

**Abstract**

The in-plane dispersion of the $X_X$ states in a GaAs/AlAs “double-barrier structure” is measured by varying the angle of an in-plane magnetic field. When $X_X$ states in the emitter AlAs layer tunnel into collector $X_X$ ($m > 1$) states, a characteristic dumbbell shape is observed for the bias shift of the resonant tunneling peak versus magnetic field angle, with the major axis along [110] or [110]. This corresponds to an elliptical constant energy surface in the collector AlAs layer which is rotated by 45° with respect to the bulk Fermi surface. We explain the new symmetry by $X_X$–$X_Y$ interface band mixing which is closely analogous to the widely studied $\Gamma$–$X_Z$ mixing. Our results provide new insight into the microscopic origin of both types of mixing. © 2000 Elsevier Science B.V. All rights reserved.

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**1. Introduction**

About 10 years ago it was predicted that in GaAs/AlAs heterostructures grown along [001] (z-direction), it is possible for mixing to occur between the AlAs $X_X$ and $X_Y$ conduction band edge states, located near the four in plane (100) boundaries of the bulk Brillouin zone [1]. In this paper we show that the effect of the mixing on the in-plane dispersion can be dramatic, particularly when an electric field is applied in the z-direction to break the four-fold symmetry in the plane. At the band edge, the four ellipses oriented along [100] and [010], which form the $X_X$ and $X_Y$ constant energy surfaces, are then replaced by a single elliptical surface oriented along either [110] or [110]. Using resonant magneto-tunneling, we are able to measure the in-plane dispersion which, to the best of our knowledge, constitutes the first observation of $X_X$–$X_Y$ mixing. We estimate the values of the mixing potentials associated with Bloch states of $X_1$ and $X_3$ symmetry, respectively. We show that interference between these two contributions to the overall mixing potential is directly responsible for the new symmetry of the constant energy surface. Contrary to a recent
theory, our results show that the $X_1$ related potential is finite.

2. Experimental

We have studied 2D → 2D tunnelling between confined states in a GaAs/AlAs structure comprising two 70 Å wide AlAs wells separated by a 30 Å wide GaAs barrier, surrounded by 150 Å spacers and doped GaAs contacts. The Ga$_{1-x}$Al$_x$As region before each spacer has been graded linearly over a distance of 1000 Å from $x = 0$ to 0.1 to enable efficient electron transfer from $\Gamma$ states in the graded region to ground $X_{X,Y}$ states in the emitter well. Fig. 1 shows the band profile in a typical structure (without grading) when the $X_{X,Y}(1)$ emitter state is in resonance with the $X_{X,Y}(3)$ collector state. The conductance is plotted versus bias in Fig. 2. $X_{X,Y}(1) \rightarrow X_{X,Y}(m)$ processes responsible for the peaks, where $m$ is the confinement quantum number, are identified in Fig. 2 by comparison with a similar ungraded sample, in which the emitter $X_{X,Y}$ states were populated using a pressure of ~9 kbar [2].

The dispersions of the $X_{X,Y}$ states were studied by applying an in-plane magnetic field which introduces a change in wave vector during tunneling, $\Delta k_y = -eB_y \Delta z/\hbar$, where $\Delta z$ is the distance between emitter and collector wave functions [3–6]. For the present sample at 15 T, $\Delta k_y \sim 0.02 \times 2\pi/a_0$, where $a_0$ is the cubic lattice constant. The resulting shift in bias allows the dispersion in the collector to be mapped out. Fig. 2 shows the shift for the $X_{X,Y}(1) \rightarrow X_{X,Y}(3)$ peak as the field is increased in the [1 0 0] direction. When the shift is plotted versus the angle of the in-plane field, a characteristic dumbbell shape is observed, as shown in Fig. 3, corresponding to an elliptical constant energy surface with its principal axes along [1 1 0] and [1 1 0]. We have also observed similar behaviour in a 60–40–60 Å sample [7]. For the sample of Fig. 3, the dumbbell axis is identical for both bias directions, although in reverse bias the ratio of the
shifts for the two (110) magnetic field directions is significantly larger (\( \sim 2.8 \) at 15 T) than in forward bias (\( \sim 1.6 \) at 10.5 T). This ratio varied between different mesas from the same wafer, particularly in reverse bias, where for three mesas the largest value at 15 T was 2.8, and the smallest 1.9.

3. Discussion

The bulk \( X_3 \) and \( Y_3 \) states have Camel’s back dispersions in the \((k_x, k_y)\) plane:

\[
E_X = \frac{\hbar^2}{2m_X} \left( \frac{k_x^2}{m_X} + \frac{k_y^2}{m_{X,Y}} \right) - E_{k,p}(k_x)
\]

and

\[
E_Y = \frac{\hbar^2}{2m_{X,Y}} \left( \frac{k_x^2}{m_X} + \frac{k_y^2}{m_{X,Y}} \right) - E_{k,p}(k_y),
\]

where \( E_{k,p}(k_x) = \sqrt{(\Delta/2)^2 + R^2k_z^2} \). \( \Delta \) is the splitting at the X-points between the bands with \( X_1 \) and \( X_3 \) symmetry, and \( R, m' \) are \( k,p \) parameters \([8]\). In the heterostructure it has been shown that the interfaces can mix the \( X_1 \) and \( X_3 \) states with a potential:

\[
V(k_x, k_y) = b^*(k_x)b(k_y)V_{X-Y} + a^*(k_x)a(k_y)V_{X-Y}^3
\]

where \( b(k_x) = \sqrt{0.5 + \Delta/4E_{k,p}} \) and \( a(k_x) = \frac{\Delta}{4E_{k,p}} \). Here,

