Effects of barrier phonons on the tunneling current in a double-barrier structure

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The effects of AlAs acoustical and optical phonons on the tunneling current in an ideal GaAs-AlAs-GaAs-AlAs-GaAs structure are discussed. The transfer Hamiltonian method was extended to inelastic tunneling current in a double-barrier structure. It is found that the current off resonance in the Tsu-Esaki model could be enhanced by orders of magnitude by inelastic tunneling due to the coupling of electrons to barrier optical phonons. The contribution to the current due to the deformation-potential coupling of electrons to barrier acoustical phonons is found to be much less important.

Semiconductor heterostructures involving GaAs and AlAs have been the subject of both theoretical and experimental studies.[1-8] In GaAs-AlAs-GaAs-AlAs-GaAs structures, AlAs layers act as energy barriers while the middle GaAs layer acts as a well. Of particular interest are GaAs-AlAs-GaAs-AlAs-GaAs double-barrier structures which are specifically doped as *n-i-i-i-n*. Observations of resonant tunneling of electrons through double-barrier structures have been reported.[1] Tsu and Esaki[2] have theoretically treated the general case of electronic tunneling through multiple barriers. In the double-barrier case, resonant tunneling was shown by them to give rise to a current maximum (J_{peak}) at the voltage bias (V_a) where the Fermi sea of an electrode is aligned in energy with one of the quasibound states in the GaAs well. The current drops very rapidly at other voltages. Subsequent works have refined the theory for calculating the barrier transmission (T) and current-voltage (J-V_a) characteristics.[3-6] Typically, the peak current they calculated agrees with the measured value. However, the measured valley current is greater than the theoretical value by at least 1 order of magnitude. Recently, Frensley has employed a transport theory approach which includes losses.[7] However, all of these theories only consider elastic tunneling. On the other hand, Tsu and Dohler[8] have considered inelastic tunneling assisted by the well phonons. In a recent study of GaAs-AlAs-GaAs structures, Collins, Lambe, and McGill[9] reported the observation of inelastic tunneling of electrons. In such tunneling, the excitation of AlAs phonons could take away finite amount of energy and momentum from the tunneling electron. Hence, the total energy and the transverse momentum of the tunneling electron are no longer conserved. As we shall show, they could enhance the current off resonance by orders of magnitude in the Tsu-Esaki model. This suggests the importance of the inclusion of inelastic tunneling assisted by barrier phonons in calculations such as the self-consistent analysis of Onishi *et al.*[6]

Here, we present the first theoretical study of the effects on the tunneling current in a double-barrier structure due to the electron interaction with barrier phonons. The transfer Hamiltonian method proposed by Bardeen[10] originally for the treatment of the tunneling of electrons through a single-barrier structure is extended to calculate phonon-induced inelastic tunneling in a double-barrier structure. For illustration, we shall consider the zero temperature case where only phonon emission is possible. In this case with proper approximations, we obtain analytical expressions which shed some light on the important effects of inelastic tunneling. These effects change *I-V* characteristics for a double-barrier structure.

We treat a standard double barrier structure consisting of a layer of GaAs followed by a barrier of $Ga_{1-x}Al_xAs$ followed by a well of GaAs followed by a second barrier of $Ga_{1-x}Al_xAs$ followed by the contact layer of GaAs. The interfaces between the layers are at x_1, x_2, x_3, and x_4, respectively. The barrier height (the conduction-band offset) is taken to be 55% of $E_g^{\text{AlAs}}-E_g^{\text{GaAs}}$, the band-gap difference.[11] The cross-section area is A. Each electrode has the thickness L. The effective mass of the electron is taken to be m^* whether in GaAs or AlAs. The left barrier and the right barrier are taken to be equally thick: $d_1=d_2=d$. w is the width of the well. The voltage bias V_a is such that the lowest quasibound level E_1 is lower in energy than the conduction-band edge of the left electrode.

