PHYSICAL REVIEW B VOLUME 46, NUMBER 19 15 NOVEMBER 1992-I

# Effects of interface-roughness scattering on resonant tunneling

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(Received 17 August 1992)

We calculate the effects of interface-roughness scattering on the current-voltage characteristics of a GaAs-$Al_xGa_{1-x}As$ double-barrier structure. We treat this scattering within the coherent-potential approximation so that the theory is nonperturbative and preserves unitarity. The scattering does not change the peak current significantly, even though the electrons are scattered many times while in the quantum well. The valley current, on the other hand, increases by several orders of magnitude in a structure with thick barriers. In good qualitative agreement with recent experiments we find that the peak-to-valley ratio grows only very slowly with barrier thickness for barriers thicker than $\approx 100$ Å.

Resonant tunneling in semiconductor double-barrier structures (DBS) has received a lot of experimental attention over the past ten years. As the bias voltage across the structure is increased the tunnel current grows and reaches a peak value. When the voltage is further increased a much smaller current, the so-called valley current, is obtained. This negative-resistance behavior can be explained by a one-dimensional theory.[1] A quantitative comparison with experimental results, however, shows that in many cases the theory predicts values of the valley current that are too small. This discrepancy is to a large extent the result of different scattering processes, such as those caused by interface roughness, impurities, and phonons, that are unavoidable in real devices.

Guéret *et al.* have reported on experiments with double-barrier structures with rather low and thick barriers.[2,3] They suggest that scattering off the rough interfaces between the barriers and the quantum well is the primary reason for the large valley currents observed. In this paper we present a calculation of the current-voltage characteristics of a DBS taking into account interface-roughness scattering. Several authors have addressed this problem before. Liu and Coon[4] assumed the interfaces to be periodically corrugated. Chevoir and Vinter[5] and Rudberg[6] used the golden rule. Fertig, He, and Das Sarma[7] and Leo and MacDonald[8] went a step further and treated the problem perturbatively employing approximations that preserve unitarity. Berkovits and Feng[9] have presented a nonperturbative theory, but they had optical applications in mind, and did not calculate the tunnel current as a function of voltage.

The point we wish to make in this paper is that a nonperturbative treatment of the interface-roughness scattering is necessary when calculating the current through a DBS with thick barriers, where one inevitably faces a multiple-scattering situation. Moreover, the approximations made must preserve unitarity, i.e., the calculated transmission and reflection probabilities of an electron should add up to 1. We achieve this by using the coherent-potential approximation.

The peak current does not change much when the effects of interface roughness are included in the calculation, but the valley current can increase by several orders of magnitude. In agreement with the experiment[3] we find a distinct change in the behavior of the peak-to-valley ($P/V$) ratio as a function of barrier thickness $d$ at $d \approx 100$ Å. For $d < 100$ Å the $P/V$ ratio exhibits a rapid exponential increase. For barriers thicker than 100 Å, on the other hand, our calculated $P/V$ ratio grows very slowly.

In elastic tunneling the tunnel current density can be calculated by a Landauer-type formula,

$$j = 2e \int_{k_z > 0} \frac{d^3k}{(2\pi)^3} \frac{\hbar k_z}{m^*} T(\mathbf{k})[n_L(\varepsilon_\mathbf{k}) - n_R(\varepsilon_\mathbf{k})] \; . \qquad (1)$$

In Eq. (1), $e$ is the elementary charge and $T$ is the transmission probability of an electron with initial wave vector $\mathbf{k}$. Since we will compare with a low-temperature experiment we evaluate the electron occupation numbers, denoted $n_L$ (in the left contact) and $n_R$, at zero temperature. We have used the GaAs value, $m^* = 0.067 m_0$, for the electron effective mass throughout the structure.

To calculate the transmission probability we model the double-barrier structure, inset in Fig. 2(b) below, by a transfer Hamiltonian with parameters calculated from a linear model potential.[10] The quantum well has one resonant level with energy $\varepsilon_0$. The electrons in the two contacts are assumed to be free with energies $\varepsilon_\mathbf{k}$ and $\varepsilon_\mathbf{p}$, respectively. We include tunneling in the model by hopping terms in the Hamiltonian; the matrix elements for hopping from the quantum well to the left (right) contact are denoted $T_{\mathbf{k}L}$ ($T_{\mathbf{p}R}$).

