Resonant tunneling via donor X states in the AlAs barrier and binding energies of donors bound to X_{XY} and X_Z valleys

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Magnetotransport in GaAs/AlAs/GaAs single-barrier heterostructures, incorporating unintentional donors in the barrier, is studied. Resonant tunneling is observed through the quasiconfined states in the AlAs layer which originate from the X_{XY} and X_Z conduction-band minima and through two distinct states of the donors bound to the X_{XY} and X_Z valleys. This allowes us to determine directly the binding energies of X_{XY}- and X_Z-related donors at the center of a 5-nm AlAs barrier as $E_B(X_{XY}) \approx 70$ meV and $E_B(X_Z) \approx 50$ meV, respectively. Furthermore, we observe an additional oscillatory fine structure of the donor resonances which we attribute to a difference in the binding energies of donors located at different position in the AlAs layer.

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Recent investigations of AlAs/GaAs heterostructures demonstrated that X-valley states in AlAs have a substantial influence on their optical and electrical properties.[1,2] For silicon donors in bulk AlAs, the central cell potential does not mix the three hydrogenic effective-mass states, which can be described as corresponding to independent X valleys. Therefore, the ground state of a silicon donor is threefold degenerated. However, in a thin AlAs layer this degeneracy is lifted due to confinement and strain, so that the threefold degenerated state splits into a twofold degenerated state associated with the X_{XY} valleys and a nondegenerated state associated with the X_Z valley.[1] The binding energies of hydrogeniclike donors bound to the X_{XY} and X_Z valleys were calculated by Weber, taking into account both the mass anisotropy and the quantum confinement.[3] Moreover, it was shown that the binding energy of the donor depends on its position in the AlAs layer and that donor resonances should occur at different voltages for impurities located at different distances from the heterointerface.

Tunneling spectroscopy allows us to measure the donor binding energy directly, provided that resonances corresponding to tunneling via both the confined state and the donor state associated with them are observed. The binding energy of Γ-related donors in the GaAs quantum well was determined reliably from tunneling studies.[4–6] Fukuyama and Waho observed a single resonance due to tunnelling via the X-related donor state in the transport characteristics of the single-barrier GaAs/AlAs heterostructure.[7] In our previous paper, we reported the detection of two X_{XY}- and X_Z-related donor resonances.[8] Apart from those papers there are only two publications on concerning tunneling via donor X states in AlAs.[9,10] Although the same experimental samples were used in both cases, the authors reported two donor resonances in the first case[9] and four donor resonances in the second case[10] in the same voltage range. Moreover, tunneling via confined X states was not detected, and the splitting of two principal X-related donor states was determined as 14 meV in Ref. 9, and as 23 meV in Ref. 10.

In this paper we report an observation of resonant tunneling both through quasiconfined X_{XY} and X_Z states and through two distinct states of donors linked to X_{XY} and X_Z valleys in the AlAs barrier. We show that the energies of donor X states are determined both by quantum confinement affecting the energies of confined X states and the binding energies of donors and by biaxial strain, which causes a splitting of X_{XY} and X_Z valleys on 23 meV.[1] In addition, it permits us to determine the binding energies of X-related donors directly. We also report an additional fine structure of the donor resonances that we attribute to resonant tunneling via states of donors located in different atomic planes of the AlAs layer with different binding energies. A study of the behavior of the fine structure when a magnetic field is applied demonstrates that the binding energy of X-related donors has an essential dependence on both the magnetic field and the donor position in the barrier, in accordance with earlier theoretical results.[3,11] Thus the possibility of the determination of the difference in binding energies of X donors located in the adjacent atomic layers of an AlAs barrier was shown.

The sample studied was a single-barrier 5 nm GaAs-AlAs-GaAs heterodiode, grown by molecular-beam epitaxy on (100)-oriented Si doped n-GaAs substrate (see Ref. 8). The AlAs layer was not intentionally doped, but donor impurities were present in the AlAs because of diffusion from the highly doped region during its growth.[12] The calculated Γ and X band profiles of the experimental structure at a bias of $V = 900$ mV are shown in Fig. 1.

Figure 2(a) shows the $dI/dV - V$ characteristic of the experimental sample measured at 4.2 K. Three strong steplike features corresponding to tunneling through quasiconfined X_Z and X_{XY} states were observed in earlier studies.[2,13,15] Two weak features A and B at a voltage below the threshold for transfer via quasiconfined X_{Z1} states are more pronounced in Fig. 2(a), which displays the voltage dependence of the second derivative $d^2I/dV^2 - V$. We attribute peaks A and B to resonant tunneling through the donor X_{XY}- and X_Z-related states.

