X-valley-related donor states and resonant tunneling in a single-barrier diode

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A δ layer of Si donors has been incorporated in the tunneling barrier of a GaAs/AlAs/GaAs single-barrier heterostructure in order to investigate the tunneling via X-valley-related donor states. The low-temperature current-voltage $I(V)$ characteristics exhibit two resonant peaks which arise due to tunneling via biaxial-strain-split donor X states. The splitting is determined as 13 ± 2 and 14 ± 2 meV for two samples, respectively, in agreement with reported piezophotoluminescence data. For a magnetic field B applied parallel to I, the tunneling current oscillates when B is tuned at a given V. The magneto-oscillations in I have been found to quench at the resonant voltage and to be *out of phase* with the oscillations in the concentration of electrons in the accumulation layer. Self-consistent calculations show that a variation of the electron attempt frequency might account for these effects. [S0163-1829(98)02712-X]

Single-barrier tunneling diodes with AlAs barriers provide an interesting example of a resonant-tunneling device: a barrier for Γ-valley electrons appears as a quantum well for X-valley electrons. The X valley in the barrier is located not much higher in energy [about 120 meV (Ref. 1)] than the Γ valley in the adjacent GaAs layers, and resonant tunneling is possible in this energy range.[2] The transition between the Γ- and X-valley states is not forbidden by momentum conservation, due to the size quantization in the growth direction of Γ-electrons in the emitter-accumulation layer. Thus resonant tunneling can be observed via the barrier states related to the X valley. Tunneling via X-valley-related states was shown to be the origin of the negative differential resistance in single-barrier tunneling devices.[2,3]

Numerous detailed studies were reported on tunneling through the X-valley-related conduction-band states, including tunneling through excited size-quantized X levels, phonon-assisted tunneling,[4] and tunneling under high pressure.[5] Tunneling via X-valley-related donor states has attracted less attention. The transition probability through a donor level should be higher than that through the X-valley edge, as the Γ-valley states contribute significantly to the strongly localized X-donor wave function. Except for our preliminary report,[6] only a single publication on X-donor-assisted tunneling exists to date.[7]

In this paper we report the investigation of resonant tunneling via X-valley-related states of Si donors incorporated in an AlAs barrier. In a typical n-i-n single-barrier device, the AlAs barrier layer and adjacent undoped GaAs layers are sandwiched between the heavily doped GaAs contact layers (see the conduction-band profile in Fig. 1). When a voltage V is applied between the contacts, a two-dimensional electron gas (2DEG) accumulates in the undoped GaAs layer near the tunnel barrier. Formation of the emitter-accumulation layer is accompanied by *nonresonant* tunneling to a continuum of electron states on the collector side of the barrier. When the applied voltage brings the 2DEG into resonance with a discrete state located in the barrier, *resonant* tunneling can occur, and manifests itself as a resonant peak in current-voltage characteristics, $I(V)$. Note that the voltage drop V_1 between the 2DEG and the resonant state in the barrier is only a small fraction of the total voltage V between the n-doped contact layers. The ratio $g=V/V_1$ gives the leverage factor which depends on V.

Due to the small lattice misfit between GaAs and AlAs bulk materials, an AlAs layer is biaxially compressed in GaAs/AlAs heterostructures grown on a GaAs substrate. The compression increases the energy of the X-valley minima which are oriented along the growth direction, X_z, relative to the minima which are oriented parallel to the layer, X_{xy}.[8,9] Reported values of the splitting between X_z- and X_{xy}-valley minima vary from 14 meV up to 23 meV.[9–13] For X-valley-related states of the Si donor, the valley-orbit interaction is negligible, because they are not mixed by the central potential,[14] so that the states can be treated as corresponding to independent valleys.[15] Therefore the splitting of