The interface roughness (IR) consists of islands, formed in the growth process,[11,12] of barrier material penetrating into the well or vice versa. The islands cause a space-dependent variation of the resonant-level energy which acts as a scattering potential in two dimensions (2D). We model this by identical delta function (in 2D) scatterers randomly distributed over the downstream inner wall of the quantum well. This gives the following interaction term in the Hamiltonian:

$$H_{\mathrm{IR}} = \sum_{\mathrm{isl.}, \mathbf{q}_\parallel, \mathbf{q}'_\parallel} e^{i\mathbf{q}' \cdot \mathbf{r}_{\parallel \mathrm{isl.}}} V_0 c^\dagger_{\mathbf{q}_\parallel + \mathbf{q}'_\parallel} c_{\mathbf{q}_\parallel} \; , \qquad (2)$$

 

where $c_{\mathbf{q}_\parallel}$ ($c^\dagger_{\mathbf{q}_\parallel}$) annihilate (create) an electron, with wave vector $\mathbf{q}_\parallel$ parallel to the barriers, in the quantum well. Since we use delta-function scatterers their Fourier transform $V_0$ is independent of the transferred momentum. We calculate $V_0$ by assuming that the islands have area $A_i = 4\times 10^4$ Å$^2$, corresponding to a linear size of 200 Å,[11] and average height 5 Å.[12] Unless otherwise stated, the areal density of scatterers used in the calculations is $n_i = 10^{-5}$ Å$^{-2}$, i.e., 40% of the interface is covered by islands. The change in resonant-level energy due to an island scales as $\delta\varepsilon \sim \varepsilon_0 \delta L/L \sim \delta L/L^3$, where $\delta L$ is the change of the well width $L$.

The transmission probability of an electron through the double-barrier structure is related to a two-electron Green's function.[13] This Green's function factorizes into a product of two one-electron Green's functions when there is no scattering mechanism present. The coherent transmission probability of an electron with total energy $\varepsilon = \varepsilon_z + \hbar^2 q_\parallel^2/2m^*$ and initial parallel momentum $\hbar\mathbf{q}_\parallel$ is then,

$$\begin{aligned} T(\varepsilon,\mathbf{q}_\parallel) &= \Gamma_L(\varepsilon_z)\Gamma_R(\varepsilon_z) G^*_{\mathbf{q}_\parallel}(\varepsilon) G_{\mathbf{q}_\parallel}(\varepsilon) \\ &= \Gamma_L(\varepsilon_z)\Gamma_R(\varepsilon_z)/\{(\varepsilon-\varepsilon_0-\hbar^2 q_\parallel^2/2m^*)^2 \\ &\quad + [\Gamma_L(\varepsilon_z)+\Gamma_R(\varepsilon_z)]^2/4\}\ , \end{aligned} \tag{3}$$

with the broadening functions $\Gamma_{L(R)}$ given by

$$\Gamma_{L(R)}(\varepsilon_z) = 2\pi \sum_{\mathbf{k}(\mathbf{p})} |T_{\mathbf{k}L(\mathbf{p}R)}|^2 \delta(\varepsilon_z - \varepsilon_{\mathbf{k}(\mathbf{p})}) \delta_{\mathbf{k}_\parallel(\mathbf{p}_\parallel),0}\ . \tag{4}$$

Allowing for scattering, the transmission probability becomes the sum of an unscattered part $T_0$, illustrated in Fig. 1(a), and a roughness-assisted part $T_{sc}$, shown in Fig. 1(b). We evaluate $T_0$ and $T_{sc}$ by calculating self energies and vertex corrections, averaged over different interface roughness configurations, by standard methods.[14] The self energy $\Sigma$ relates the full Green's function $G$, to the bare one $G^{(0)}$, through $G = G^{(0)} + G^{(0)}\Sigma G$, as shown in Fig. 1(c). We calculate $\Sigma$ self-consistently in the spirit of the coherent-potential approximation,[15] i.e., the full Green's function appears in the expression for the self energy. This procedure, illustrated in Fig. 1(d), is necessary in order to get an approximation that preserves unitarity when one considers multiple scattering. The self energy is a sum of tunneling (not shown) and interface-roughness contributions,

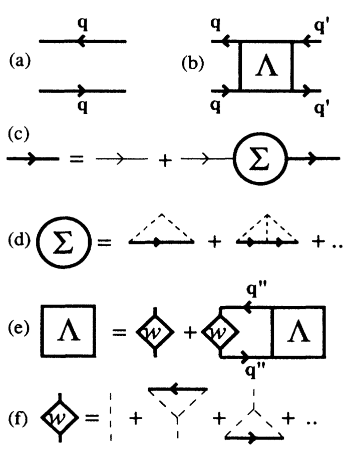


FIG. 1. Diagrammatic illustration of the calculations. Contributions to the transmission probability from (a) unscattered electrons, and (b) tunneling assisted by interface roughness. (c) The Dyson equation. (d) The electron self energy is evaluated self-consistently and gets contributions from interface-roughness scattering to all orders. (e) Ladder summation of multiple scattering events. (f) Evaluation of the irreducible vertex.

