Boundary electronic states in stressed semiconductor heterostructures

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Two-dimensional electronic states with a linear spectrum appear in a stressed heterostructure with internal polarization fields induced by an elastic strain. These states appear regardless of the arrangement of bands of the semiconductors. They exist in only limited intervals of the energy and the transverse momentum.

The elastic strain which arises in stressed periodic heterostructures can substantially change the electronic structure of these heterostructures, giving rise to many new features in the physical characteristics of the semiconductor system. In this letter we analyze the electron energy spectrum of stressed heterostructures made from piezoelectric semiconductors.

Since piezoelectric materials do not have a symmetry center, static polarization fields are generated in stressed multilayer structures made from them. The magnitude and orientation of these fields depend on the growth direction of the structure.[1] Stressed superlattices have a situation in which one of the alternating layers is stretched, while the other is compressed. As a result, the polarization may in fact have opposite signs in the different layers of the heterostructure. The polarization $P_{a,b}$ induced by a uniform strain of the layers (a and b) is determined by the piezoelectric tensor $e_{14}^{a,b}$, by the elastic constants of the constituent semiconductors, and by the ratio of layer thicknesses. This polarization is comparable in magnitude to the spontaneous polarization in weak ferroelectrics.[1] Static polarization fields may also arise in structures made of semiconductors with a symmetry center, as the result of a flexometric effect, when there is a gradient of the strain fields.

The simplest model in which the effect of the polarization on the energy spectrum can be taken into account is the two-band kp scheme. In the case of mirror-symmetry bands, this scheme takes the form of the modified Dirac equation

$$\begin{bmatrix} \Sigma(z) & \vec{\sigma}(\vec{p}+i\vec{\Delta}(z)) \\ \vec{\sigma}(\vec{p}-i\vec{\Delta}(z)) & -\Sigma(z) \end{bmatrix} \Psi = [E-V(z)]\Psi, \tag{1}$$

where $\Sigma(z) = E_g(z)/2$, the function $\Delta(z)$ is related to the displacement of the sublattices and is proportional to the magnitude of the polarization, σ are the Pauli matrices $\vec{p} = -i\hbar(v_\perp \nabla_x, v_\perp \nabla_y, v_\parallel \nabla_z)$, $v_{\perp,\parallel}$ are the electron Fermi velocities, and $V(z)$ is the potential, which incorporates the change in the work function in the structure. We could also incorporate in $V(z)$ terms associated with electric fields generated by the polarization. The direct effect of strain on the spectrum can also be taken into account through renormalized gap parameters.

In the case of a homogeneous semiconductor, the eigenvalues of Eq. (1) deter-

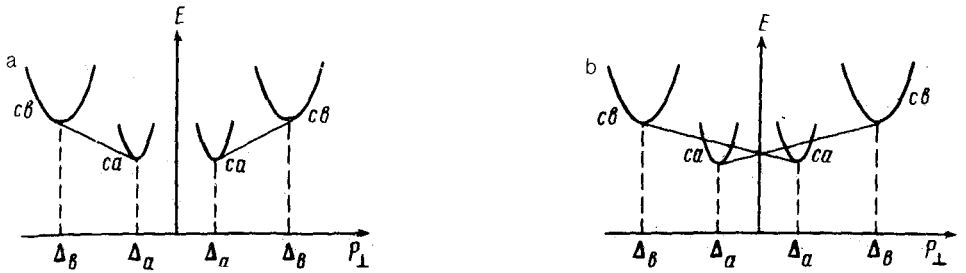

FIG. 1. Rough sketch of the spectrum of boundary states in a stressed semiconductor heterostructure with a normal arrangement of bands ($E_{ga}E_{gb}>0$). a—Case of a heterojunction with identically oriented polarizations in the layers ($\Delta_a\Delta_b>0$); b—case of a heterojunction with oppositely directed polarizations in the layers ($\Delta_a\Delta_b<0$). Here *ca*, *cb*, *va*, and *vb* are the bulk bands in the semiconductors.

mine four spin-split energy branches[2] (Fig. 1). In an inhomogeneous semiconductor structure, the quantities Σ, Δ, and V (among others) are functions of the coordinates. The vector quantity $\vec{\Delta}$ may be oriented in different ways with respect to the z axis of the structure. We consider the case in which $\vec{\Delta}$ is directed along the z axis: $\vec{\Delta}=[0,0,\Delta(z)]$. According to Ref. 1, this case corresponds to an orientation of the structure along the trigonal axis of a cubic semiconductor. We assume that the spatial variation of the quantities Σ, Δ, and V is determined by the same function $f(z)$. We also assume that the parameters $v_{\perp,\parallel}$ are identical for the two semiconductors making up the structure. The spatial variation of the quantities Σ, Δ, and V for an individual heterojunction can thus be written

$$\Sigma(z)=\Sigma_+ +\Sigma_- f(z),\quad \Delta(z)=\Delta_+ +\Delta_- f(z),\quad V(z)=\varphi_0/2f(z), \tag{2}$$

where $\Sigma_\pm=(E_{gb}\pm E_{ga})/4$, $\Delta_\pm=(\Delta_b\pm\Delta_a)/2$, and $f(z\to\pm\infty)=\pm 1$.