\[
V_{X-Y}^1 = \beta_1 \Sigma_2 \Sigma_X^+(z) \Sigma_X^-(z) \exp(i2\pi z/a_0) \quad \text{and} \quad V_{X-Y}^3 = \beta_2 \Sigma_2 \Sigma_Y^+(z) \Sigma_Y^-(z) \exp(i2\pi z/a_0)
\]

are mixing potentials in which \( \Sigma_X, \Sigma_Y \) are envelope functions of the unmixed \( X_3,Y_3 \) states, \( \beta_1 < \beta_3 \) are constants related to the interface potential, \( a_0 \) is the cubic lattice parameter, \( z_i \) are the interface positions and \( P(z_i) = 1(-1) \) for AlAs on GaAs (GaAs on AlAs) \([7-10]\). The energies of the mixed states are obtained by diagonalising the Hamiltonian:

\[
H_{XY} = \begin{bmatrix} E_X & \frac{\pi}{\alpha_0} \\ \frac{\pi}{\alpha_0} & E_Y \end{bmatrix}.
\]

In Fig. 4, we plot the dispersion and constant energy contours in the \((k_x, k_y)\) plane using the \( k,p \) parameters \( R = 1 \text{ eV A}, \Delta = 0.35 \text{ eV}, m'_{m}/m_e \approx 1.56 \) of Ref. \([8]\), and potentials \( V_{X-Y}^1 = 30 \text{ meV}, V_{X-Y}^3 = 850 \text{ meV} \). We take \( m_X/m_e = 0.24 \) \([2,11]\). It can be seen that the contours are elliptical with their major axis along [110]. The sub-band kinetic energy in Fig. 4 at constant \( k_\parallel \) should be proportional to the bias shift plotted in Fig. 3 when \( k_\parallel \) is at right angles to the magnetic field. In Fig. 5, we show kinetic energy plots for \( k_\parallel = 0.02 \times 2\pi/a_0 \) with \( V_{X-Y}^1 = 6 \) or 30 meV and \( V_{X-Y}^3 = 850 \text{ meV} \). The value of \( V_{X-Y}^3 \) was chosen by noting that the ratio of kinetic energies for the two \( \langle 110 \rangle \) directions is very sensitive to \( V_{X-Y}^3 \). Fig. 5 shows that \( V_{X-Y}^3 \) hardly affects this ratio but it does influence the shape of the kinetic energy plot. We find good correspondence between Figs. 3 and 5(b) suggesting that for these \( k,p \) parameters, \( V_{X-Y}^3 \sim 30 \text{ meV} \) is a good estimate for the collector well of the 70\textdegree\textdegree–70 sample in reverse bias.

The \( \langle 111 \rangle \) orientation of the elliptical contours in Fig. 3 is due to interference between the \( V_{X-Y}^1 \) and \( V_{X-Y}^3 \) terms in the expression for \( V(k_x, k_y) \), since \( a^*(k_x)a(k_y) > 0 \) for \( k_\parallel \) along [110] but \( a^*(k_x)a(k_y) < 0 \) for \( k_\parallel \) along [1 1 0]. The interference shows that both mixing potentials are finite. A finite \( V_{X-Y}^1 \) is consistent with Ref. \([1]\) but not with Ref. \([10]\) which predicts \( \beta_1 = 0 \). The result \( V_{X-Y}^1 < V_{X-Y}^3 \) is consistent with theory \([9,10,12]\), while the relatively large size of both \( V_{X-Y}^1 \) and \( V_{X-Y}^3 \) is due in part to the large amplitudes of \( \Xi_X \) and \( \Xi_Y \) at the last interface of the collector quantum well. Even so, we
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Fig. 5. Kinetic energy at $k_1 = 0.02 \times 2\pi/a_0$ for field angles in the $(k_x,k_y)$ plane, calculated with $\tilde{V}_3^{X-Y} = 850$ meV and (a) $\tilde{V}_1^{X-Y} = 6$ meV (b) $\tilde{V}_1^{X-Y} = 30$ meV. Zero angle corresponds to [100].

note that $\beta_3$ is much greater than the expected range of $\sim 0.5$ eV Å estimated in Ref. [10]. Therefore, we have re-examined the $k.p$ parameters and find that $K \sim 2.5$ eV Å and $m'_Z/m_e \sim 0.3$ are consistent with recently measured confinement energies for $X_Z$ states in narrow quantum wells [7,13], whereas those in Ref. [8] are not. With these new parameters we obtain a fit to the angular dependence of the kinetic energy virtually identical to that in Fig. 5(b), but with $\tilde{V}_1^{X-Y} = 30$ meV, $\tilde{V}_3^{X-Y} = 120$ meV. These potentials yield a $\beta_1$ value comparable with $\sim 0.4$ eV Å deduced from tight binding calculations in Ref. [1], but $\beta_3$ is still several times greater than expected [7,10]. It suggests that further refinement might be needed for the envelope function theory of interface band mixing.

In conclusion we have observed the first clear evidence for mixing between AlAs $X_X$ and $X_Y$ states predicted in Ref. [1]. We have shown that the mixing leads to a rotation of the constant energy surface from the two in-plane $(100)$ directions to one of the $(110)$ directions. Which of the $(110)$ directions depends on the details of the interface structure and the bias conditions. The rotation is a consequence of interference between the $X_1$ and $X_3$ contributions to the mixing potential. This shows that $\beta_1$ cannot be zero, as recently suggested in Ref. [10]. We find $\tilde{V}_3^{X-Y} > \tilde{V}_1^{X-Y} \sim 30$ meV in the collector well of our biased sample. By considering the microscopic interface potential, a close analogy exists between $X_X-X_Y$ and $\Gamma-X_Z$ mixing [9]. It follows that the $X_1$ related $\Gamma-X_Z$ mixing potential must also be finite, contrary to the models in Refs. [8,12].

References