$$\begin{aligned} \Sigma_{\mathbf{q}_\parallel}(\varepsilon) &= -\frac{i}{2}[\Gamma_L + \Gamma_R](\varepsilon - \hbar^2 q_\parallel^2/2m^*) \\ &\quad + n_i A_i^2 V_0^2 \left[1 - A_i V_0 \int \frac{d^2 q''_\parallel}{(2\pi)^2} G_{\mathbf{q}''_\parallel}(\varepsilon)\right]^{-1} \\ &\quad \times \int \frac{d^2 q'_\parallel}{(2\pi)^2} G_{\mathbf{q}'_\parallel}(\varepsilon)\ . \end{aligned} \tag{5}$$

The real parts of the integrals are divergent as a consequence of the use of a delta-function potential. We therefore use a cutoff corresponding to an energy of 100 meV in all parallel-momentum integrals. The ladder summation in Fig. 1(e) yields an integral equation which reduces to an algebraic equation when using a delta-function potential, so $\Lambda$ does not depend on momentum,

$$\Lambda(\varepsilon) = w(\varepsilon)\left[1 - w(\varepsilon)\int \frac{d^2 q''_\parallel}{(2\pi)^2} |G_{\mathbf{q}''_\parallel}(\varepsilon)|^2\right]^{-1}\ . \tag{6}$$

An evaluation of the irreducible vertex $w$ along the lines of Fig. 1(f) yields

$$w(\varepsilon) = n_i A_i^2 V_0^2 \left|1 - A_i V_0 \int \frac{d^2 q''_\parallel}{(2\pi)^2} G_{\mathbf{q}''_\parallel}(\varepsilon)\right|^{-2}\ . \tag{7}$$

The contribution from the diagram in Fig. 1(b) to the transmission probability is now

$$\begin{aligned} T_{sc}(\varepsilon,\mathbf{q}_\parallel) &= \int \frac{d^2 q'_\parallel}{(2\pi)^2} \Gamma_L(\varepsilon - \hbar^2 q_\parallel^2/2m^*) \\ &\quad \times \Gamma_R(\varepsilon - \hbar^2 q'^2_\parallel/2m^*) G^*_{\mathbf{q}_\parallel}(\varepsilon) G_{\mathbf{q}_\parallel}(\varepsilon) \\ &\quad \times \Lambda(\varepsilon) G^*_{\mathbf{q}'_\parallel}(\varepsilon) G_{\mathbf{q}'_\parallel}(\varepsilon)\ . \end{aligned} \tag{8}$$

The unscattered part, $T_0$, of the transmission probability is still formally given by the first line of Eq. (3). However, for thick barriers the self energy is dominated by the scattering contributions. This suppresses $T_0$ very much. The interface roughness assists tunneling by transferring energy, from an electron's perpendicular motion, to the motion parallel to the barriers or vice versa. In this way some electrons are brought into resonance. The parallel-motion energy can never become negative, so $T_{sc}$ can only contribute substantially to the transmission probability of electrons whose total energy $\varepsilon$ is above resonance, i.e., $\varepsilon > \varepsilon_0$. $T_{sc}$ is very small when $\varepsilon < \varepsilon_0$. All in all, scattering replaces the sharp Lorentzian transmission peak, characteristic of coherent resonant tunneling, by a suppressed, inhomogeneously broadened transmission line. In a structure with the parameter values given in Fig. 2 the scattering lifetime of an electron, $\tau_{sc} = -\hbar/2\,\mathrm{Im}\Sigma_{sc}$, is $\approx 0.5$ ps. The time the electron spends inside the quantum well is, on the other hand, $\approx 5$ ns (200-Å barriers). Thus, we are in the regime of sequential tunneling,[16] and a multiple-scattering treatment of the interface roughness is clearly needed.

Figure 2 shows the results of our calculations. The parameter values are taken from the experiment by Guéret *et al.*[3,17] Note first that the peak current in Fig. 2(a) does