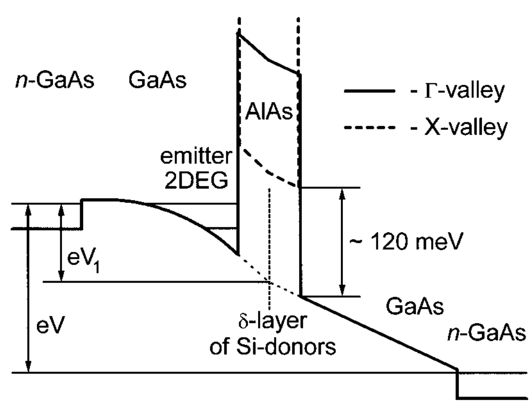

FIG. 1. A schematic conduction-band diagram of a single-barrier tunneling device under an applied voltage V. The kink within the barrier arises due to the charge of ionized donors.

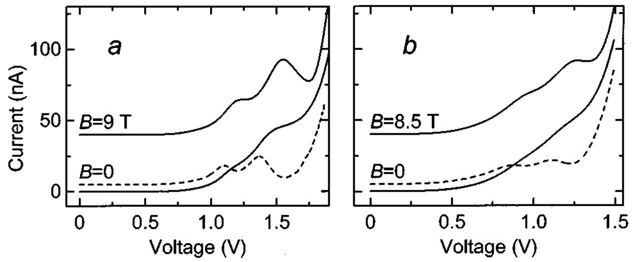

FIG. 2. Solid curves—$I(V)$ characteristics at $T=4.2$ K at zero and high B: (a) sample *1*, (b) sample *2*. Dashed curves—$I(V)$ derivatives at $B=0$. Curves are offset.

Si donor levels reflects the strain-induced X_z-X_{xy} splitting. In $I(V)$ characteristics of our device we observe this splitting, which was not resolved in Ref. 7.

There is an interesting effect which appears in single-barrier devices in magnetic field B applied parallel to the tunneling current. If the voltage V between the contact layers is fixed, variation of B causes oscillations, periodic in $1/B$, in the 2DEG concentration n_e and in the tunneling current I (Refs. 16–18) (these provide a reasonable estimate of n_e). The oscillations arise because the chemical potential μ_e in the Landau-quantized 2DEG is pinned to that in the heavily doped n-type GaAs emitter, so the variation of B results in a redistribution of electrons between the 2DEG and the emitter and a modification of the potential profile in the device. The tunneling current was previously reported[16–18] to oscillate *in phase* with n_e. A striking feature of our devices is that they exhibit magneto-oscillations in I which are *out of phase* with n_e. With the help of self-consistent calculations, we have successfully explained this observation, as well as the fact that, at resonance voltage, the magneto-oscillations are strongly quenched in amplitude.

Two samples were grown on a (100) n^+-type GaAs substrate, and comprise the following layers: 1 μm of heavily doped GaAs with a Si concentration of 2×10^{18} cm^{-3}; 100 nm of GaAs with 2×10^{16} cm^{-3} of Si; 100 nm of undoped GaAs; 5 nm of AlAs; a δ layer of Si donors; 5 nm of AlAs; 100 nm of undoped GaAs; 100 nm of GaAs with 2×10^{16} cm^{-3} of Si; and 1 μm of heavily doped GaAs. Thus the total width of the AlAs barrier is 10 nm. The Si concentrations in the δ layer was 1×10^{10} and 5×10^{10} cm^{-2} for samples 1 and 2, respectively. A control sample lacking the δ layer of donors was also grown. Circular mesas of various diameters, from 50 to 200 μm, were produced using optical lithography, and AuGe was alloyed into the n^+-type GaAs layer to form an ohmic contact. Figure 1 shows the conduction-band profile of our device. The kink in the barrier potential profile is due to the charge of the ionized donors.

Figure 2 shows the $I(V)$ characteristics of both samples at 4.2 K. Each $I(V)$ exhibits two resonant peaks. The peaks are broad and relatively weak at zero magnetic field. The $I(V)$ change drastically at high $B\|I$: the two peaks become narrower and much better resolved, with a negative differential resistance for $B>6$ T. In sample 2, with higher δ-layer-donor concentration, the peaks are shifted to lower voltage with respect to sample 1. The peaks are absent in the $I(V)$ of the control sample.

