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Observation by resonant tunneling of high-energy states in GaAs-$Ga_{1-x}Al_xAs$ quantum wells

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The current-voltage characteristics of $Ga_{1-x}Al_xAs$-GaAs-$Ga_{1-x}Al_xAs$ double-barrier devices show, in addition to resonant tunneling via quasibound Γ states, well-defined structures corresponding to energies higher than the barrier height. These new features are interpreted as resonant tunneling through confined states in $Ga_{1-x}Al_xAs$, at the X point of the Brillouin zone.

The states of a particle confined to a one-dimensional potential well form a discrete set of levels whose energies depend on the width and depth of the well. This energy quantization has been exploited extensively in semiconductor physics, since the first demonstrations, by resonant tunneling[1] and optical absorption,[2] of quantum-state formation in $Ga_{1-x}Al_xAs$-GaAs-$Ga_{1-x}Al_xAs$ heterostructures (where the GaAs conduction-band edge, which lies lower in energy than that of $Ga_{1-x}Al_xAs$, provides electron confinement).

In addition to these bound states, there is a set of resonant states at energies above the well, for which the transmission probability of a particle scattered by the well, has a maximum. For instance, in the simple case of a rectangular well with infinitely wide barriers, the resonant energies depend only on the width of the well, given by $E_n=(\pi^2\hbar^2/2m^*L^2)n^2$, where m^* is the mass of the particle, L is the width of the well, and n is an integer. Recent optical measurements in semiconductor heterostructures have been interpreted on the basis of these resonant states,[3,4] sometimes called delocalized or virtual bound states. To avoid confusion, in this paper we will call them virtual states.

In this Rapid Communication we investigate the possibility of observing the virtual states by resonant tunneling through $Ga_{1-x}Al_xAs$-GaAs-$Ga_{1-x}Al_xAs$ double barriers. Experimental results show, in fact, well-defined features in the current-voltage characteristics, corresponding to energies above the well barrier. However, effective-mass calculations for the transmission probability through Γ-point barriers cannot explain the observed structures, which are interpreted as resulting from resonant tunneling through confined states in $Ga_{1-x}Al_xAs$, at the X point of the Brillouin zone.

The experiments were done on three samples, prepared by molecular beam epitaxy on n^+-GaAs (100) substrates, which consisted of two identical undoped $Ga_{1-x}Al_xAs$ layers separated by an undoped layer of GaAs. The structures were completed with a top n^+-GaAs region, which, together with the substrate, constituted the electrodes. In two heterostructures the thickness of the $Ga_{1-x}Al_xAs$ barriers was 100 Å, and that of the GaAs well was either 40 Å (sample A) or 60 Å (sample B). The Al mole fraction x was in the range 0.4–0.45. A third structure (sample C) had a 50-Å well and 50-Å barriers with $x\sim 0.30$–0.35. Circular devices, 250 μm in diameter, were prepared using standard metallization and etching techniques.

Tunneling-current measurements through the double-barrier structures were done, at 77 and 4 K, by applying a voltage between the two electrodes. At small voltages the wide barriers prevent the flow of any significant amount of current, except at those for which the quantum states in the well coincide in energy with the electrode Fermi energy. At those voltages, the electrons tunnel resonantly, giving rise to a dramatic increase in the current flow. The resonance persists until the quantum state is lower in energy than the conduction-band edge in the electrode, when the requirement of conservation of momentum parallel to the interfaces prevents the flow of any further current.[5] For even higher voltages, the effective narrowing of the barriers introduced by the electric field leads to an increase in the nonresonant tunneling current. The different regimes are illustrated in Fig. 1, showing the current-voltage characteristics for samples A and B. The reasonable symmetry of the I-V characteristics, with respect to the voltage polarity, reflects the identity of the two barriers.

