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Tunneling via Impurity States Related to the *X* Valley in a Thin AlAs Barrier

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Abstract—Special features corresponding to resonance tunneling of electrons from the Γ valley of GaAs to the *X* valley of AlAs were observed in the current–voltage characteristics of single-barrier GaAs/AlAs/GaAs heterostructures. Tunneling both via the states related to the two-dimensional X_{xy} and X_z subbands and via the related impurity states was detected. It is shown that the energy position of such impurity states is largely controlled by two factors: (i) spatial confinement of the AlAs layer, which influences both the size-quantization energy levels of the X_{xy} and X_z subbands and the corresponding binding energies of impurity states, and (ii) the biaxial compression of the AlAs layer due to a mismatch of the AlAs and GaAs lattice parameters, which results in the splitting of the X_{xy} and X_z valleys. This made it possible to determine directly the binding energy of the impurity states; this energy was found to be ~50 meV for the X_z valley and ~70 meV for the X_{xy} valley. © *2001 MAIK "Nauka/Interperiodica".*

It is known that AlAs (unlike GaAs) is an indirect-gap semiconductor (the minimum of the conduction band is located in the vicinity of the *X* point of the Brillouin zone) and represents a quantum well (QW) for the *X*-valley electrons and a barrier for the Γ-valley electrons in AlAs/GaAs heterostructures (Fig. 1). The offset of the conduction-band bottom between the GaAs *X* valley and the AlAs Γ valley amounts to ~0.12 eV. Such a combination of properties has rendered the AlAs/GaAs-based heterosystems convenient objects for experimental studies of transitions between the states corresponding to the different symmetry points (Γ and *X*) of the Brillouin zone. It has been found experimentally that quantum states related to the *X* valley in AlAs exert a pronounced effect on the optical and transport properties of AlAs/GaAs-based heterosystems [1–4]. This has motivated interest in the mechanisms of transitions between the Γ and *X* states and in the spectra of states in the *X* valley of AlAs and the related impurity states.

Experimental studies of the optical [1, 2] and transport [3, 4] properties of AlAs/GaAs heterosystems have shown the following. The *X* valleys that are sixfold degenerate in the bulk AlAs are transformed into two types of two-dimensional (2D) *X* subbands with different energies if thin AlAs films are considered (i.e., under the conditions of size quantization in a single direction). This phenomenon is often referred to as the splitting of the *X* valleys and is caused by the following. First, for a thin AlAs layer (the *X* wells), the X_z and X_{xy} valleys (Fig. 1) are no longer equivalent owing to a difference in effective masses that govern the motion of electrons in the direction perpendicular to the heteroboundaries (the QW walls). The effective mass is $1.1m_0$ for the X_z valleys, whereas it is $0.19m_0$ for the X_{xy} valley. Therefore, the energy positions of 2D electron subbands belonging to the X_z and X_{xy} valley are different. Second, due to a 0.12% mismatch between the lattice constants of AlAs and GaAs, the lattice is compressed in the well plane in the AlAs layer and is extended in the perpendicular direction in accordance with the Poisson ratio. The compression leads to a descent of the X_{xy} valley, whereas the Poisson tension results in an ascent of the X_z valley. Thus, the X_z valley is located below the X_{xy} valley for AlAs layers less than 60 Å thick; the reverse situation is observed for an AlAs layer thicker than 60 Å [1].

The presence of donors in AlAs leads to the emergence of impurity states. The ground state of a silicon donor in bulk AlAs is triply degenerate [2]. The nature of these states is such that each of them may be independently related to a specific pair of *X* valleys. In the conditions of a thin AlAs layer, the triplet states are split into a doubly degenerate state (related to the X_{xy} valleys) and a singly degenerate state (related to the X_z valleys); this occurs in addition to the splitting of the *X* states. The binding energies of such impurity states have been calculated previously [5] with allowance made for the mass anisotropy and the size-quantization effect.