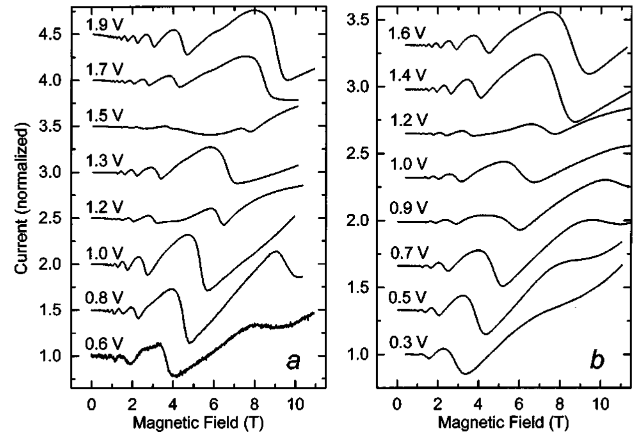

FIG. 3. $I(B)$ characteristics at various biases: (a) sample *1*, (b) sample *2*. The current is normalized to the values at $B=0$. Curves are offset.

Peaks in $I(V)$ indicate the resonances between the 2DEG and the states in the barrier. The observation of peaks in the doped samples lead us to attribute the peaks to tunneling through donor states. The donor levels which exist in the energy range corresponding to the peak voltage are related to the X valley. Since in-plane momentum conservation is not important for tunneling through confined X-donor states, all occupied emitter 2DEG Γ electron states contribute to the current. Therefore both sample inhomogeneity and the spread of emitter 2DEG kinetic energy contribute to a broadening of the peaks at $B=0$; a narrowing of the peaks at $B\|I$ reflects Landau quantization in the 2DEG.

To determine quantitatively the energy position of the levels which give rise to the resonant peaks, we need to know the electron concentration in the 2DEG. This was obtained from magneto-oscillations of the tunneling current in $B\|I$, i.e., $I(B)$ recorded at various constant V.[16–18] A representative set of $I(B)$ for the two samples is shown in Fig. 3. The curves exhibit strong magneto-oscillations as B increases, with relatively smooth increases and sharp falls. Note also that the oscillations are strongly quenched at the resonant voltages [1.2 and 1.5 V in (a), and 0.9 and 1.2 V in (b)]. Figure 4 shows how the oscillation amplitude depends on the applied voltage both for samples 1 and 2 and for the control sample. With a background of weak variations observed in all samples, the doped samples show sharp and strong minima in the oscillation amplitude at the resonances.

The $I(B)$ dependences allow us to determine with a reasonable accuracy[18] the values of n_e for a given V. The magneto-oscillations observed in our sample are consistent with an assumption that sharp falls in current, which are periodic in $1/B$, correspond to an integer even filling factor ν (this will be discussed in detail later). The strongest fall, which appears in sample 1 at 3.8–4 T at 0.6 V and evolves to 8.7–9.3 T at 1.9 V, corresponds to $\nu=2$. We pointed out earlier that in sample 2 the peaks in $I(V)$ are shifted to smaller voltage with respect to sample 1. Nevertheless note that in sample 2 a smaller voltage is required to obtain the same n_e: the fall in $I(B)$, which corresponds to $\nu=2$, evolves to ≈ 9 T at smaller V, around 1.6 V. This results from the contribution of the charge of ionized donors in the barrier to the sample potential profile, due to which the le-

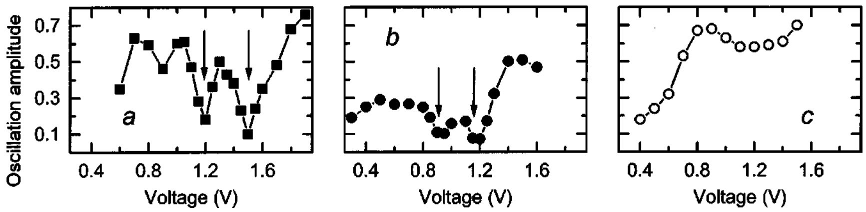

FIG. 4. Amplitude of current magneto-oscillations at filling factor $\nu=2$ at various voltages: (a) sample *1*, (b) sample *2*, and (c) control sample. The current is normalized to values at $B=0$.

