Hole tunneling times in GaAs/AlAs double-barrier structures

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We have calculated hole tunneling times in GaAs/AlAs double-barrier structures taking quantum well band-mixing effects into account. Our results indicate that for sufficiently high hole temperatures and concentrations, band-mixing effects reduce average hole tunneling times from the pure heavy hole value to values comparable to electron tunneling times in the same structure. For very low hole temperatures and concentrations, band mixing is less important and average hole tunneling times should approach the pure heavy hole value. These results provide an explanation for previously reported experimental results in which electrons and holes were found to be characterized by very similar tunneling times.

The high-frequency behavior of the double-barrier heterostructure proposed by Tsu and Esaki\(^1\) has been a subject of intense study recently due to interest in the use of double-barrier structures in high-speed devices, such as oscillators and switching elements. Several experimental\(^2\)\(^-\)\(^4\) and theoretical\(^5\)\(^-\)\(^9\) studies have focused on the characteristic time scale for electron tunneling processes, an issue of both practical and fundamental physical importance. In a recent experiment of Jackson\textit{et al.},\(^2\) an excitation correlation method was used to study the decay of photoexcited electron and hole populations in double-barrier heterostructures. An unexpected result in this experiment was that electrons and holes were observed to have very similar tunneling times; if all the photoexcited holes in the quantum well are assumed to relax to the lowest heavy hole subband, a simple model of hole tunneling would suggest that the holes should be characterized by a much longer tunneling time than the electrons, due to the large effective mass of the heavy holes.

In this letter we propose an explanation for this anomaly. By including quantum well band-mixing effects in our calculations of hole tunneling times, we have found that for sufficiently high hole temperatures and concentrations, average hole tunneling times are obtained that are comparable to electron tunneling times in the same structure. Our calculated electron and hole tunneling times are thus in good agreement with previously reported experimental results.\(^2\)

We begin by calculating the valence-band structure in a GaAs quantum well with AlAs barriers; we assume that in the double-barrier structure, the finite barrier thickness has a negligible effect on the quantum well band structure. Assuming that spin-orbit coupling can be neglected, the valence bands can be described by the \(4\times4\) Luttinger–Kohn Hamiltonian,\(^10\)

\[
\hat{H} = \begin{pmatrix} P + Q + V(z) & L & M & 0 \\ L^* & P - Q + V(z) & 0 & M \\ M^* & 0 & P - Q + V(z) & -L^* \\ 0 & M^* & -L & P + Q + V(z) \end{pmatrix}, \tag{1}
\]

where

\[
P = \frac{\hbar^2}{2m_0} \gamma_1 \left( k_x^2 + k_y^2 - \frac{d^2}{dz^2} \right),
\]

\[
Q = \frac{\hbar^2}{2m_0} \gamma_2 \left( k_x^2 + k_y^2 + 2 \frac{d^2}{dz^2} \right),
\]

\[
L = \frac{\hbar^2}{2m_0} \sqrt{2} \gamma_3 (k_x - ik_y) \frac{d}{dz},
\]

\[
M = -\frac{\hbar^2}{2m_0} \sqrt{3} \sqrt{\gamma_1 (k_x^2 - k_y^2) + i2\gamma_3 k_x k_y},
\]

and \(V(z)\) is the quantum well potential due to the AlAs barriers. The basis elements are \((j,m)\), with \(j = 3/2\) and \(m = \pm 3/2, \pm 1/2, 3/2, \pm 3/2\) are heavy hole states, and \(3/2, \pm 1/2\) are light hole states. \(\gamma_1, \gamma_2, \) and \(\gamma_3\) are the Luttinger parameters; for simplicity, we employ the spherical approximation\(^11\) \((\gamma_2 = \gamma_3 = \gamma)\), with the values of \(\gamma_1\) and \(\gamma\) determined by the known heavy and light effective masses for GaAs and AlAs.\(^12\) We assume a valence-band offset of 0.55 eV\(^13\) between GaAs and AlAs, and a direct band gap of 3.13 eV\(^12\) in AlAs at 80 K.

The quantum well subband structure is obtained by substituting the Hamiltonian (1) for fixed \(k_x, k_y\) into the time-independent Schrödinger equation:

\[
\sum_{j=1}^{4} \hat{H}_{ji} \psi_i(z) = E \psi_i(z), \quad i = 1, ..., 4 \tag{2}
\]

and solving for the eigenvalues \(E\). We impose the following boundary conditions on the problem: (a) all wave functions should decay exponentially as \(z \to \pm \infty\), (b) the wave function components \(\psi_i(z)\) should be continuous at the GaAs/AlAs interfaces, and (c) the probability current density should be continuous at the interfaces.\(^14\)

For \(k_x = k_y = 0\), the Hamiltonian (1) is diagonal and there is no mixing between the light holes and heavy holes.
For \( k_i \neq (k_y, k_z) \neq 0 \), however, the Hamiltonian is no longer diagonal, and interactions occur between the light hole and heavy hole bands. The lowest valence subbands for a 58 Å GaAs quantum well are shown in Fig. 1, and the light hole and heavy hole probability densities in the lowest subband for \( k_y = 0 \) and \( k_y \neq 0 \) are shown in Figs. 2(a) and 2(b), respectively. The total probability density for each basis component \( \rho_{\ell} \) at a given energy, \( \rho_{\ell}(E) \), is obtained by integrating the spatial probability density across the entire structure.