We use the transfer Hamiltonian method proposed by Bardeen[10] and extend the method to treat the inelastic tunneling of an electron through the excitation of an AlAs phonon. We choose the states ψ_r and ψ_l so that ψ_r is matched to the correct solution for $x\geq x_2$ but decays in the region $x\leq x_1$ instead of satisfying the wave equation, and, similarly, ψ_l continues to decay for $x\geq x_2$. Then ψ_r is a correct solution for the Hamiltonian H for $x\geq x_1$ and ψ_l is correct for $x\leq x_2$. With WKB approximation, we have

$$\begin{aligned}\psi_l(x)&=\left[\frac{2}{AL}\right]^{1/2}e^{ik_\parallel x_\parallel}\sin(k_lx+\gamma_l),\quad x\leq x_1\\ \psi_l(x)&=\left[\frac{k_l}{\kappa_l}\right]^{1/2}\frac{e^{ik_\parallel x_\parallel}e^{-\kappa_l(x-x_1)}}{\sqrt{2AL}}\\ &=\frac{e^{ik_\parallel x_\parallel}}{\sqrt{AL}}\chi_l(x),\quad x\geq x_1\end{aligned}\tag{1}$$

where k_l is the wave vector of the electron in the left electrode, $i\kappa_l$ is the imaginary wave vector in the left barrier, and $\chi_l(x)$ is defined in the equation. Similarly,

$$\psi_r(x)=\left[\frac{2}{AL}\right]^{1/2} e^{ik_\parallel x_\parallel}\sin(k_r x+\gamma_r), \quad x\ge x_4$$

$$\psi_r(x)=\left[\frac{2}{AL}\right]^{1/2}\left[\frac{k_r}{\kappa_r}\right]^{1/2}\frac{e^{ik_\parallel x_\parallel}e^{-\kappa_r(x-x_1)}}{\{[\sin(k_w w)]^2 e^{-2\kappa_2 d_2}+[4\cos(k_w w)]^2 e^{2\kappa_2 d_2}\}^{1/2}} \tag{2}$$

$$=\left[\frac{1}{AL}\right]^{1/2} e^{ik_\parallel x_\parallel}\chi_r, \quad x\le x_2$$

where k_r is the wave vector in the right electrode, $i\kappa_r$ is the imaginary wave vector in the left barrier, k_w is the wave vector in the well, $i\kappa_2$ is the imaginary wave vector in the right barrier, and $\chi_r(x)$ is defined in the equation. The electron-phonon coupling in the left AlAs barrier gives arise to the interaction Hamiltonian

$$H^a_{\text{e-ph}}=iD_\Gamma\left[\frac{\hbar q}{2\rho v_s V_{\text{AlAs}}}\right](a^\dagger_{q\lambda}e^{i\mathbf{q}\cdot\mathbf{r}}+a_{q\lambda}e^{-i\mathbf{q}\cdot\mathbf{r}}) \tag{3}$$

for the deformation-potential (DP) coupling due to the longitudinal-acoustic (LA) phonon mode $\mathbf{q}\lambda$, where $\mathbf{q}$ is the phonon wave vector and λ specifies the polarization.[12] Here, D_Γ is the deformation potential for Γ-valley electrons, ρ is the density, v_s is the sound velocity in AlAs, and V_{AlAs} is the volume of the left barrier. On the other hand,

$$H^o_{\text{e-ph}}=\frac{4\pi i}{q}\left[\frac{\hbar\omega}{8\pi V_{\text{AlAs}}}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right]\right]^{1/2} \times(a^\dagger_{q\lambda}e^{-i\mathbf{q}\cdot\mathbf{r}}-a_{q\lambda}e^{i\mathbf{q}\cdot\mathbf{r}}) \tag{4}$$

for the polar-optical (PO) coupling due to the longitudinal-optical (LO) phonon mode $\mathbf{q}\lambda$.[12] ϵ_0 and ϵ_∞ are the dielectric constants at zero and optical frequencies, respectively. Other kinds of electron-phonon coupling, piezoelectric coupling for example, are much weaker and much less important.[12] They are not considered here. The transition rate can be calculated easily by the application of Fermi's golden rule. The temperature is taken to be zero to simplify our analysis; hence, only phonon emission needs to be considered. The inelastic tunneling current is

$$J_{\text{inel}}=\frac{4\pi e}{\hbar}\sum_{\mathbf{q},\lambda}\sum_{\mathbf{k}}\sum_{\mathbf{k},l}|M|^2 f(\varepsilon_k) \times[1-f(\varepsilon_{k'})]\delta(\varepsilon_k+eV_a-\varepsilon_{k'}-\hbar\omega)\ , \tag{5}$$

