2_{\perp,\text{max}}} - L)(0, 0, L),
\]
where \(p_{\perp,\text{max}}\) is defined by the condition (16). That is the average spins of the \(\Psi^+\) and \(\Psi^-\) states are opposite directed along \(z\)-axis.

As it follows from (14) when \(f(+\infty) > 0, f(-\infty) < 0\) under the condition \(\Delta_0^2 > V_0^2\) the energy level \(\epsilon_i^+\) is situated higher than \(\epsilon_i^-\) while under the condition \(V_0^2 > \Delta_0^2\) they switch their positions. So the state with the average spin down is higher than the state with the spin up. For another asymptotics: \(f(+\infty) < 0, f(-\infty) > 0\), the state \(\epsilon_i^-\) with the spin down is higher than the state \(\epsilon_i^+\) with the spin up.

Comparing the expression (4) for the energy levels of the homogeneous semiconductors and (14) for interface heterojunction states one gets that the interface states are situated nearer to the middle of the gap of the constituents. Thus if in the studied semiconductor
heterojunctions the Fermi level, for example by means of doping, gets into one of the two-dimensional interface bands, then it leads to the magnetic ordering into the interface plane. The magnetic moment as it follows from (15) is exponential attenuated moving away from the interface plane.

Figures 1 and 2 show the rough sketch of the interface energy spectrum arising in the stressed inverted contact with antiferromagnetic ordering for both types of the functions \( f(z) \) asymptotics. Solid lines correspond to the bulk semiconductor bands while dashed lines to the interface states. Arrows show the average spin direction. Note that in accordance with the taken geometry of the studied heterojunctions the energy branches of the constituents are the same but their spin directions are opposite in the initials semiconductors.

The interface magnetization effect investigated in this work can be observed also in the normal semiconductor heterojunction when the gaps of the initial semiconductors have the same signs. But in this situation as it have been shown \cite{3} for stressed semiconductor heterostructure the interface states appear inside either the bulk valence or conduction bands of the original semiconductors, and they are restricted in the momentum space. So in this case the effect of the interface magnetization might take place under more rigorous conditions.

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References

[1] Smith D.L., Mailhiot C. Reviews of Modern Physics, 1990, 62, N1, p.173-234.

[2] Tagantsev A.K., Sov. Phys. Usp., 1987, 30, N3, p.588-602.

[3] Kantser V.G., Malkova N.M. JETP Lett., 1991, 54, N7, p.384-389.

[4] Volkov B. A., Pankratov O. A., JETP Lett., 1985, 42, p.178.

[5] Pankratov O.A., Pakhomov S.A., Volkov B.A. Solid State Comm. 1987, 61, N 2, p.93-96.

[6] Litvinov V.,Oszwaldowki M.,Berus T.,Mironov O., Phys.Stat. Sol.(a), 1994, 145, N2, p.503-508.

[7] Yuan S., Frank N.,Bauer G.,Kriechbaum M., Phys.Rev.B, 1994, 50, N8, p.5286-5294.

[8] Yuan S.,Springholz G.,Bauer G.,Kriechbaum M., Phys.Rev.B, 1994, 49, N8, p.5476-5489.

[9] Olver M. M., Pastalan J. Z., Romaine S. E., et.al., Solid State Comm., 1994, 89, N8, p.693-696.

[10] Pankratov O.A., Physics letters A, 1987, 121, N7 p.360-366.

[11] Volkov B.A., Kopaev Yu.V., Rusinov A.I., Sov Phys. JETP, 1975, 41, N 5, p.952-959.

[12] Dimmock J.O., Wright G.B. Phys. Rev., 1964, 135, N 3A, p.A821-830.

[13] Mitchell D.L., Wallis R.F., Phys. Rev., 1966, 151, N 2, p. 581-595.

[14] Acquarone M., Magnetic properties of Matter (Proc. of the National School held in L’Aquila, September 3-14, 1990), World Scientific Publishing, Singapore.New-Jersey.London.Hong Kong, 1991, p.3.
LIST CAPTIONS

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

Fig. 2 The same as in the fig.1 but for the asymptotics $f(+\infty) < 0$, $f(-\infty) > 0$. 
Fig. 1. The interface energy spectrum for the first type asymptotics. Solid lines show the energy branches of the constituents and dashed lines show the interface states. The arrows show the average spin direction.
Fig. 2. The same as in Fig. 1 but for the second type asymptotics.