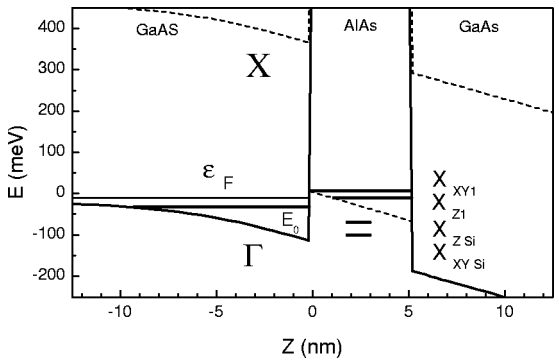

FIG. 1. Band profile diagram for the for the Γ (solid line) and X (dashed line) minima around the AlAs layer of a single-barrier AlAs/GaAs heterostructure at bias $V=900$ mV. The two lowest quasiconfined states in the X quantum well and two states of the donors linked to them are denoted by X_{XY1}, X_{Z1}, and X_{XYSi}, X_{ZSi}.

The key to the attributions of the experimental features in Fig. 2 is a Schrödinger-Poisson modeling of the conduction-band profile and of the electronic levels, from which the applied bias required for a given resonant process may be calculated. The most important input parameter of the model is the variation of the electric field across the emitter/barrier region (or the electron concentration in the accumulation layer) as a function of the bias. The electron concentration

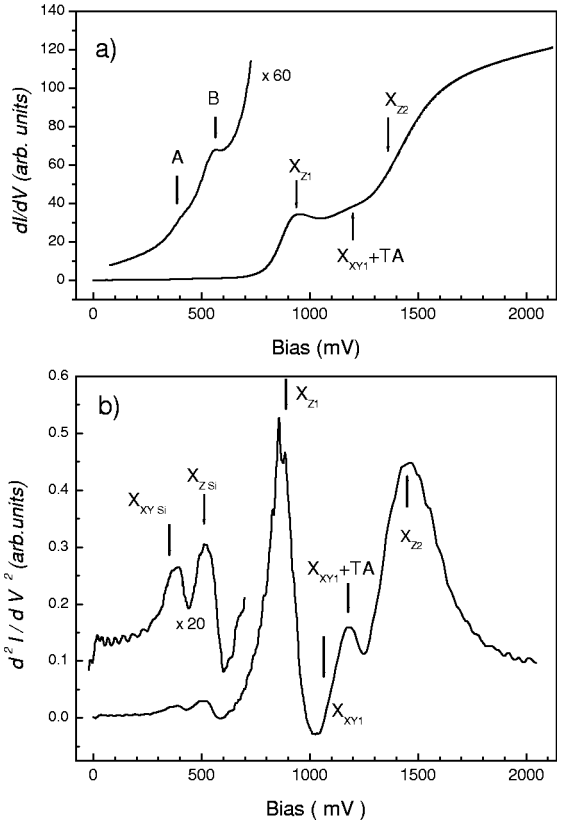

FIG. 2. dI/dV (a) and d^2I/dV^2 characteristics (b) of the experimental device at 4.2 K. Features A and B correspond to resonant tunneling via X-related donor states. The calculated threshold voltages are denoted by arrows.

was obtained from Shubnikov–de Haas-like magnetotransport ($I-B$) measurements. These data were reported in our previous publication[12] and are not presented here. The X_Z and X_{XY} electronic levels were calculated as a function of the applied bias. The threshold voltages for tunnelling through the X_Z- and X_{XY}-related donor states were calculated using the data reported in Ref. 3. It was shown that the binding energies of X_Z- and X_{XY}-related donors at the center of a 5-nm AlAs barrier are 51 and 68 meV, respectively.

