Effective Mass Anisotropy of Γ Electrons in GaAs/AlGaAs Quantum Wells

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Resonant magnetotunneling in GaAs/Al_{0.28}Ga_{0.72}As double barrier structures is used to demonstrate that the effective mass of confined Γ conduction electrons becomes anisotropic when an electric field is applied perpendicular to the interfaces. Although several authors have previously reported Γ -related optical anisotropy, this is the first example of a corresponding *electrical* anisotropy. The results are explained using a quantum mechanical model involving interface band mixing that contains additional features not found in the optical case.

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In the past few years, it has become evident that the interfaces in semiconductor heterostructures can play a subtle but highly significant role which goes beyond the obvious one of phonon or electron confinement [1–4]. For example, anisotropy has recently been reported in the polarization of light along the two in-plane $\langle 110 \rangle$ directions for optical transitions in quantum wells (QWs) [5–8]. It has been proposed that such behavior arises from the interface induced mixing between zone center Γ_{15x} and Γ_{15y} valence states [9].

Recently, some of the authors have reported very strong electrical anisotropy in AlAs QWs, where the in-plane effective mass of X electrons is different for the two $\langle 110 \rangle$ directions. This electrical anisotropy is caused by interface band mixing of zone boundary X_X and X_Y electrons, and can thus also be characterized by an "x-y" mixing mechanism [10]. To our knowledge there has been no report of a similar electrical anisotropy for Γ electrons. Such anisotropy is to be expected since all of the above optical and mass anisotropies should relate to the orthogonal $\langle 110 \rangle$ orientations of bond planes at opposite interfaces of the QW (Fig. 1). Anisotropy will occur when the equivalence of the two $\langle 110 \rangle$ directions is destroyed, e.g., by the application of an electric field along [001]. In this Letter we present the first observation of effective mass anisotropy for Γ_1 electrons. However, unlike in the previous cases of optical anisotropy, we show that two mixing contributions are required: Γ_{15x} with Γ_{15y} states ("x-y" mixing) and Γ_1 with Γ_{15z} states (" Γ -*z*" mixing).

Resonant magnetotunneling spectroscopy $(B \perp J)$ has been used widely in double barrier structures (DBSs), to probe the in-plane dispersions of QW states [10–12]. We apply this technique here to sample the in-plane dispersion anisotropy of two symmetric DBSs grown by molecularbeam epitaxy along [001], consisting of 80 Å spacers, 80 Å Al_{0.28}Ga_{0.72}As barriers, and a 120 Å wide GaAs QW. The emitter and collector regions, including spacers, were Al_xGa_{1-x}As with $x \sim 0.05$ and 0.06, respectively. Silicon doping of 2×10^{17} cm⁻³ was present in the emitter and collector. I(V) measurements were performed at T = 1.5 K.

Figure 2(a) shows the I(V) characteristics of the x =0.05 sample as a function of magnetic field up to B =10 T, applied parallel to a (100) direction. Note the high degree of symmetry between bias directions. The $\Gamma(2)$ resonant tunneling peaks, at approximately ± 0.2 V, are easily discernible and they shift to higher bias, and also broaden, with increasing magnetic field. In Fig. 2(b), the peak positions are plotted against B^2 . According to the semiclassical interpretation of resonant magnetotunneling [12,13], the peak bias shift should be proportional to the dispersion energy of the confined state in the well, at a wave vector whose magnitude and direction are proportional and perpendicular, respectively, to those of the magnetic field [10,12]. Deviations from this behavior are known to occur at small magnetic fields [11,14]. For $B \ge$ 5 T, the measured data in Fig. 2(b) exhibit a parabolic



FIG. 1. The bonding arrangement in an AlAs-GaAs-AlAs quantum well.





FIG. 2. (a) I(V) characteristics (100 μ m mesa) showing the $\Gamma(2)$ resonances in the x = 0.05 sample as a function of magnetic field along a (100) direction between B = 0 T (bottom) and 10 T (offset for clarity). Inset: the $\Gamma(1)$ resonances. (b) $\Gamma(2)$ peak position plotted against B^2 —the dotted lines show a linear fit to the data for $B \ge 5$ T.

field dependence, consistent with the parabolic dispersion relation for electrons in the well. In this region, the shift of the peak position from a bias value found by extrapolating back the parabolic dependence to B = 0 is thus a true measure of the dispersion energy.

