Anisotropic exchange splitting in type-II GaAs/AlAs superlattices

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The anisotropic splitting of the exciton emission doublet, seen experimentally in a type-II GaAs/AlAs superlattice, is analyzed. The splitting is shown to result from nonconservation of the hole spin component normal to the boundary upon reflection from an ideal heterojunction, because of the low symmetry (C_{2v}) of this junction.

The lower electron states in GaAs/AlAs (001) superlattices are formed either primarily from electron states near the Γ minimum in the GaAs layer (type I) or primarily from states near the X minimum in the AlAs layer (type II), depending on the ratio of layer widths.[1] In either case, the heterostructure has point symmetry D_{2d}, and the fourfold-degenerate lower exciton level should be split by the exchange interaction into an emission doublet E and two optically inactive singlets. Experimentally, on the other hand, it has been found that the exciton doublet level E in the photoluminescence spectra of a type-II GaAs/AlAs superlattice is split into sublevels, which are dipole-active along the [110] and [1$\bar{1}$0] directions.[2–4] The occurrence of an anisotropic interaction of this sort is puzzling in itself; adding to the mystery is the extremely large energy gap $\Delta = \epsilon_{[110]} - \epsilon_{[1\bar{1}0]}$, between the levels, which approaches the size of the basic exchange splitting, between the doublet and the singlets, Δ_0 (the difference is by a factor of only 2 or 3, according to Ref. 2). It has also been found that two classes of excitons coexist in a common structure; the absolute values of Δ for these excitons are the same, and fixed, but the signs are opposite.

These facts cannot be explained by the suggestion that the anisotropy stems from an extrinsic lowering of the symmetry, e.g., a lowering caused by step distortions of the heterojunction[2] or a uniaxial deformation.[5] In this letter we offer an explanation based on an examination of the low symmetry (C_{2v}) of an ideal heterojunction. For such a symmetry, there can be a mixing of states of heavy and light holes, even when a hole is incident normally on a heterojunction. When this mixing is taken into account, the simplest boundary conditions for the envelopes (φ_j) of the hole wave function ($j = \pm 3/2, \pm 1/2$) which are allowed by the summetry C_{2v}, which are also allowed by time-reversal symmetry, and which maintain the continuity of the total flux of particles across the interface are

$$\varphi_j^A = \varphi_j^B, \quad \nabla_z^j \varphi_j^A - \nabla_z^j \varphi_j^B = \frac{2}{\sqrt{3}} t_{l-h} \sum_{j'} [J_x J_y]_{jj'} \varphi_{j'}^B. \tag{1}$$

Here t_{l-h} is a real coefficient; $\varphi^{A,B}$ is the value of the function at the boundary, on the side of layer A (GaAs) or layer B (AlAs); x is parallel to the [100] axis; y is parallel to [010]; a is parallel to [001]; and

$$\nabla_z^{\pm 3/2} = a_0 \frac{m_0}{m_{hh}} \frac{\partial}{\partial z}, \quad \nabla_z^{\pm 1/2} = a_0 \frac{m_0}{m_{lh}} \frac{\partial}{\partial z},$$

where m_0 is the mass of a free electron, m_{hh} and m_{lh} are the effective masses of a heavy hole (for simplicity, we ignore the differences between these masses in layers A and B), and a_0 is the lattice constant. In addition, J_α are the angular-momentum matrices in the basis of the Γ_8 representation of the T_d group of the bulk crystal. The only elements of the matrix $[J_x J_y] = (J_x J_y + J_y J_x)/2$ which are nonzero are the off-diagonal elements with $|j - j'| = 2$. The incorporation of the additional term in (1) is equivalent to incorporating a contribution $\pm V_{l-h} a_0 [J_x J_y]/\sqrt{3}) \delta(z - z_i)$ in the hole Hamiltonian for AB and BA heterojunctions, respectively, where z_i is the coordinate of the boundary plane, and we have $V_{l-h} = t_{l-h} \hbar^2/(m_0 a_0^2)$.

We can now show that this mixing of hole states leads to an anisotropic exchange splitting. An exciton in a type-II superlattice consists of an electron in an A layer and a hole in a neighboring B layer. The two are coupled by the Coulomb interaction (Fig. 1). Tunneling of carriers between neighboring layers of the same type can be ignored because of the large mass of a heavy hole and the large longitudinal mass of an X electron. The trapped exciton is then quasi-two-dimensional, and its wave function can be written in the form

$$\Psi_{exc} = f(\vec{R}) \sqrt{\frac{2}{\pi}} \frac{1}{\rho_0} \exp(-\rho/\rho_0) \psi_e(z_e) \psi_h(z_h), \tag{2}$$