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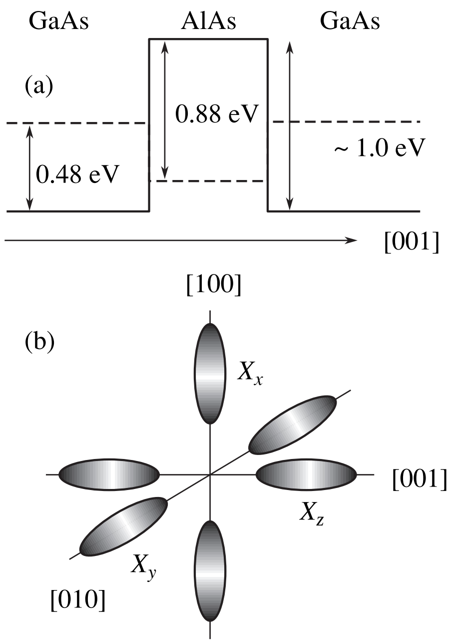

Fig. 1. (a) The profile of the conduction-band bottom of a GaAs/AlAs/GaAs heterostructure. (b) A schematic representation of the constant-energy ellipsoids in reference to the point X in the Brillouin zone in the k space for AlAs.

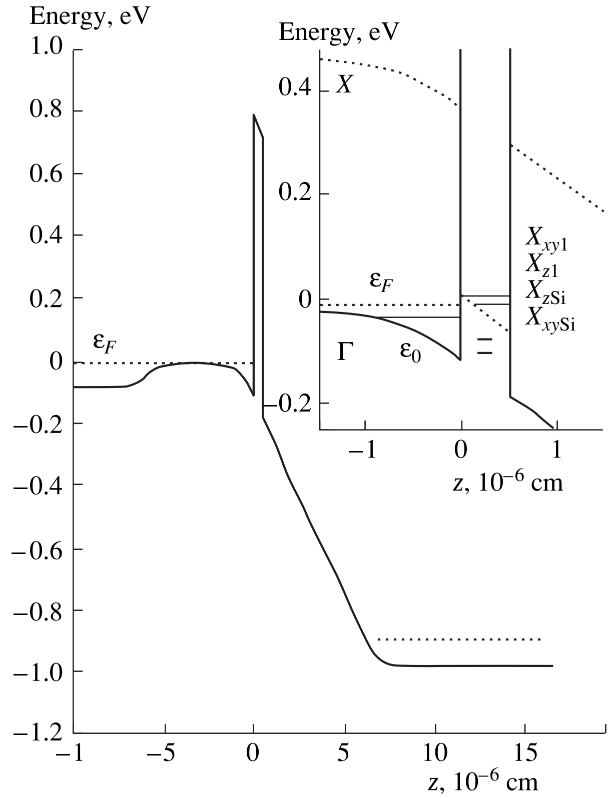

Fig. 2. Calculated profile of the conduction-band bottom (for the Γ point in the Brillouin zone) for a single-barrier GaAs/AlAs structure under a bias voltage of V = 900 mV. The profiles of the Γ- and X-band bottoms in the vicinity of the AlAs layer are shown in the inset. The positions of the Fermi level ε_F, the size-quantization level ε_0 in the 2D accumulation Γ layer in GaAs, and the size-quantization energy levels of the X_{xy} and X_z subbands in the AlAs barrier are shown. The energy positions of the X_{xySi} and X_{zSi} impurity states generated by the X_{xy} and X_z valleys in AlAs are also shown.

Tunneling spectroscopy makes it possible to directly measure the binding energy of the donor state if we observe the tunneling both via the ground state and via the impurity state and if we can convert the measured voltages to the energy values (i.e., if we know the potential distribution over the structure). Tunneling via the Si donor state in GaAs QWs in two-barrier resonance-tunneling GaAs/Al_xGa_{1-x}As-based diodes has been observed previously [6–8]; the experimentally determined value of binding energy [6–8] for such a donor state is in excellent agreement both with the calculated value for a QW with corresponding width and with the results of optical measurements. As far as we know, there have so far been only two publications [10, 11] (in addition to our preliminary study [9]) where the impurity states in the AlAs X valley have been reported. However, the results of the above studies do not give an accurate idea either of the impurity-state structure in the X valley or of the value of the corresponding binding energy.