To study the energy spectrum of a nonuniform structure consisting of a heterojunction, we transform Eq. (1) into an equation of supersymmetric quantum mechanics, as in Refs. 3 and 4. For this purpose, we first let the matrix operator on the left side of Eq. (1) operate on both sides. The matrix equation found in this manner can be diagonalized by means of the following unitary transformation when the spatial variations $\Sigma(z)$, $\Delta(z)$, and $V(z)$ are all identical:

$$\hat{S}=\begin{pmatrix}\cos\theta & i\sin\theta\\ i\sin\theta & \cos\theta\end{pmatrix},\quad \tan\theta=\frac{\Delta_- +(\Sigma_-^2+\Delta_-^2-V_0^2)}{(\Sigma_- +V_0)}. \tag{3}$$

This transformation commutes with the operator $\hat{p}_z$. As a result, the matrix equation which determines the electronic state of the nonuniform structure takes the form of an equation of supersymmetric quantum mechanics:

$$\left\{\left[p_z^2+W^2(z)+\hbar v_{\parallel}\sigma_z\otimes\tau_z\frac{dW(z)}{dz}\right]+\Sigma_+^2+(\pm p_\perp+\Delta_+)^2-E^2\right.$$

$$\left.\frac{[\Sigma_+\Sigma_- +\Delta_-(\pm p_\perp+\Delta_+)+EV_0]^2}{\Sigma_-^2+\Delta_-^2-V_0^2}\right\}\Phi(z)=0. \tag{4}$$

Here $\Phi(z)$ is the envelope of the wave function $\Psi = \exp(ik_{\perp\rho})\hat{S}^{-1}\Phi(z)$; τ_z is the Pauli matrix acting in the space of the wave functions which determine the conduction and valence bands; $p_\perp = v_\perp |k_\perp|/\hbar$; and, finally the supersymmetric potential $W(z)$ is given by

$$W(z) = (\Sigma_-^2 + \Delta_-^2 - V_0^2)^{1/2}\left[f(z) + \frac{\Sigma_+\Sigma_- + \Delta_-(\pm p_\perp + \Delta_+) + EV_0}{\Sigma_-^2 + \Delta_-^2 - V_0^2}\right]. \quad (5)$$

According to a theorem of supersymmetric quantum mechanics,[5] when the asymptotic expressions for the superpotential $W(z \to \pm\infty)$ have opposite signs, i.e., when

$$\left|\frac{\Sigma_+\Sigma_- + \Delta_-(\pm p_\perp + \Delta_+) + EV_0}{\Sigma_-^2 + \Delta_-^2 - V_0^2}\right| \leq 1, \quad (6)$$

Eq. (4) has a so-called zero mode as eigenvalues. This solution determines two-dimensional boundary electronic states of the Weyl type, which are localized near the interface.[4] For the asymptotic behavior which we have selected, $W(\infty) > 0$ and $W(-\infty) < 0$, the zero mode of Eq. (4) arises in the case $\sigma_z \otimes \tau_z = -1$. Accordingly, the energy spectrum of the boundary states is not degenerate in terms of spin. It is determined from

$$E = \{-\Sigma_+(V_0\Sigma_- + D\Delta_-) + (\Delta_+ \pm p_\perp)(D\Sigma_- - V_0\Delta_-)\}(\Sigma_-^2 + \Delta_-^2)^{-1}, \quad (7)$$

for $(V_0 D - \Sigma_-\Delta_-)(\Delta_-^2 - V_0^2)^{-1} \geqslant 0$, and

$$E = \{-\Sigma_+(V_0\Sigma_- - D\Delta_-) - (\Delta_+ \pm p_\perp)(D\Sigma_- + V_0\Delta_-)\}(\Sigma_-^2 + \Delta_-^2)^{-1}, \quad (8)$$

for $(V_0 D + \Sigma_-\Delta_-)(\Delta_-^2 - V_0^2)^{-1} \leqslant 0$, where $D = (\Sigma_-^2 + \Delta_-^2 - V_0^2)^{1/2}$ and $|V_0| \leqslant (\Sigma_-^2 + \Delta_-^2)^{1/2}$.