For the 40-Å well, the existence of a single bound state is highlighted in the I-V curve of Fig. 1(a), with a peak-to-valley ratio of 10 for the resonant structure. (At 77 K this ratio is 8.) The peak position of 0.259 ± 0.002 V is in reasonable agreement with the calculated energy of 0.101 eV, for the bound state under flat-band conditions. (Note that the energy of the quantum state is determined by halving the peak voltage, corresponding to the voltage drop between the two electrodes.) The calculation was done using the envelope-wave-function formalism[6] with a barrier height of 0.296 eV, and effective masses of $0.066m_0$ and $0.101m_0$ for GaAs and $Ga_{0.6}Al_{0.4}As$, respectively. (More realistic calculations, taking into account the applied bias, are described below.) Even better agreement was found for sample B [see Fig. 1(b)], indicating that the voltage drop, away from the double-barrier structure, is negligible. The existence of two bound states (estimated to be at 0.063 and 0.241 eV) is revealed by the presence of two negative-resistance regions at 0.115 ± 0.015 and 0.455 ± 0.025 V.

In addition to the negative-resistance regions, both heterostructures show a distinct feature in their I-V characteristics at high voltage: ~ 1.0 V for the 40-Å well, and ~ 0.9 V for the 60-Å well. The features, which appear for both polarities at about the same voltage, are superimposed on a large background of tunneling current, making difficult the precise determination of their voltage position. Their presence, already observable at 77 K, is better illustrated in conductance measurements, as shown in Fig. 1(a). As in the case of resonant tunneling associated with bound states, these new features represent additional current channels, for which the tunneling probability exhibits a maximum. In

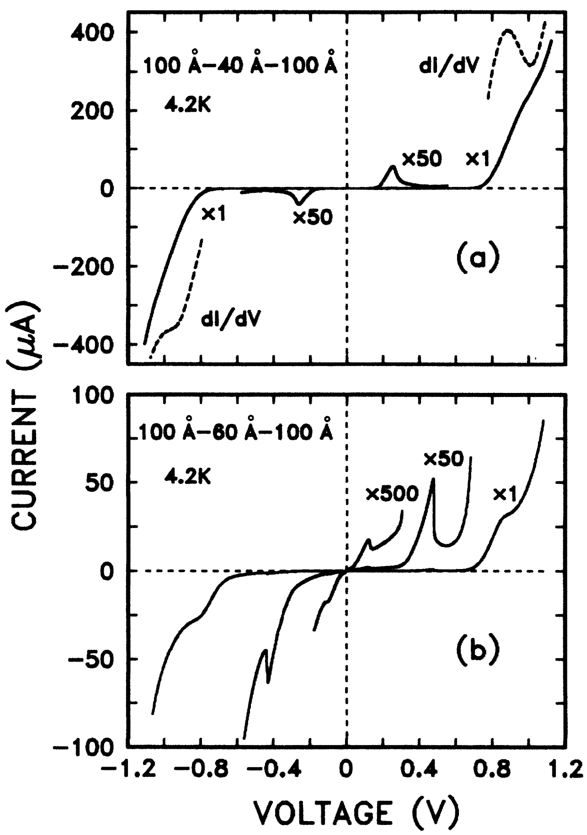

FIG. 1. Experimental current-voltage characteristics of $Ga_{1-x}Al_xAs$-GaAs-$Ga_{1-x}Al_xAs$ heterostructures with identical barriers of 100 Å and a quantum well of either (a) 40 Å (sample A), or (b) 60 Å (sample B). In (a), the conductance dI/dV is also shown at high bias, emphasizing the weak resonant-tunneling structure corresponding to energies above the Γ-point barrier.