To within the resolution ($\approx 100 \ \mu eV$) of our setup, the bias position of the $\Gamma(1)$ resonance [inset of Fig. 2(a)] was isotropic with respect to the angle of the in-plane magnetic field. Figure 3 shows the angle dependence of the $\Gamma(2)$ peak position. The field was aligned initially along a $\langle 100 \rangle$ direction. Subsequent I(V) characteristics were measured every 10° up to 240° from this position. Figure 3 reveals a twofold anisotropy in both forward and reverse bias. The main axes of the anisotropy are oriented along the two orthogonal $\langle 110 \rangle$ directions, with a clear 90° rotation



FIG. 3. Dependence of the peak bias position on the in-plane magnetic field direction for the $\Gamma(2)$ resonance in the x = 0.05 sample. Magnetic fields of 8.4 and 9.25 T were applied in (a) the forward and (b) the reverse bias directions, respectively. Insets: peak current vs magnetic field direction.

between forward and reverse bias. This shows that the constant energy surface of the $\Gamma(2)$ subband is *anisotropic*, with its principal axes oriented along the $\langle 110 \rangle$ directions and that the constant energy surface rotates by 90° on changing the bias polarity. Further, we find that the peak current shows the same anisotropy and 90° rotation (insets of Fig. 3).

Figure 4 shows a plot of the peak position vs magnetic field direction for the forward bias $\Gamma(3)$ resonance in the x = 0.06 sample at B = 5 T. For $B \ge 4$ T, this resonance shifts to higher bias linearly in B^2 , as shown in the inset. Figure 4 shows similar behavior to that seen for the $\Gamma(2)$ resonance in Fig. 3(a). We obtain a mass difference between the [110] and [110] directions of ~1% for the $\Gamma(2)$ resonance and ~3% for the $\Gamma(3)$ resonance. The $\Gamma(1)$ resonance in both samples showed no bias shift but only a small current anisotropy (similar to the insets of Fig. 3), indicating that weak anisotropy exists even for the $\Gamma(1)$ resonance. From the behavior of all three resonances, we conclude that the size of the effective mass anisotropy increases with electric field.



FIG. 4. Behavior of the $\Gamma(3)$ resonance in the forward biased x = 0.06 sample. Inset: peak bias vs B^2 for $B \parallel \langle 100 \rangle$. The dotted line shows a linear fit to the data for $B \ge 4$ T.

In the remainder of this Letter, we present a simple quantum mechanical model to explain our results. In a typical GaAs/AlAs QW or superlattice, the bonding Γ_{15v} (antibonding Γ_{15c}) profile has a type-I (type-II) alignment ~1.5 eV below (~1 eV above) the Γ_{1c} conduction band. In such a structure, the planes containing the Ga-As and As-Al interfacial bonds are orthogonal and oriented along the [110] and [110] directions, denoted x' and y', respectively. If we define a virtual crystal, whose microscopic potential is the average of those for GaAs and AlAs, the Ga and Al atoms will acquire equal and opposite charges $\pm \delta q$, relative to the virtual crystal. We can also define a microscopic interface potential, $V_{\rm INT}$, which extends $\pm a_0/4$ in the z direction from the interface plane of As atoms at z_i (a_0 is the cubic lattice parameter), and which, when added to the potential of the virtual crystal, yields that of the actual crystal in that region [15,16]. The tetrahedral bonding of the atoms then leads to the relation $V_{INT}(x', y', z - z_i) = -V_{INT}(y', x', -z + z_i)$. From this it follows that $\langle X'|V_{\rm INT}|X'\rangle = \alpha$, $\langle Y'|V_{\rm INT}|Y'\rangle =$ $-\alpha$, and $\langle \Gamma_1 | V_{\rm INT} | Z \rangle = -i\beta$, where $|X'\rangle$ is a crystal periodic function (CPF) of the virtual crystal with its porbital oriented along x' (analogous definitions apply to $|Y'\rangle$ and $|Z\rangle$), where α , β are real constants, and where $|\Gamma_1\rangle = |iS\rangle$ is a CPF based on antibonding s orbitals. Throughout this discussion, we use the CPF basis of Ref. [17] for the virtual crystal. We consider only the spin up Γ_1 state, since the analogous treatment for the spin down case is obvious. With a simple transformation of coordinates, it is found that