The zero mode of Eq. (4) exists when the asymptotic expressions for superpotential (5) as $z \to \pm\infty$ have opposite signs, i.e., when conditions (6) hold. Correspondingly, boundary electronic states exist in limited intervals of the energy and of the transverse momentum $p_\perp = \hbar v_\perp k_\perp$. These intervals are defined by

$$-V_0 - \frac{(\Sigma_+ - \Sigma_-)}{\Delta_-^2 - V_0^2}(\Delta_- D - V_0\Sigma_-) \leq E \leq V_0 - \frac{(\Sigma_+ + \Sigma_-)}{\Delta_-^2 - V_0^2}(\Delta_- D - V_0\Sigma_-),$$
$$-\Delta_- - \frac{(\Sigma_+ + \Sigma_-)}{\Delta_-^2 - V_0^2}(\Delta_-\Sigma_- - DV_0) \leq \Delta_+ \pm p_\perp \leq \Delta_- - \frac{(\Sigma_+ - \Sigma_-)}{\Delta_-^2 - V_0^2}(\Delta_-\Sigma_- DV_0) \quad (9)$$

for energy branch (7) and

$$V_0 + \frac{(\Sigma_+\Sigma_-)}{\Delta_-^2 - V_0^2}(\Delta_- D + V_0\Sigma_-) \leq E \leq -V_0 + \frac{(\Sigma_+ - \Sigma_-)}{\Delta_-^2 - V_0^2}(\Delta_- D + V_0\Sigma_-),$$
$$\Delta_- - \frac{(\Sigma_+ - \Sigma_-)}{\Delta_-^2 - V_0^2}(\Delta_-\Sigma_- - DV_0) \leq \Delta_+ \pm p_\perp \leq -\Delta_- \quad (10)$$
$$+ \frac{(\Sigma_+ + \Sigma_-)}{\Delta_-^2 - V_0^2}(\Delta_-\Sigma_- + DV_0)$$

for energy branch (8).

Two-dimensional electronic states of a boundary type were first predicted and studied by Volkov and Pankratov[3] for a heterostructure based on a junction between two semiconductors with mutually inverted bands ($E_{ga}E_{gb}<0$). It follows from (7) and (8) that boundary electronic states may exist in any semiconductor heterostructure, i.e., in the case $E_{ga}E_{gb}>0$. For an unstressed heterostructure ($\Delta_a=\Delta_b=0$), the only necessary condition is that the difference between the work functions be finite[6-8] ($V_0\neq 0$). In the case of a heterojunction with a normal arrangement of bands ($E_{ga}E_{gb}>0$), branches of boundary states appear either inside the bulk valence bands (in the case $V_0\Sigma_-<0$) or inside the bulk conduction bands (in the case $V_0\Sigma_->0$); (Fig. 1) (in contrast with the case of a heterojunction with an inversion of bands,[3,4] in which the energies of the boundary states fall in energy gaps of the original semiconductors).

The picture of boundary energy branches is richer in the case of stressed semiconductor heterostructures, i.e., with $\Delta_a\neq 0$ and $\Delta_b\neq 0$. We first analyze the case of a heterojunction with a normal arrangement of bands, $E_{ga}E_{gb}>0$ and $\Sigma_+>0$. We note that with $E_{ga}=E_{gb}$, $V_0=0$, and $\Delta_+=0(\Delta_a=-\Delta_b)$ we find from (7) and (8) a spectrum of two-dimensional "heavy fermions." These entities have been studied previously in a so-called supersymmetric ferroelectric domain wall.[9] For $V_0\neq 0$, two-dimensional boundary bands acquire width, and the heavy-fermion spectrum[9] becomes dispersive. In the case $\Delta_- V_0>0$, its two-dimensional energy branches lie against the background of the bulk valence bands, while in the case $\Delta_- V_0<0$ they lie against the background of the conduction bands (Fig. 1).

To analyze the picture of the boundary states in the general case ($\Sigma_-\neq 0$, $\Delta_-\neq 0$, $V_0\neq 0$), it is important to consider the particular case $\Sigma_-\neq 0$, $\Delta_-\neq 0$, but $V_0=0$. We easily see from (7) and (8) that boundary electronic states arise only if $\Sigma_-\Delta_-\leqslant 0$. Consequently, if $\Sigma_-\Delta_->0$, two-dimensional electronic states appear at the heterojunction only at finite values of the difference between work functions ($V_0\neq 0$). In this case, the two-dimensional boundary bands lie against the background of either bulk conduction bands, for $\Sigma_->0$, $\Delta_->0$, $-(\Sigma_-^2+\Delta_-^2)^{1/2}\leqslant V_0\leqslant\min\{-|\Delta_-|,-|\Sigma_-|\}$ and for $\Sigma_-<0$, $\Delta_-<0$, $\max\{|\Sigma_-|,|\Delta_-|\}\leqslant V_0\leqslant(\Sigma_-^2+\Delta_-^2)^{1/2}$, or valence bands, for $\Sigma_-<0$, $\Delta_-<0$, $\max\{|\Sigma_-|,|\Delta_-|\}\leqslant V_0\leqslant(\Sigma_-^2+\Delta_-^2)^{1/2}$ and for $\Sigma_-<0$, $\Delta_-<0$, $-(\Sigma_-^2+\Delta_-^2)^{1/2}\leqslant V_0\leqslant\min\{-|\Delta_-|,-|\Sigma_-|\}$. In the case $|V_0|=|\Sigma_-|$, the two-dimensional bands become dispersion-free, as in the case of ferroelectric domain wall.[9]