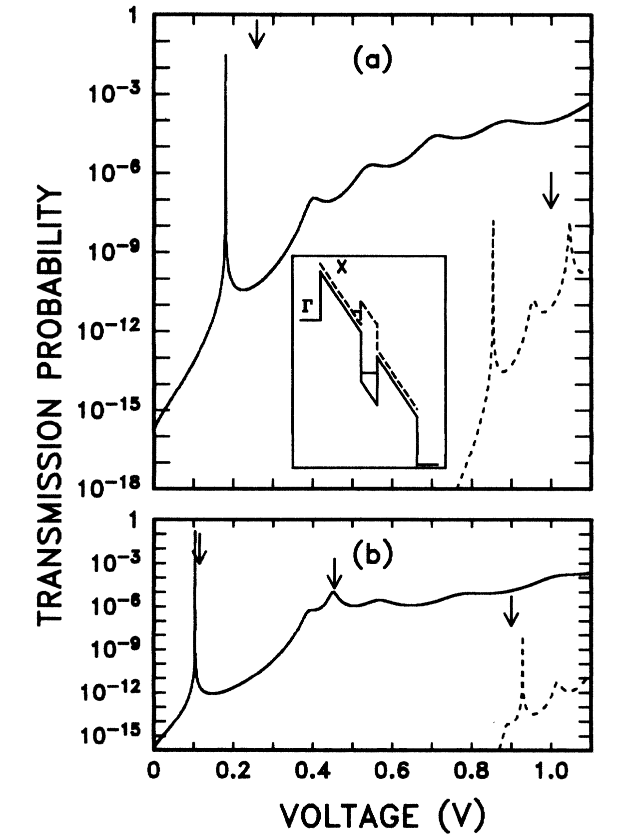

FIG. 2. Calculated transmission probability vs applied voltage for samples A and B. Continuous and discontinuous lines correspond to intravalley tunneling (through a $\Gamma\rightarrow\Gamma\rightarrow\Gamma\rightarrow\Gamma\rightarrow\Gamma$ path) and intervalley tunneling (via a $\Gamma\rightarrow X\rightarrow X\rightarrow\Gamma\rightarrow\Gamma$ path), respectively. The two different potential profiles, for the 40-Å configuration, are sketched in the inset. The arrows indicate the positions of the experimental conductance minima. Effective-mass values used in the calculations are $m^{\Gamma}_{\rm GaAs}=0.066m_0$, $m^{\Gamma}_{\rm GaAlAs}=0.101m_0$, $m^{X}_{\rm GaAs}=m^{X}_{\rm GaAlAs}=0.85m_0$. The Γ- and X-barrier heights are taken to be 0.296 and 0.174 eV, respectively.

contrast, sample C, which is not shown, exhibited two negative-resistance regions, at 0.16 and 0.60 V (the latter much weaker than the former), corresponding to two quasibound states in the GaAs well, but no additional features up to 1 V, the highest bias applied to it.

In order to interpret the observed extra structures of samples A and B, we have calculated the transmission probability through a double-barrier potential under applied bias, by numerical integration of the Schrödinger equation, taking into account appropriate boundary conditions at the interfaces. The total external bias is assumed to be applied entirely across the barrier-well-barrier structure. We have evaluated the transmission probability for a monochromatic beam of electrons incident upon the first barrier at various energies and parallel wave vectors ($\mathbf{k}_{\parallel}$), from which the I-V characteristics can be computed. For simplicity, we present here only the results for the transmission probability for electrons with $\mathbf{k}_{\parallel}=0$ and at low energies (10 meV), in the bias region of incipient negative conductance. More detailed results, including the calculated I-V characteristics and a comparison between theoretical and experimental line shapes will be published elsewhere.

Figure 2 (continuous lines) shows calculated transmission probabilities for potential profiles derived exclusively from Γ states (intravalley tunneling), assuming a single parabolic band. As can be seen, there is reasonable quantitative agreement with the experimental data (indicated by arrows in Fig. 2), especially for sample B, regarding the bias at which negative conductance sets in, for applied bias smaller than 0.5 V. For sample A the peak is at 0.18 V, while for sample B there are two peaks, at 0.10 and 0.45 V. For both samples, at higher bias, this simple model is unable to explain, even qualitatively, the observed conductance anomalies. The transmission probability at higher bias (see Fig. 2) shows oscillations, originating from tunneling through virtual levels and quantum-mechanical reflections at the interfaces, but the calculated structures bear no resemblance to the experimental results. Hence, it seems unlikely that this is the origin of the features observed at high bias.