$$\langle X|V_{\rm INT}|X\rangle = \langle Y|V_{\rm INT}|Y\rangle = \langle Z|V_{\rm INT}|Z\rangle = \langle \Gamma_1|V_{\rm INT}|\Gamma_1\rangle = 0,$$
(1)
$$\langle X|V_{\rm INT}|Y\rangle = \langle Y|V_{\rm INT}|X\rangle = \alpha,$$
(1)
$$\langle \Gamma_1|V_{\rm INT}|Z\rangle = -i\beta.$$

It has been shown in Refs. [15,16] that matrix elements which contain V_{INT} and the relevant CPFs, such as those derived in Eq. (1), can lead to δ -function–like interface band mixing.

We will now show that both mixing potentials, α and β , contribute to the observed mass anisotropy, unlike in the optical case discussed later, where only α contributes [5,7]. Here, we use standard $\mathbf{k} \cdot \mathbf{p}$ theory [17], in which the mixing between Γ_1 and any one of the Γ_{15} states, denoted $\Gamma_{15\sigma}$, has the matrix element: $H_{k\cdot p}^{\Gamma_{1,\sigma}} = -\sum_{x_i=x,y,z} \frac{\hbar^2}{m_0} \langle u_{\Gamma_1} | \frac{d}{dx_i} | u_{\Gamma_{15\sigma}} \rangle \frac{d}{dx_i}$. For example, if $u_{\Gamma_{15\sigma}}$ represents the CPF $| \mathbf{j}, \mathbf{m}_{\mathbf{j}} \rangle = |3/2, 3/2\rangle$, then $H_{k\cdot p}^{\Gamma_{1,\sigma}} = i \frac{P_0}{\sqrt{2}} (\frac{\partial}{\partial x} + i \frac{\partial}{\partial y})$, where P_0 is a real constant. For particular Γ_1 and Γ_{15} states, $|\nu\rangle$ and $|\sigma\rangle$, with envelope functions $\Psi_{\Gamma_1}^{\nu} = e^{ik_x x} e^{ik_y y} \phi(z)$ and $\Psi_{\Gamma_{15}}^{\sigma} = e^{ik_x x} e^{ik_y y} \theta(z)$, respectively, this gives a matrix element: $\langle \nu | H_{k\cdot p}^{\Gamma_{1,\sigma}} | \sigma \rangle = -\frac{P_0}{\sqrt{2}} (k_x + ik_y) \langle \phi | \theta \rangle$, which is finite only when ϕ and θ have the same parity. The wave functions of the confined states, E(n), in the QW conduction band, thus have the form

$$\begin{aligned} |\Gamma(n)\rangle &= \{\phi_n(z) |\Gamma_1\rangle + \theta_n(z) (k_x + ik_y) | X + iY \rangle \\ &+ \vartheta_n(z) (k_x - ik_y) | X - iY \rangle \\ &+ \Psi_n(z) | Z \rangle \} e^{ik_{\parallel} \cdot \rho}, \end{aligned}$$
(2)

where the second term contains contributions from the Γ_{15v} or Γ_{15c} CPFs $|3/2, 3/2\rangle$, the third from $|3/2, -1/2\rangle$ and $|1/2, -1/2\rangle$, and the fourth from $|3/2, 1/2\rangle$ and $|1/2, 1/2\rangle$. In Eq. (2), ρ and k_{\parallel} are the in-plane position and wave vectors, respectively. Rearranging, we have

$$\begin{aligned} |\Gamma(n)\rangle &= \{\phi_n(z) |\Gamma_1\rangle + [\Xi_n(z)k_x + i\Theta_n(z)k_y] |X\rangle \\ &- [\Xi_n(z)k_y - i\Theta_n(z)k_x] |Y\rangle \\ &+ \Psi_n(z) |Z\rangle \} e^{ik_{\parallel}\cdot\rho}, \end{aligned}$$
(3)

where $\Xi_n(z) = \theta_n(z) + \vartheta_n(z)$ and $\Theta_n(z) = \theta_n(z) - \vartheta_n(z)$. In Eq. (3), all the envelope functions are real except the Ψ_n , which are purely imaginary. The parities with respect to the center of the GaAs layer are given in Table I.