The conditions for the existence of boundary states in stressed heterostructures with a normal arrangement of bands ($E_{ga}E_{gb}\geqslant 0$) are less stringent in the case $\Sigma_-\Delta_-\leqslant 0$. As we have already mentioned, these conditions include the point $V_0=0$. Depending on the particular situation, the energy levels of these states also lie against the background of either the valence bands of the original semiconductors or the conduction bands.

In the analysis up to this point we have considered only heterostructures with a normal arrangement of bands ($E_{ga}E_{gb}>0$). For a heterojunction with a band inversion ($E_{ga}E_{gb}<0$, i.e., $|\Sigma_+|<|\Sigma_-|$), the energy interval in which the boundary elec-

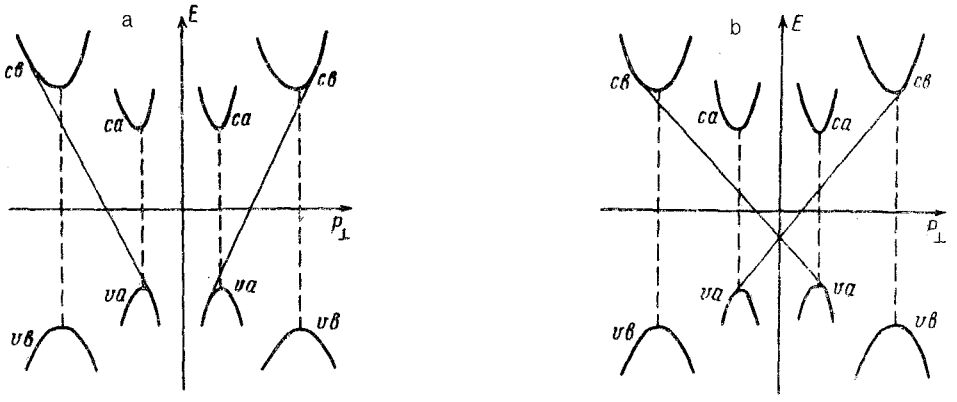

FIG. 2. Energy branches of boundary states in a stressed heterostructure with an inversion of bands. The notation is the same as in Fig. 1.

tronic states exist is far wider, as can be seen from (9) and (10). The two-dimensional energy branches stretch from one of the spin-split bulk valence bands to one of the conduction bands (Fig. 2). In the case $\Delta_a = \Delta_b = 0$ we find from (7) and (8) the energy branches which were discussed previously in Refs. 4 and 5. According to (9) and (10), the region in which the boundary states exist is limited not only along the energy scale but also along the scale of the magnitude of the transverse momentum $p_\perp$. Analysis of the second conditions in (9) and (10) shows that the $p_\perp$ interval in which these states exist is determined to a large extent by the signs of the polarization in the semiconducting layers making contact. If $\Delta_a \Delta_b > 0$, i.e., if $|\Delta_+| > |\Delta_-|$, the boundary electronic states can arise only at finite values of the transverse momentum (Figs. 1a and 2a). In the case $\Delta_a \Delta_b < 0$, on the other hand, i.e., with $|\Delta_+| < |\Delta_-|$, energy levels exist even in the case $p_\perp = 0$, and the existence domain is correspondingly far broader (Figs. 1b and 2b).

We have mentioned in this letter only the Weyl boundary electron states of a stressed semiconductor junction which are associated with a null mode of supersymmetric potential (5). These states are not degenerate in terms of spin; they are gapless; and they have a linear dispersion. Along with the Weyl states, other states localized at the interface may arise. In contrast with the Weyl states, these other states will be spin-degenerate and will have a finite spectral gap, as in a heterojunction with an inversion of bands.[4,5] The number of these states and their energy spectrum will be determined by the particular function $f(z)$ in (1). In the case of a sharp heterojunction [a stepped change in $f(z)$], only states of the Weyl type corresponding to a zero mode will appear.

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