A second calculation has been performed under the assumption that at the interfaces there is a finite amplitude for transmission from states with wave vectors near the Γ valley to states with wave vectors near the X valley (intervalley tunneling). [For (100)-grown heterostructures, only one of the three X-valley minima is accessible by conservation of $\mathbf{k}_{\parallel}$. Although surface roughness and alloy scattering are elastic processes that may break this selection rule, the process of Γ to X transfer that we envisage here takes place even when $\mathbf{k}_{\parallel}$ is fully conserved.] This process can take place as soon as, at high bias, there are propagating states derived from the X-valley minimum in the $Ga_{1-x}Al_xAs$ barrier, at the same energy as the electrons incident from the electrode, as has been pointed out by Mailhiot, McGill, and Schulman.[7] It gives origin to resonant tunneling because, for states derived from the X valley, the GaAs layers act as potential barriers and the $Ga_{1-x}Al_xAs$ layers act as wells, as sketched in the inset of Fig. 2. There are, thus, bound X-like states in the $Ga_{1-x}Al_xAs$ layers, through which resonant tunneling can proceed.

Schematically, we indicate the tunneling path by the appropriate label of the electron wave vector through the various layers, so that the intravalley model of Fig. 2(a) reads $\Gamma \rightarrow \Gamma \rightarrow \Gamma \rightarrow \Gamma \rightarrow \Gamma$. For intervalley tunneling, we tried different paths: ($\Gamma \rightarrow X \rightarrow X \rightarrow X \rightarrow X$, $\Gamma \rightarrow X \rightarrow X \rightarrow X \rightarrow \Gamma$, $\Gamma \rightarrow X \rightarrow X \rightarrow \Gamma \rightarrow \Gamma$). As might be expected, the transmission probability curves, for the various cases, differ only in detail from each other, but not on the position of the resonant peaks. This simple model, which can be regarded as a "density of states" calculation, is unable to establish the relative weight of the various tunneling channels, for which matrix elements must be computed in the framework of an electronic structure calculation.

The results for the intervalley tunneling model are in better agreement with the experiment at high bias than the intravalley model, as can be seen on Fig. 2 (discontinuous lines). Up to 1.1 V, for the potential profile of sample A there are two sharp peaks, at ~0.85 and ~1.05 V, and one at ~0.9 V for sample B. These maxima correspond to resonant tunneling through quasibound states of the X valley, in the triangular barrier potential formed by the first $Ga_{1-x}Al_xAs$ layer and the GaAs layer. (Additional oscillations result from quantum-mechanical reflections in subsequent interfaces.)

The voltage predicted by the intervalley model for the X-point bound state is, for sample A, significantly lower than the observed one. Such a discrepancy can be due to serious resistance, to the inherent uncertainty in layer thickness or to a somewhat smaller Al mole fraction in the $Ga_{1-x}Al_xAs$ barriers, which would increase the energy difference between the Γ point in GaAs and the X point in $Ga_{1-x}Al_xAs$, shifting the resonant structures to higher bias. A comparison of the tunneling current at high bias, for samples A and B, shows indeed a larger current for sample A, suggesting a lower Γ barrier, and consequently a smaller Al content. This interpretation also explains the absence of any additional features, up to 1 V, in the I-V characteristic of sample C, where the Al mole fraction is substantially smaller than in samples A and B.

Finally, let us discuss an alternative mechanism that, in principle, could account for our observations. Since the L point lies, in GaAs, ~0.30 eV above the Γ point,[8] it is conceivable that the high-voltage structures reported here could have their origin in nonresonant $\Gamma \rightarrow L$ intervalley tunneling. However, several arguments are against this interpretation. First, the voltage would be at least 0.25 V lower than the observed values. Second, the onset of that tunneling path would lead to a reduction—not an increase—of current. Third, such a mechanism would violate the $\mathbf{k}_{\parallel}$-conservation law.

The results presented in this work point out that, as the quality of samples improve and new phenomena come to light, a more complete theory of resonant tunneling is needed.

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