In this study, we detected tunneling both via the states corresponding to the 2D X_{xy} and X_z subbands in the AlAs layer and via the related impurity states. This made it possible to directly determine the binding energies of the impurity states and to demonstrate that the energy positions of such impurity states is largely governed by the following two factors:

(i) The spatial confinement of the AlAs layer, which influences both the size-quantization levels in the X_{xy} and X_z subbands and the impurity-state binding energies.

(ii) The biaxial compression of AlAs layer due to the mismatch between the AlAs and GaAs lattice constants, which results in the splitting of the X_{xy} and X_z valleys by ~23 meV.

Heterostructures used in the fabrication of the samples were grown by molecular-beam epitaxy on the heavily doped n^+-GaAs(100) substrates at 570°C and had the following sequence of layers: an n^+-GaAs layer with $n = 2 \times 10^{18}$ cm^{-3} and a thickness of 400 nm; an n^--GaAs layer with $n = 2 \times 10^{16}$ cm^{-3} and a thickness of 50 nm; an undoped GaAs layer 10 nm thick; an undoped AlAs layer 5 nm thick; an undoped GaAs layer 10 nm thick; an n^--GaAs layer with a thickness of 50 nm and $n = 2 \times 10^{16}$ cm^{-3}; and an n^+-GaAs layer with a thickness of 400 nm and $n = 2 \times 10^{18}$ cm^{-3}. Silicon was used as a dopant. Nonrectifying contacts were formed by the consecutive deposition of AuGe, Ni, and Au layers with subsequent thermal annealing at 400°C. In order to form a mesa structure 100 μm in diameter, we used the conventional technology of chemical etching. The calculated profile of the conduction-band bottom (for the Γ point in the Brillouin zone) in an experimental structure for a bias voltage of V = 900 mV is shown in Fig. 2. The profiles of the Γ and X bands in the vicinity of the AlAs layers are shown in the inset.

We measured the dependences of the current I, the differential conductance dI/dV, and the second derivative d^2I/dV^2 on the bias voltage in a magnetic field with an induction of up to 8 T at temperatures of T = 1.5–4.2 K. The dependences of differential conductance dI/dV and the second derivative d^2I/dV^2 on the bias voltage were measured using the modulation technique.

An experimental current–voltage (I–V) characteristic of the sample is shown in Fig. 3a. As the voltage increases, a drastic increase in the current is observed. Such a shape of I–V characteristic in single-barrier GaAs/AlAs heterostructures is unambiguously related to tunneling via the X states in the AlAs barrier [10, 12]. For individual AlAs barriers 5 nm thick, the magnitudes of the effect observed in this study (the current density increases from 10 to 100 A/cm^2 when the tunneling via the X valley becomes effective) and those reported in previous publications [10, 12] are the same. In addition, an excess current (indicated by an arrow in Fig. 3a) is distinct below the threshold corresponding to the onset of tunneling via the X valley in the AlAs barrier. A similar special feature has been observed in the I–V characteristics of single-barrier GaAs/AlAs heterostructures with a δ-doped barrier and has been attributed to resonance tunneling via the zero-dimensional impurity states belonging to the X valley in the AlAs barrier [10].

Figure 3b shows the bias-voltage dependence of the differential conductance dI/dV. The special features corresponding to the transitions via the 2D X subbands are denoted by C, D, and E. As will be shown below, the resonance C corresponds to tunneling via the X_{z1} subband; we attribute the resonance D to tunneling via the subband X_{xy1} with the emission of a transverse acoustic (TA) phonon in AlAs, and the transition E is attributed to tunneling via the subband X_{z2}.

For the bias voltages below the threshold of tunneling via the ground state in the AlAs X valley, two low-intensity peaks (A and B) are observed in Fig. 3b. These special features are clearly distinguishable in Fig. 4, which shows the dependence of the second derivative of the current with respect to the voltage d^2I/dV^2 on the voltage V. We relate the peaks A and B to the resonance tunneling via the Si donor states belonging to the X_{xy} and X_z valleys, respectively, in the X-AlAs QW. It should be noted that, in our case, the barrier was not intentionally doped; however, the presence of impurities in the barrier was caused by the diffusion of Si from the heavily doped regions during heterostructure growth and also by residual (background) doping that amounted to 10^{15} cm^{-3} in the case under consideration.