verage factor depends on the donor concentration. The greater the donor concentration, the greater the kink in the potential profile in the barrier (see Fig. 1); so for a *given* resonance between the 2DEG and the barrier state, the smaller the voltage drop in the collector region of the device. Due to this, each of the resonant peaks in $I(V)$ has been found to occur at similar values of n_e in the two samples despite the difference in voltage.

Self-consistent calculations have been performed in order to relate n_e to the voltage drop between the chemical potential in the 2DEG and the layer of donors in the barrier. These give the following energies of the two resonant levels, E_1 and E_2, referred to as the conduction-band edge in GaAs: $E_1=75\pm3$ meV and $E_2=88\pm3$ meV for sample 1, and $E_1=71\pm3$ meV and $E_2=85\pm3$ meV for sample 2. The splitting between the peaks is determined as $\Delta E=13\pm2$ meV for sample 1 and $\Delta E=14\pm2$ meV for sample 2. This is in excellent agreement with the value of the biaxial-strain-induced splitting between the minima of the X_z and X_{xy} valleys, ≈ 14 meV, obtained by piezophotoluminescence spectroscopy.[9] Due to strong localization of the X-donor-state wave function, size quantization in the 10-nm AlAs layer does not contribute to the donor-level energies, so, in the absence of valley-orbit interaction for group-IV donors,[14,15] the splitting between the X-donor levels gives the splitting between the valley minima. This is not the case for exciton states,[9,10] and the valley-orbit interaction may contribute to the larger splitting value, ≈ 23 meV which was reported in Ref. 11.

The lower- and higher-voltage peaks in $I(V)$ correspond to tunneling through X_{xy} and X_z levels, respectively. This may account for the larger amplitude of the higher-voltage peak, despite the double degeneracy of the X_{xy} level. For tunneling through X-valley conduction-band states, transitions from the emitter 2DEG Γ states to X_z (X_{xy}) valleys are allowed (forbidden) due to in-plane momentum conservation.[4] Both transitions are allowed in donor-level tunneling because of the contribution of Γ states to the strongly localized donor wave function, but for the X_z level the transition probability can be still expected to be significantly larger than for X_{xy} levels. If we assume that the X-valley edge in the AlAs barrier is located at ≈ 120 meV (Refs. 1 and 4) above the GaAs Γ-valley minimum, we obtain $E_B\approx 45-50$ meV for the binding energy of the donor ground X state, which is consistent with the earlier reported values.[19]

Now we discuss the magneto-oscillations in the tunneling current in our device. They arise because the chemical potential in the 2DEG is pinned to that in the n-doped GaAs emitter. The magnetic field determines the energy of the highest occupied electron Landau level in the 2DEG, and hence the chemical potential position. This has to be compensated for by charge redistribution between the 2DEG and the emitter, changing both n_e and the potential profile, and therefore the tunneling current in the device. There are two possible states of the 2DEG in the sample for $B\|I$, with μ_e positioned either *between* maxima in the Landau-level (LL) density of states or *within* a LL. The former state corresponds to integer filling factor ν (more accurately to even ν, as we neglect the spin splitting). With increasing B, the 2DEG alternates between these two states, with n_e growing at integer ν and falling when ν is a noninteger.

What parts of $I(B)$ curves correspond to integer ν? The increase of both B and n_e contributes to the enhancement of the 2DEG energy in this case, and qualitatively we can expect that these are the parts which exhibit a *sharp* change in current. Conversely, for noninteger ν the contributions to the 2DEG energy of B and n_e oppose each other, and a *smooth* change in the current can be expected. These arguments were discussed in detail in Ref. 17. Analysis of our devices shows that an integer ν really does correspond to *sharp* falls in the current (otherwise the required change in n_e would be inconsistent with the device parameters). This implies out-of-phase oscillations in I and n_e: an increase in n_e results in a decrease in I, and vice versa. Although only in-phase oscillations were reported to date,[16–18] self-consistent calculations for our devices indicate that this behavior is reasonable.