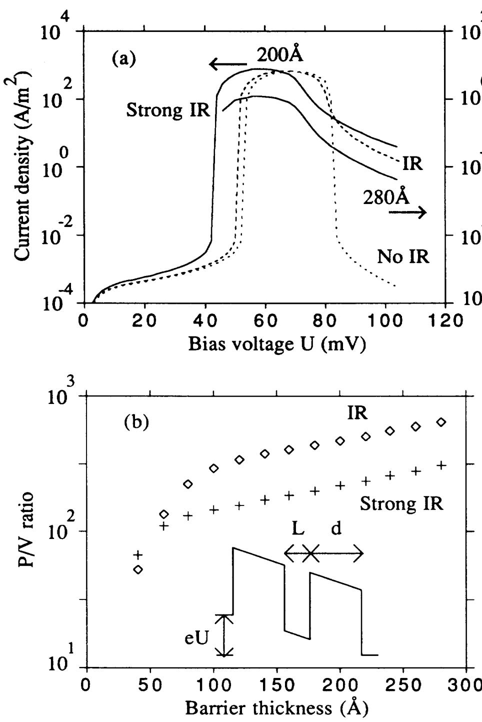


FIG. 2. (a) The current-voltage characteristics. The short-dashed curve shows the current through a double-barrier structure with barriers that are 120 meV high and 200 Å thick when there is no interface roughness (IR). The well is 70 Å wide and the contact Fermi energy is 15 meV. The long-dashed curve was calculated with IR with islands of barrier material of area $A_i = 4\times10^4$ Å$^2$, height 5 Å, and areal density $n_i = 1\times10^{-5}$ Å$^{-2}$. When calculating the solid curves $n_i$ was increased to $2\times10^{-5}$ Å$^{-2}$ and the roughness islands were assumed to consist of material from a 240-meV barrier. The lower of these curves corresponds to 280-Å-thick barriers. (b) The peak-to-valley ratio as a function of varying barrier thickness for the two sets of roughness parameter values. We have taken $j$(105 meV) as the valley current. Inset: Schematic illustration of the double-barrier structure.

not change significantly when scattering is included in the model. Still the tunneling electrons undergo many scattering events. This corroborates the statement that coherent and sequential tunneling give essentially the same *peak* current, unless, of course, the energy distribution of the incoming electrons is more narrow than the broadened resonance.[18,19]

The valley current, on the other hand, increases by several orders of magnitude in the presence of scattering. The strong interface roughness parameter values have been chosen in an attempt to approximately account for alloy disorder near the interfaces, scattering at more than one interface, etc. The current-voltage curves corresponding to these parameter values resemble the experimental curves reasonably well. Notice that changing the barrier thickness from 200 to 280 Å basically leaves the shape of the current-voltage curve unchanged. The same thing is seen in the experiment.

In Fig. 2(b) the $P/V$ ratio crosses over from a rapid exponential increase up to $\approx 100$ Å to a much slower increase for thicker barriers.[20] This is in good qualitative agreement with the experiment.[3] The basic physics behind the crossover is the change, from a situation where an electron is scattered just once, or a few times, to a multiple-scattering situation. Quantitatively the experiment gave a maximum $P/V$ ratio of $\approx 20$. In view of the present calculation it seems difficult to explain such a small $P/V$ ratio as the result of interface-roughness scattering alone.

We should mention that the transfer Hamiltonian formalism does not describe tunneling just below the barrier tops well. One loses a "field emission" contribution to the valley current, so the $P/V$ ratios in Fig. 2(b) for barriers thinner than 100 Å are actually too large. For thicker barriers, however, $j$(105 meV) should be a reliable estimate of the valley current.

We have investigated some other mechanisms that we believe can be ruled out as the cause of the large valley current in this particular case: (i) Emission of LO phonons: The DBS enters the field-emission regime before the phonon emission sideband of the transmission probability reaches the Fermi energy of the emitter, so this effect does not play any role here. In situations where the phonon sideband can assist tunneling, on the other hand, this mechanism is in general stronger than roughness scattering.[5,13,21] (ii) Fluctuating barrier thickness: This is another effect of interface roughness. It is important for tunneling through metal oxides.[22] Here we find that the thinner parts of the upstream barrier could cause the $P/V$ ratio to decrease by $\approx 10\%$ but not more. (iii) Weak localization: This causes strong scattering from $\mathbf{q}_\parallel$ to $-\mathbf{q}_\parallel$,[9] but it does not help to bring any electrons into resonance. It should therefore not change the valley current much.

In conclusion, we have presented a calculation of the effects of interface-roughness scattering on the tunnel current through a GaAs-$Al_xGa_{1-x}As$ double-barrier structure. We have treated this scattering nonperturbatively by using the coherent-potential approximation. Our results are in agreement with experimental observations on a number of points: The peak current in the presence of scattering is basically the same as the one calculated without scattering. The scattering increases the valley current through a DBS with thick barriers by several orders of magnitude. Finally, the peak-to-valley ratio as a function of barrier thickness grows only slowly for barriers thicker than 100 Å.

I have benefited from discussions with Jean-Pol Vigneron, Amand Lucas, Göran Wendin, and Peter Apell. This work was supported by the Belgian Program on Interuniversity Attraction Poles initiated by the Belgian State–Prime Minister's Office–Science Policy Programming.

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