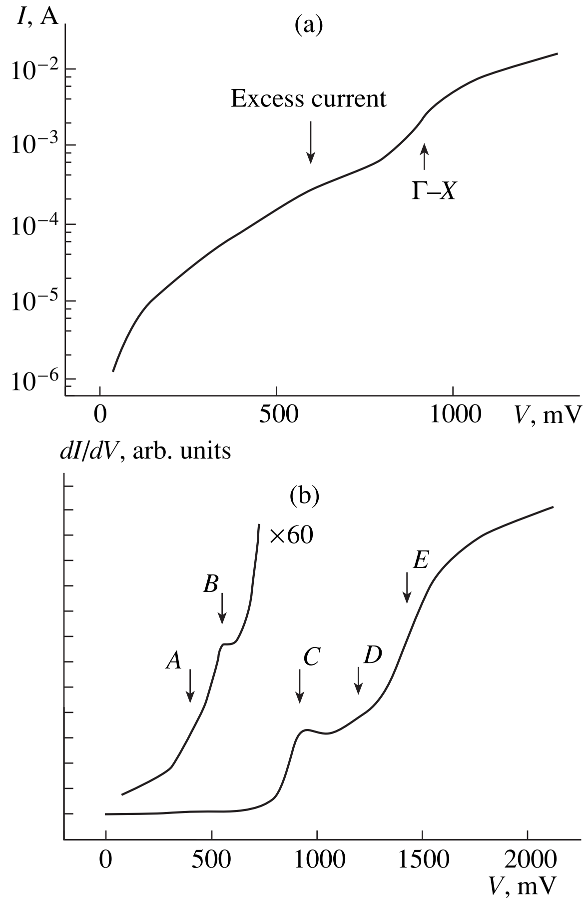

Fig. 3. (a) The I–V characteristic of GaAs/AlAs/GaAs heterostructure. (b) The dependence of differential conductance on the applied voltage.

The existence of a large amount of impurities in the barrier in the structures used is verified both by the presence of the zero-voltage anomaly (a conductance peak) [13] and by the experimental voltage dependence of electron concentration in the accumulation layer (this dependence was obtained as a result of processing the tunneling-current Shubnikov–de Haas oscillations in a magnetic field perpendicular to the 2D electron layer). Extrapolation of concentration to the zero external bias indicates that a large density of built-in positive charge (~1×10^{11} cm^{-2}) is present in the barrier. However, the absolute value of concentration determined from the measured period of the tunneling-current oscillations yields only the upper bound of the built-in charge, because the true value of the Fermi energy in a 2D layer may be smaller than the measured value [14].

In Fig. 4, the arrows indicate the calculated values of voltages for which the Fermi level ε_F in the accumulation layer coincides with the impurity level ε_i in the AlAs-layer X well ($X_{xy\mathrm{Si}}$ or $X_{z\mathrm{Si}}$) or with the size-quantization level (X_{z1} and X_{xy1}); i.e., a new channel of tunneling becomes effective. The voltage corresponding to the condition $\varepsilon_F = \varepsilon_i$ is referred to as the threshold of