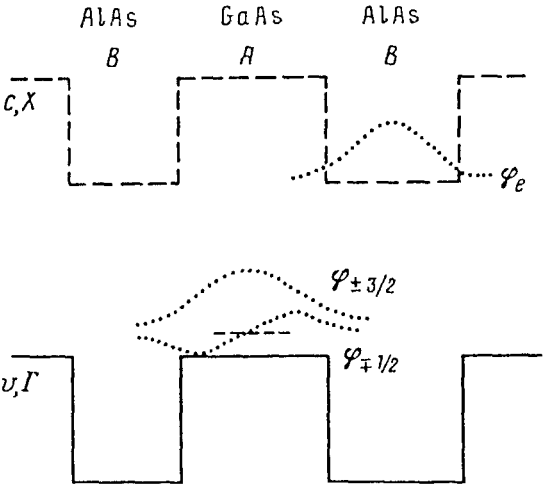

FIG. 1. Energy diagram and envelopes of the electron and hole wave functions for an AB exciton in a type-II GaAs/AlAs superlattice. Solid and dashed lines—Spatial profiles of the top of the Γ_8^v band and the bottom of the X_7^c band; dotted lines—the electron envelope (φ_c) and the hole envelopes $\varphi_{\pm 3/2}$, $\varphi_{\pm 1/2}$, which are given in layer A by $C_h \cos kz$, $C_l \sin qz$, where $\hbar k = (2m_{hh}E_1)^{1/2}$, $\hbar q = (2m_{lh}E_1)^{1/2}$, and E_1 is the energy of the size quantization of the hole. For a 17Å/17Å structure the ratio C_l/C_h is $\approx 0.1 t_{l-h}$.

where $\psi_{e,h}$ are spinor functions which describe the motion of the electron and the hole, respectively, along the axis of the superlattice, ρ_0 is the radius of a quasi-2D exciton, $\vec{\rho}$ is the relative position of the electron and the hole, $\vec{R}$ is the position of the center of mass of the exciton in the plane of a layer, and the function $f(\vec{R})$ characterizes the motion of the center of mass of the exciton. The two following wave functions satisfy boundary conditions (1) and are transformmed by the Γ_6 spinor representation:

$$\psi_h^{(\pm)}(z_h) = C(z_h)|\mp 3/2> \mp iS(z_h)|\pm 1/2>, \tag{3}$$

where C and S are real functions satisfying $C(-z) = C(z)$ and $S(-z) = -S(z)$. The origin of coordinates is at the center of the layer in which the hole is trapped (Fig. 1). We write the exchange-interaction Hamiltonian $\mathscr{H}_{\text{exch}}$ as follows:

$$\mathcal{H}_{exch} = a_0^3 V_0 \delta(\vec{r}_e - \vec{r}_h)\left(1 - \frac{2}{3}\vec{\sigma}\vec{J}\right), \tag{4}$$

where V_0 is a constant. The nature of the exchange splitting does not depend on the function describing the motion of the center of mass of the exciton. Applying operator (4) to functions (2) and (3), we find the following expression for the ratio of the anisotropic exchange splitting Δ to the basic splitting Δ_0, in the lowest approximation in t_{l-h}

$$\frac{\Delta}{\Delta_0} = \frac{4}{\sqrt{3}} \frac{\int C(z)S(z)\varphi_e^2(z)dz}{\int C^2(z)\varphi_e^2(z)dz}. \tag{5}$$

If the X electron is distributed uniformly between two B layers, the corresponding exciton has symmetry D_{2d}, so there is of course no splitting of the emission doublet. On the other hand, excitons trapped at defects of the heterostructure (e.g., fluctuations in width of the B layer) participate in a low-temperature luminescence. Let us assume that the potential in which the exciton is trapped is asymmetric with respect to the center of the A layer and that the trapping energy is greater than the overlap integral which determines the width of the X miniband in the ideal superlattice. Then there is an overwhelmingly large probability that the electron in the trapped exciton will lie either to the right or to the left of the layer in which the hole is excited (Fig. 1). In this case, expression (5) is nonzero, and it has opposite signs for AB and BA excitons. Accordingly, the two types of excitons, with exchange splittings of opposite signs, are trapped AB and BA excitons. That assertion is the basic assertion of this letter. The anisotropy axes of the exchange interaction are set by the direction of the reflection planes of the C_{2v} group, i.e., by the direction of the chemical bonds at the interface.

For a 17 Å/17 Å superlattice and for the band parameter values used in Refs. 1 and 6, the value of ratio (5) is $\approx 0.2 t_{l-h}$. A first-principles calculation of t_{l-h} remains an open question, but a comparison with experimental results[2] yields an estimate $t_{l-h} = 1$–2.

The boundary conditions which we have proposed here [conditions (1)] describe a mixing of the u_x and u_y Bloch states of the Γ_{15} representation of the T_d group. The boundary conditions are similar in structure to those found in Ref. 7 (see also Ref. 6)

for describing a mixing of Γ_1^c and X_3^c electron states in GaAs/AlAs superlattices. A calculation carried out[7] by the strong-coupling method yields $t_{\Gamma-X} \sim 1$. The estimate of t_{l-h} given above thus looks realistic.

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