Effective Mass Anisotropy of \( \Gamma \) 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 \( \Gamma \) conduction electrons becomes anisotropic when an electric field is applied perpendicular to the interfaces. Although several authors have previously reported \( \Gamma \)-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.

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 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 \( \Gamma_{15x} \) and \( \Gamma_{15y} \) 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 \( X_y \) 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 \( \Gamma \) 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 \( \Gamma_1 \) electrons. However, unlike in the previous cases of optical anisotropy, we show that two mixing contributions are required: \( \Gamma_{15x} \) with \( \Gamma_{15y} \) states (“\( x-y \)” mixing) and \( \Gamma_1 \) with \( \Gamma_{15z} \) states (“\( \Gamma-z \)” 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 molecular-beam 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\(_x\)Ga\(_{1-x}\)As with \( x \sim 0.05 \) and 0.06, respectively. Silicon doping of \( 2 \times 10^{17} \) 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 \( \langle 100 \rangle \) direction. Note the high degree of symmetry between bias directions. The \( \Gamma(2) \) resonant tunneling peaks, at approximately \( \pm 0.2 \) 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 \( B \gtrsim 5 \) T, the measured data in Fig. 2(b) exhibit a parabolic

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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 \( B = 0 \) T 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 (100) 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 (110) directions, with a clear 90° rotation 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 (110) 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 \( B \geq 4 \) 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 \{1 \overline{1} 0\} directions of \( \approx 1\% \) for the \( \Gamma(2) \) resonance and \( \approx 3\% \) 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 weak anisotropy 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.
It has been shown in Refs. [15,16] that matrix elements which contain $V_{\text{INT}}$ and the relevant CPFs, such as those derived in Eq. (1), can lead to $\delta$-function–like interface band mixing.

We will now show that both mixing potentials, $\alpha$ and $\beta$, contribute to the observed mass anisotropy, unlike in the optical case discussed later, where only $\alpha$ contributes [5,7]. Here, we use standard $k \cdot p$ theory [17], in which the mixing between $\Gamma_1$ and any one of the $\Gamma_{15}$ states, denoted $\Gamma_{15r}$, has the matrix element: $H_{k\parallel}^{r} = -\sum_{\alpha=x,y,z} \frac{\hbar^2}{m_a} (u_{r1\alpha}^2 \frac{d}{dx} u_{r1\alpha}) \frac{d}{dx}$. For example, if $u_{r1\alpha}$ represents the CPF $|j, m\rangle = |3/2, 3/2\rangle$, then $H_{k\parallel}^{r} = i \frac{\hbar^2}{m_a} (\beta_{1/2} \gamma_{3/2} + i \gamma_{1/2})$, where $P_0$ is a real constant. For particular $\Gamma_1$ and $\Gamma_{15}$ states, $|\nu\rangle$ and $|\sigma\rangle$, with envelope functions $\Psi_{\Gamma_1}^{\nu} = e^{ik_{x\nu} e^{ik_{y\nu}} \phi(z)}$ and $\Psi_{\Gamma_{15}}^{\sigma} = e^{ik_{x\sigma} e^{ik_{y\sigma}} \phi(z)}$, respectively, this gives a matrix element: $\langle \nu | H_{k\parallel}^{r} | \sigma \rangle = -\frac{\hbar^2}{m_a} (2 \gamma_{1/2} + i \gamma_{3/2})(\phi | \theta)$, which is finite only when $\phi$ and $\theta$ have the same parity. The wave functions of the confined states, $E(n)$, in the QW conduction band, thus have the form

$$\Gamma(n) = \{ \phi_n(z) | \Gamma_1 \} + \theta_n(z) (k_x + i k_y) | X + i Y \}
+ \theta_n(z) (k_x - i k_y) | X - i Y \}
+ \Psi_n(z) | Z \} e^{ik_{y\parallel} \rho},$$

(2)

where the second term contains contributions from the $\Gamma_{15}$, or $\Gamma_1$, 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), $\rho$ and $k_{\parallel}$ are the in-plane position and wave vectors, respectively. Rearranging, we have

$$\Gamma(n) = \{ \phi_n(z) | \Gamma_1 \} + \{ \Xi_n(z) k_x + i \Theta_n(z) k_y | X \}
- \{ \Xi_n(z) k_y - i \Theta_n(z) k_x | Y \}
+ \Psi_n(z) | Z \} e^{ik_{y\parallel} \rho},$$

(3)

where $\Xi_n(z) = \theta_n(z) + \theta_n(z)$ and $\Theta_n(z) = \theta_n(z) - \theta_n(z)$. In Eq. (3), all the envelope functions are real except the $\Psi_n$, 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 $2 \times 2$ Hamiltonian with diagonal elements, $E_1$ and $E_2$, and off-diagonal elements, $V_{12}(k_x, k_y)$ and $V_{12}^T(k_x, k_y)$, in

$\begin{array}{c|c|c|c}
\text{Even} & \text{Odd} \\
\hline
\phi_1(z) & \Xi_1(z) & \Theta_1(z) & \Psi_2(z) \\
\phi_2(z) & \Xi_2(z) & \Theta_2(z) & \Psi_1(z)
\end{array}$

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

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 $\Gamma_{15r}$ (antibonding $\Gamma_{13c}$) profile has a type-I (type-II) alignment ~1.5 eV below (~1 eV above) the $\Gamma_{1c}$ conduction band. In such a structure, the planes containing the GaAs and As-Al interfacial bonds are orthogonal and oriented along the [110] and [\overline{1}10] 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, $V_{\text{INT}}$, which extends $\pm a_0/4$ in the $z$ direction from the interface plane of As atoms at $z = a_0$ (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 $V_{\text{INT}}(x', y', z - z_0) = -V_{\text{INT}}(y', x', z + z_0)$. From this it follows that $\langle X' | V_{\text{INT}} | X' \rangle = \alpha$, $\langle Y' | V_{\text{INT}} | Y' \rangle = -\alpha$, and $\langle \Gamma_1 | V_{\text{INT}} | Z \rangle = -i \beta$, where $|X'\rangle$ is a crystal periodic function (CPF) of the virtual crystal with its $p$ orbital oriented along $x'$ (analogous definitions apply to $|Y'\rangle$ and $|Z\rangle$), where $\alpha$, $\beta$ are real constants, and where $|\Gamma_1\rangle = |\varpi\rangle$ 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 $\Gamma_1$ state, since the analogous treatment for the spin down case is obvious. With a simple transformation of coordinates, it is found that

$$\langle X | V_{\text{INT}} | X \rangle = \langle Y | V_{\text{INT}} | Y \rangle = \langle Z | V_{\text{INT}} | Z \rangle = \langle \Gamma_1 | V_{\text{INT}} | \Gamma_1 \rangle = 0,$$

(1)

$$\langle X | V_{\text{INT}} | Y \rangle = \langle Y | V_{\text{INT}} | X \rangle = \alpha,$$

$$\langle \Gamma_1 | V_{\text{INT}} | Z \rangle = -i \beta.$$
The anisotropy is caused by interference between contributions from
x and \(\Gamma\)-z interface band mixing. Our results contrast with the large mass anisotropy observed for
electrons, recently related to interference between two different x-y contributions, having \(X_1\) and \(X_3\) symmetry. Interference between two contributions thus appears to be
a common characteristic of mass anisotropy in QWs.

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