The arrows in Fig. 2(b) show the calculated values of the threshold voltages at which the Fermi energy in the accumulation layer is aligned with the energies of X states in the barrier. As shown in Fig. 2(b) the peak positions of the second derivative d^2I/dV^2 are in good agreement with the calculated values. It should be noted that the resonant alignment of states corresponds to the maximum of the second derivative d^2I/dV^2 with good accuracy (see Ref. 14). In the calculations we employed the commonly used values of transverse and longitudinal effective masses in the X valleys of AlAs, which are $m_l=1.1m_0$ and $m_t=0.19m_0$, respectively. The Γ(GaAs)-X(AlAs) conduction-band offset was taken to be 120 meV in accordance with Ref. 13. The splitting of the X_{XY} and X_Z valleys due to the biaxial strain on the AlAs layer was taken to be 23 meV.[1] In order to confirm the identification of the feature C in $dI/dV-V$ dependence as a $\Gamma-X_{Z1}$ resonance, we also studied the $\Gamma-X$ magnetotunneling in the magnetic field parallel to the transport direction. An analysis of the resonant structure corresponding to $\Gamma-X$ inter-Landau-level transitions carried out in accordance with the approach proposed in Ref. 15 enabled us to determine the transverse X valley effective mass $[m_t=m_{X_{XY}}=(0.2\pm0.02)m_0]$ in AlAs, and confirmed the identification of the main low-voltage resonant feature obtained by self-consistent modelling as corresponding to the $\Gamma-X_{Z1}$ transfer.

It should be noted that, unlike structures with a δ-doped layer in the center of the AlAs barrier,[7] our structures were doped randomly. Because the binding energy of the donor depends on its position in the AlAs layer,[3] the resonances should occur at different voltages for impurities located at different distances from the heterointerface. However, it was shown that tunneling through impurities near the center of the barrier gives the main contribution to the total current.[16] In addition, we suppose that there is insignificant variation in the concentration of the impurities in the AlAs layer in the growth direction. Therefore, an accurate identification of the experimental resonances permits us to determine the binding energies of central X_Z- and X_{XY}-related donors directly as ≈ 50 and ≈ 70 meV, respectively.

The additional fine structure of the X_{XY}-related donor resonance in magnetic fields applied along the direction of the current, $B \| J$, from 12.75 to 14 T and $T=0.4$ K, is displayed in Fig. 3(a). A similar additional fine structure in the X_Z-related donor resonance was observed. We assume that the fine structure is related to the resonant tunneling via states of the donors located in different atomic layers within the AlAs barrier. It should be noted that the fine structure exists in the absence of the magnetic field, and intensifies

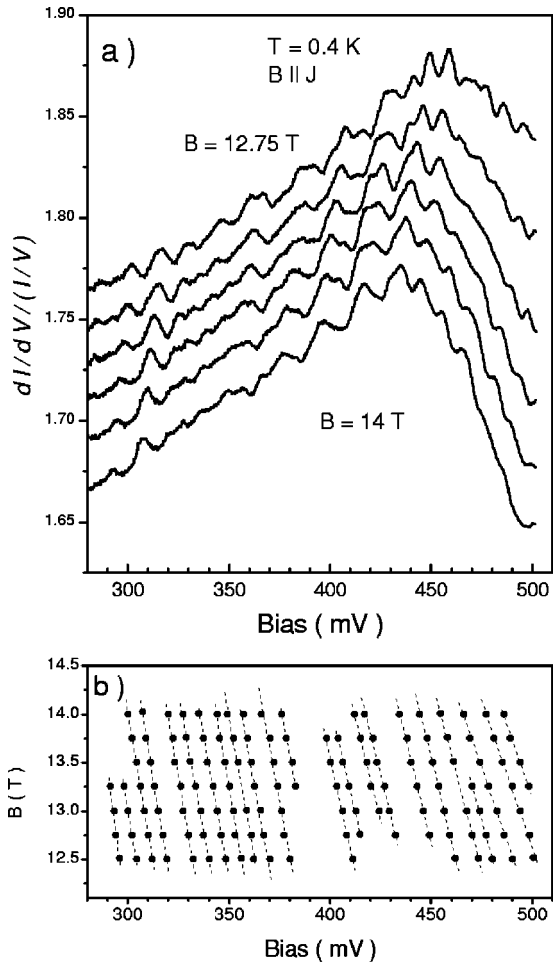

FIG. 3. (a) Normalized conductance-voltage curves for magnetic fields from 12.75 to 14 T at $T=0.4$ K. The curves are vertically offset for clarity. (b) Fan diagram of the fine-structure peak positions as a function of the magnetic field.

with increasing magnetic field. The structure is sample specific, but is precisely reproducible for a given sample, even after thermal recycling. All devices from a single wafer show the same basic features. The average period of this structure is about 15 mV, corresponding to an energy separation of approximately 1.2 meV. When the temperature was increased to 20 K ($kT \approx 1.25$ meV), the fine structure disappeared due to the thermal broadening of the Fermi distribution function in the accumulation layer. Note that the amplitudes of the peaks of the fine structure did not vary significantly when the temperature was decreased from 4.2 to 0.4 K. The number of peaks of the fine structure over the bias range of interest does not vary with an increase in temperature from 0.4 to 20 K. This indicates that, in this temperature range, the differences in energy of adjacent donor states exceeds kT.