Tunneling times are calculated assuming that all the holes in the quantum well have relaxed to the lowest subband, and that the hole distribution is characterized by a carrier temperature \( T_c \). In an actual experiment, \( T_c \) need not be equal to the lattice temperature and may be determined primarily by other experimental parameters, such as photoexcitation energy. A Fermi level \( \mu \) for the holes is determined from the condition

\[
p = \frac{1}{\rho} \int_0^\infty \mathcal{D}(E)f(\mu, E, T_c)E dE,
\]

where \( \mathcal{D}(E) \) is the density of states in the quantum well, \( f(\mu, E, T_c) \) is the Fermi distribution function, and \( p \) is the total hole population. The probability density for each basis component averaged over the entire hole distribution is then given by

\[
\rho_{\ell}(E) = \frac{1}{\rho} \int_0^\infty \mathcal{D}(E)f(\mu, E, T_c)P_{\ell}(E) dE.
\]

To obtain an average hole tunneling rate \( 1/\tau_h \), we simply take an average of the tunneling rates for the individual light and heavy hole components, weighted by the probability density for each basis component given by Eq. (4). The heavy and light hole tunneling times are calculated from the full widths at half maximum (FWHM) of the transmission probability resonances in the double-barrier structure using the relation \( \tau \sim \hbar/\Delta E_{\text{FWHM}} \). Transmission probabilities were computed using the transfer matrix method of Kane, modified to account for different hole effective masses in GaAs and AlAs. Wave vectors in the AlAs barriers were estimated using a two-band kp model for the light hole components and a one-band model for the heavy-hole components. For GaAs/AlAs double-barrier structures, tunneling times for light holes were found to be somewhat shorter than for electrons and several orders of magnitude shorter than for heavy holes; thus, even a small amount of band mixing can have a large effect on the average hole tunneling time.

Our results indicate that valence-band mixing plays an important role in determining tunneling times for holes. In Fig. 3 we have plotted, for \( T_c = 80 \) K, theoretical average hole tunneling times as a function of hole population and barrier thickness, theoretical electron tunneling times, and experimental carrier decay times measured at \( T = 80 \) K. Electron and hole densities for these measurements were estimated to be approximately \( 10^{11} \) cm\(^{-2}\). At the estimated experimental carrier concentrations, the calculated hole and electron tunneling times are in good agreement with these experiments. Jackson et al. have discussed other effects, such as diffusion and quantum well charging, that may conspire to make the electron and hole tunneling escape times exactly equal, but these effects will be small compared to the reduction in hole tunneling times caused by mixing of the valence subbands.

In Fig. 4 we have plotted the hole tunneling time as a function of hole concentration and hole temperature for a barrier width of 28 Å. These results indicate that for sufficiently low hole temperatures and concentrations, band-mixing effects are diminished and the average hole tunneling time approaches the pure heavy hole value. This is exactly

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**FIG. 1.** Valence subband structure for a 58 Å GaAs quantum well surrounded by AlAs barriers. The two lowest subbands (labeled hh1 and hh2) correspond to pure heavy hole states at \( k = 0 \). The third subband (lh1) corresponds to a pure light hole state at \( k = 0 \).

**FIG. 2.** Four individual components of the quantum well wave function in the lowest valence subband for (a) \( k_y = 0 \) and (b) \( k_y \neq 0 \), the components corresponding to the lowest heavy hole and lowest light hole states are labeled hh1 and lh1, respectively. For \( k_y = 0 \), the band is purely heavy hole in character. For \( k_y \neq 0 \), the band is primarily heavy hole in character with a small component from the lowest light hole subband; smaller contributions from higher subbands (unlabeled) can also be seen.

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Yu, Jackson, and McGe! 745
the result one would expect, since for low carrier temperatures and concentrations, the holes are very close to the bottom of the band \( (k_z = 0) \), where the band is almost entirely heavy hole in character. For higher carrier temperatures and concentrations, however, calculated hole tunneling times rapidly drop to values comparable to electron tunneling times, since even a small light hole component in the hole population causes a very significant reduction in the average hole tunneling time.

In summary, we have calculated average hole tunneling times for GaAs/AlAs double-barrier heterostructures, taking into account band-mixing effects in the lowest valence subband in the quantum well. These calculations yield hole tunneling times that are in good agreement with experimental observations which had indicated that, under certain conditions, tunneling times for holes were much shorter than expected for the lowest heavy hole subband, and comparable in fact to electron tunneling times. Specifically, we have found that for sufficiently high hole temperatures and concentrations, band-mixing effects lower the average hole tunneling times to values comparable to electron tunneling times, whereas for very low hole temperatures and concentrations, band mixing becomes less important and the hole tunneling time approaches the pure heavy hole value.

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