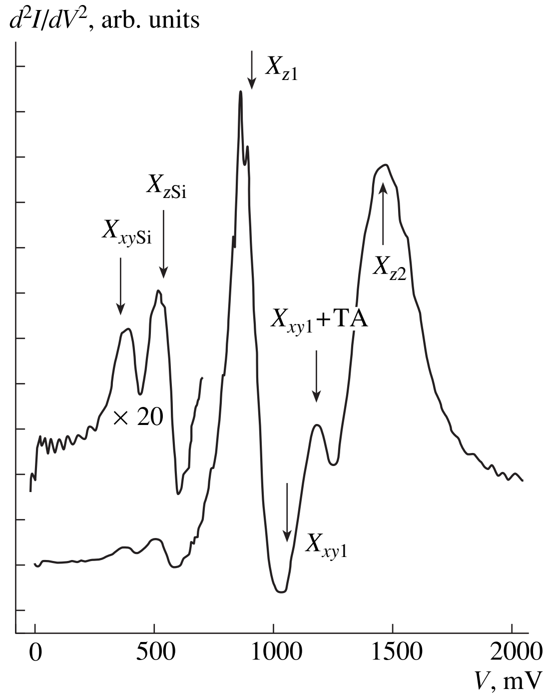

Fig. 4. Dependence of the second derivative d^2I/dV^2 on the applied voltage. The arrows indicate the calculated values of voltages for which the Fermi level in the accumulation layer coincides with the impurity level in the X well in the AlAs layer (X_{xySi} or X_{zSi}) or with the size-quantization level (X_{z1} or X_{xy1}) (i.e., when a new channel for tunneling becomes available).

tunneling via the ith level in the well [3]. The maximum of the second derivative d^2I/dV^2 corresponds to such a condition in the I–V characteristic [15]. As can be seen from Fig. 4, the positions of the peaks in the $d^2I/dV^2(V)$ curve coincide with the calculated values. When calculating the thresholds of tunneling via the size-quantization levels X_z and X_{xy}, the electron effective masses (the longitudinal m_l and the transverse m_t ones) in the AlAs X valley were assumed to be $m_l = 1.1m_0$ and $m_t = 0.19m_0$ and the energy difference between the GaAs Γ band and the AlAs X band was taken to be 120 meV in accordance with [3]. In addition, the influence of biaxial compression of AlAs as a result of the mismatch between the GaAs and AlAs lattice constants on the energy levels in the X well was taken into account. We note that the special features related to tunneling via the X_{xy1} level were not observed experimentally; however, the special feature corresponding to tunneling via this level with emission of a TA phonon with an energy of $\hbar\omega_{TA} = 12$ meV was observed in AlAs. Such a relation between the magnitudes of experimental features corresponding to tunneling transitions $\Gamma \longrightarrow X_z$, $\Gamma \longrightarrow X_{xy}$, and $\Gamma \longrightarrow X_{xy}$ + TA has been observed previously [3] and has been attributed to different probabilities of the processes $P_{\Gamma \to X_z} \gg P_{\Gamma \to X_{xy} + TA} \gg P_{\Gamma \to X_{xy}}$. Such a relation between the probabilities is independently supported by the experiments concerned with studying the photoluminescence spectra for the GaAs/AlAs-based structures [1]. A low probability of elastic transition to the side X_{xy} valley is caused by the fact that, in this case, a large change in the transverse electron momentum (by a value of $q \approx 2\pi/a$, where a is the lattice constant) is required.

Voltages corresponding to tunneling via impurities belonging to the X_z and X_{xy} valleys were calculated using the results reported in [5], according to which the binding energy of the impurity located at the center of the 5-nm-thick AlAs barrier is 51 meV for the X_z valley and is 68 meV for the X_{xy} valley. The calculated values of the tunneling thresholds for such impurities are 551 mV for the X_z valley and 358 mV for the X_{xy} valley and agree closely with the positions of the peaks in the curve for the second derivative d^2I/dV^2. It should be noted that, in contrast to the structures with a δ-doped layer in the AlAs-barrier center [6–8, 10], the structures we used were randomly doped. Since the impurity energy depends on its position in the QW [5], the resonance should occur at somewhat different bias voltages for the impurities located at different distances from the heteroboundary. However, as has been shown previously [16], only tunneling via impurities located in the vicinity of the barrier center contributes significantly to the current. Thus, we may state that, in our heterostructures, the binding energy of a Si impurity is ~50 meV for the X_z valley and is ~70 meV for the X_{xy} valley.

Thus, in this study, we detected for the first time tunneling both via the states belonging to the 2D X_{xy} and X_z subbands in the AlAs layer and via the related impurity states, which made it possible to directly measure the binding energies of these donor states.

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