Limiting ourselves to the basis { $|\Gamma(1)\rangle$, $|\Gamma(2)\rangle$ }, we can now illustrate the changes caused by the interface band mixing. The conduction band is then described by a simple 2×2 Hamiltonian with diagonal elements, E_1 and E_2 , and off-diagonal elements, $V_{12}(k_x, k_y)$ and $V_{12}^{\dagger}(k_x, k_y)$, in

TABLE I. Parity properties of the envelope functions for the $|\Gamma(1)\rangle$ and $|\Gamma(2)\rangle$ states.

Even				Odd			
$\phi_1(z)$	$\Xi_1(z)$	$\Theta_1(z)$	$\Psi_2(z)$	$\phi_2(z)$	$\Xi_2(z)$	$\Theta_2(z)$	$\Psi_1(z)$

which

$$V_{12}(k_x, k_y) = \langle \Gamma(1) | V_{\text{INT}} | \Gamma(2) \rangle$$

= $\sum_i \alpha P_i \{ [\Theta_1^*(z_i) \Theta_2(z_i) - \Xi_1^*(z_i) \Xi_2(z_i)] 2k_x k_y + i [\Xi_1^*(z_i) \Theta_2(z_i) - \Theta_1^*(z_i) \Xi_2(z_i)] (k_x^2 - k_y^2) \}$
 $- i \beta P_i [\phi_1^*(z_i) \Psi_2(z_i) + \phi_2(z_i) \Psi_1^*(z_i)]$
= $A_{12}k_x k_y + i B_{12}(k_x^2 - k_y^2) + C_{12},$ (4)

where the summation is over both QW interfaces and $P_i =$ 1 (-1) for a normal (inverted) interface. Here, A_{12} , B_{12} , and C_{12} are real. In zero electric field, $A_{12}, B_{12} \neq 0$, but $C_{12} = 0$, so the dispersions in the two (110) directions are identical. However, in a nonzero electric field all three coefficients become finite, so that if the contributions from A_{12} and C_{12} add for the [110] direction, they will cancel for the [110] direction, and vice versa. This leads to anisotropy in the constant energy surface, so that the effective masses along [110] and $\overline{[110]}$ are no longer the same. It is also clear from Eq. (4) that, on reversing the electric field, the sign of C_{12} changes, thereby interchanging the dispersions for [110] and $\overline{[110]}$ and rotating the constant energy surface of each subband by 90°. The interchange and rotation still occur if more basis states are included. This follows from the fact that for a given pair of subbands, i and j, either A_{ij} or C_{ij} change sign with a reversal in the electric field, but not both at the same time.

The preceding model, based on *x*-*y* and Γ -*z* mixing, explains well the key features of our measurements, namely, the existence of a mass anisotropy that increases with perpendicular electric field, and that rotates by 90° when the field is reversed. We also note that *x*-*y* mixing as in Eq. (1) leads to mixing between heavy and light holes [9]. Using a basis of the first confined heavy-hole and the first two confined light-hole states, we obtain excellent agreement with the optical anisotropy measurements of Kwok *et al.* [5] if $\alpha \approx 0.5$ eV Å, a value consistent with Ref. [16].

In conclusion, we have observed a small (110) effective mass anisotropy for Γ electrons in GaAs/AlGaAs QWs. The anisotropy is caused by interference between contributions from x-y and Γ -z interface band mixing. Our results contrast with the large mass anisotropy observed for X electrons, recently related to interference between two different x-y contributions, having X₁ and X₃ symmetry. Interference between two contributions thus appears to be a common characteristic of mass anisotropy in QWs.

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