There are two other possible causes of the fine structure. The first possibility is that the fine structure of resonances in devices with large lateral dimensions may be caused by interface roughness, as demonstrated from studies of $\Gamma-\Gamma$ tunneling in double-barrier AlAs-GaAs heterostructures.[17] However, the binding energy of donor states has a stronger dependence on the donor's position in the barrier than on the width of the barrier itself. When the thickness of the 5-nm AlAs barrier varies on 2 ML [a typical value of the molecular-beam-epitaxy (MBE) technology interface roughness] the binding energies of the central X_Z- and X_{XY}-related donors vary by 2 and 4 meV, respectively. The difference in binding energies of donors located at the center of the 5-nm AlAs barrier and at the heterointerface is 30 meV for X_Z-related donors and 20 meV for X_{XY}-related donors.[3] Thus we assume that, in our experimental situation, the interface roughness cannot cause the fine structure. The second explanation is mesoscopic conductance fluctuations due to the statistical fluctuations in the quasicontinuous density of the localized states. Such fluctuations were seen in the conductance of a resonant tunneling diode with donors in the GaAs quantum well.[18,19] The statistical fluctuations in the density of the localized states are a consequence of a random distribution of impurity states in energy due to strong random variations of the electrostatic potential in the quantum well induced by a partially depleted region of the doped collector contact. Both the amplitudes and number of the observed conductance fluctuations, i.e., their typical period, decreased with an increase in the temperature from $T \approx 0.5$ K, where $kT=\Gamma$ (where Γ is the linewidth of the donor state) to $T=4.2$ K, where the fluctuations disappeared. In contrast, the donor states in AlAs are much more strongly localized than in GaAs, and the binding energies of Si donors located in the adjacent atomic layer of the AlAs barrier differ more strongly than in GaAs.[3] Therefore, random variations of the electrostatic potential have a small influence on the spectrum of impurity states in AlAs. As a result, the spectrum of donor states in the AlAs barrier is determined predominantly by the dependence of the binding energy on the position of the donor in the barrier. Both the regular displacement of peaks of the fine structure and the coincidence of a number of observed peaks with a number of possible position of Si donors in the 5-nm AlAs layer confirm the minor influence of the random variations of the electrostatic potential on the spectrum of donor states in the AlAs barrier. The fine structure reveals 22 peaks, whereas Si donors in a 5-nm AlAs barrier can be located in 20 different atomic planes. The difference in binding energies of donors located at the center of the barrier and at the heterointerface for our structures is 35 meV.[3] Therefore, the average difference between donors energy levels is 1.75 meV. In our experiment, the average voltage distance between adjacent peaks of the fine structure is 15 mV, which corresponds to an energy separation by 1.2 meV which is in good agreement with the above estimate. Also, the temperature does not change the number of the observed resonances, but just their amplitude. From the above, we suppose that the random potential causes only an additional nonuniform broadening of the donor states located in different atomic planes, but does not leads to a quasicontinuous density of the localized states.

The conductance curve shows complex changes with the magnetic field $B \| J$. These are partly due to Landau-level quantization in the emitter, and partly due to the fine structure. Therefore, we studied the fine structure in a strong magnetic field when Landau-level quantization leads only to monotonic moving of the resonant peaks[8] [see Fig. 3(a)]. The

fine structure shows a shift to a lower bias with increasing magnetic field. The fan diagram of the observed peak position as a function of the magnetic field is shown in Fig. 3(b). Fine-structure peaks in the voltage range from 300 to 500 mV near X_{XY}-related donor resonance move to a lower bias as the magnetic field increases at a rate from 8 to 20 mV/T, and the rate is a monotonically increasing function of the voltage [see Fig. 3(b)]. It should be noted that Landau quantization should lead to the same voltage shift for all resonant peaks. On the other hand, our self-consistent Poisson-Schrodinger calculations show that, over the bias range of interest (300–500 mV), the ratio of the total voltage drop in the structure to that in the barrier region (leverage factor) varies slightly from 12 to 12.7. Therefore, we conclude that the significant difference in shift rates of the peaks is due to the fact that the binding energy of the more extended state of the donor located at the heterointerface has a stronger dependence on the magnetic field than that of the more localized state of the donor located at the center of the barrier.[3,11] In other words, the behavior of the fine structure with a magnetic field is further evidence that the fine structure is related to the resonant tunneling through the states of the donors located at different atomic layer in the AlAs barrier.

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