In the semiclassical approximation, the tunneling current is given by $I=n_e e f_e T$, where f_e is the attempt frequency of the 2DEG and T is the transmission coefficient. Here T is determined by the electron-wave-function penetration in the barrier, while f_e is closely related to the spatial extent Δz of the electron wave function in the tunneling direction, roughly proportional to $1/\Delta z^2$. This follows just from the uncertainty relation: the electron energy $hf_e\approx\Delta p^2/2m^*\approx\hbar^2/2m^*\Delta z^2$, where Δp is the uncertainty in electron momentum and m^* is the electron effective mass.

In the case of increasing voltage V at fixed values of B, an *increase* in n_e is followed by an *increase* both in T and f_e. The former results from the increased transparency of the barrier, and the latter is due to a *sharpening* of the potential which confines the 2DEG. These result in the well-known superlinear $I(V)$ dependence. However, if n_e is changed by a variation of magnetic field at *fixed* V, an *increase* in n_e results in a *flattening* of the 2DEG confining potential. This should be followed by an increase in Δz and a *reduction* in f_e. Therefore the enhancement in n_e and T competes with the reduction in f_e, and a fall in the tunneling current with n_e increase is possible.

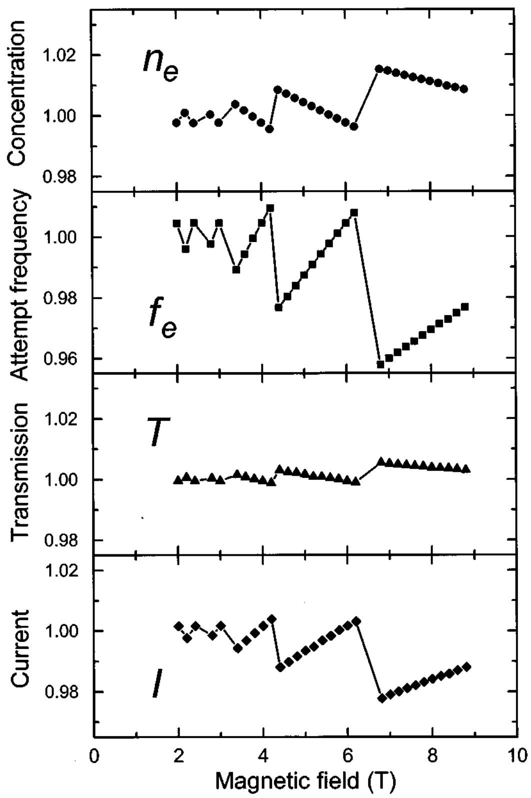

FIG. 5. Self-consistent calculations: magneto-oscillations at given voltage in 2DEG concentration n_e, attempt frequency f_e (i.e., $1/\Delta z^2$), barrier transmission coefficient T, and in the tunneling current I. All values are normalized to those at $B=0$.

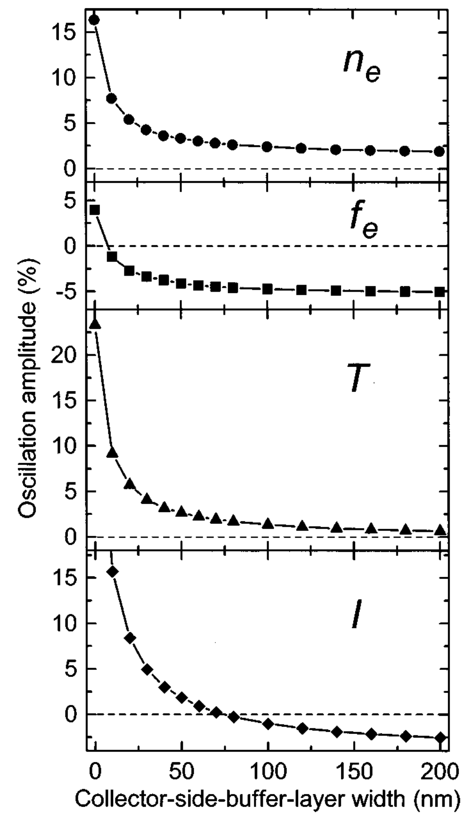

FIG. 6. Self-consistent calculations: amplitude of magneto-oscillations at $\nu=2$ in 2DEG concentration n_e, attempt frequency f_e, and barrier transmission coefficient T, and in the tunneling current I as a function of the width of the buffer layer on the collector side of the device.

Although our self-consistent calculations cannot explain the large amplitude of the current oscillations, they show that the observation of out-of-phase oscillations in I and n_e is reasonable for our samples. Figure 5 shows calculated relative changes in n_e, $1/\Delta z^2$, and T when B is varied at given V [here T is taken semiclassically as $T=\exp(-2/\hbar\int|p_z|dz)$, with the integral taken within the barrier]. One can see that the change in $1/\Delta z^2$ exceeds the sum of changes in n_e and T, so the current is expected to oscillate out of phase with n_e (see the lowest plot in Fig. 5).

Our calculations were performed for nonresonant tunneling. Under resonant conditions the wave function of 2D electrons penetrates strongly into the barrier. This increases the wave-function spatial extent, which hence becomes less sensitive to the sharpness of the confining potential. In the competition between the enhancement in n_e and T and the reduction in f_e, the contribution of f_e becomes less important, and the oscillations quench.

Finally, we consider why only in-phase oscillations in I and n_e have been observed to date. The principal difference between our samples and the heterostructure investigated theoretically in Ref. 17 is in the thickness of the collector-side buffer layer d_c. This is ≈ 200 nm for our samples, as the slightly doped GaAs layer is fully depleted at our measured voltages. In Ref. 17 the collector n-doped layer was taken very close to the barrier. In that case the shape of the barrier was much more sensitive to a change in the potential profile than in our samples, as practically all the additional voltage drop between the 2DEG and the collector occurred within the barrier. The thicker the collector buffer layer, the smaller the fraction of the voltage drop within the barrier and the less sensitive the sharpness of the barrier edge is to a change in the potential profile. Figure 6 shows the effect of d_c on the amplitude of the oscillation in n_e, f_e, and T at $\nu=2$. For the calculations we assume the potential profile in the collector and barrier regions of the device is the same in all cases. Hence the 2DEG concentration at $B=0$ is also the same, while the total voltage applied between the contact layers is different for each of the points. The negative sign for the f_e amplitude corresponds to an oscillation out of phase with that of n_e. For $d_c\approx 15$ nm the magneto-oscillations in f_e change sign, while those in n_e and T are strong. This results in strong oscillations in the tunneling current in phase with n_e which were investigated in Ref. 17. With increasing d_c the oscillations in n_e and T are quenched gradually, while the amplitude of the out-of-phase oscillations in ν_e saturates. Thus the in-phase oscillations in I should quench around $d_c\approx 75$ nm, and reappear out of phase as d_c increases; see the lowest plot in Fig. 6.

As our calculations predict the correct sign, but a much smaller amplitude of the effect than that observed in the experiment, a more detailed theory is required for a comprehensive understanding of our data.

To conclude, we have observed resonant tunneling through strain-field-split X-valley-related states of the Si donor in the AlAs barrier of a single-barrier GaAs/AlAs/GaAs tunneling diode. The magnitudes of the splitting are determined as 13±2 and 14±2 meV for two samples, respectively, in agreement with piezophotoluminescence data.[9] The magneto-oscillations in the tunneling current are found to be out of phase with oscillations in the electron concentration in the emitter-accumulation layer. It has been shown that the variation of the 2DEG attempt frequency might account for this effect.

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