where $\hbar\omega$ is the phonon energy, ε_k and $\varepsilon_{k'}$ are the kinetic energies of the electrons in the left and right electrode, respectively, and M is the matrix element. Here, $\mathbf{k}$ and $\mathbf{k}'$ are wave vectors of the electron at left and right electrodes, respectively, and $f(\varepsilon)$ is the Fermi distribution function. The general expression for J_{inel} at a finite temperature may be derived with the use of many-body theory. Bennett *et al.*[12] have given the derivation of the formula for the single-barrier case. We do not attempt to treat finite temperature case, however. Replacing $\sum$ with $\int$, we have

$$J_{\text{inel}}=\frac{4\pi e}{\hbar}A\sum_\lambda\int d^3q\frac{1}{(2\pi)^3}|U_q|^2\int d^3k\frac{1}{(2\pi)^3}\int d^3k'\frac{1}{(2\pi)^3}|T(q_\perp;k_\perp,k'_\perp)|^2 f(\varepsilon_k)[1-f(\varepsilon_{k'})] \times\delta(\mathbf{k}_\parallel-\mathbf{k}'_\parallel-\mathbf{q}_\parallel)(2\pi)^2\delta(\varepsilon_k+eV_\alpha-\varepsilon_{k'}-\hbar\omega)\ . \tag{6}$$

Here, we have

$$U_q=4\pi e[\hbar\omega(1/\epsilon_0-1/\epsilon_\infty)/8\pi]^{1/2}/q \tag{7}$$

for PO coupling, and

$$U_q=D_\Gamma(\hbar q/2\rho v_s)^{1/2} \tag{8}$$

for DP coupling. T is the overlap integral

$$T(q_\perp;k_\perp,k'_\perp)=\int_{x_1}^{x_2}e^{iq_\perp x}\chi_l^*\chi_r dx\ . \tag{9}$$

Suppose now the electron is scattered into the quasibound level, then ψ_r in the left barrier would be enhanced by the exponential factor $e^{\kappa_2 d_2}$. This can be verified by setting $\cos(k_w w)$ to zero in Eq. (2) when near resonance. This would in turn increase T by the same factor. Therefore, the contribution to the inelastic current due to such a process would be dominant. It turns out that for PO coupling, we have

$$J_{\text{inel}}\ge\frac{2Aem^{*2}d_1^2}{(2\pi)^3\hbar^5\kappa_0^2}e^{-2\kappa_0 d_1}e^{E_1/V_b}\frac{E_1}{2} \times\frac{2}{\pi}e^2\hbar\omega\frac{k_F^4}{q_0}(1/\epsilon_0-1/\epsilon_\infty)\tan^{-1}(1/q_0 d_1)\ , \tag{10}$$

For DP coupling, we have

$$J_{\text{inel}}\ge\frac{2Aem^{*2}d_1^2}{(2\pi)^3\hbar^5 k_0^2}e^{-2\kappa_0 d_1 e^{E_1/V_b}}\frac{E_1}{2}\frac{\pi k_F^4}{2\pi^2}\frac{D_\Gamma^2\hbar}{2\rho v_s} \times\{d_1^{-1}(d_1^{-2}+q_0^2)^{1/2}+q_0^2\sinh^{-1}[(q_0 d_1)^{-1}]\}\ . \tag{11}$$

Here, E_b is the zero-bias barrier height, $\kappa_0 = (2m^* E_b/\hbar^2)^{1/2}$, $V_b = 2E_b/\kappa_0 d_1$, and q_0 satisfies $\hbar^2 q_0^2/2m^* = eV_a/2 - \hbar\omega - E_1$.

We now compare contributions to the current from the elastic and the inelastic process. We consider only the inelastic process induced by PO coupling or DP coupling. Inelastic processes induced by other couplings will further increase the inelastic current. Therefore, the inelastic current we consider here is a lower bound of the actual value. However, even without a complete knowledge of the inelastic current, we can still demonstrate the dramatic change in order of magnitude of the current which is due to the inelastic processes.

In Fig. 1, we plot the lower limit of $J_{\text{inel}}/J_{\text{el}}$, the ratio of inelastic current to elastic current, versus barrier thickness for biased symmetric structures with $w = 50$ Å, $E_f = 50$ meV, and $V_a = 0.4$ V. Both LO and LA phonon-induced effects are shown. For thin barrier cases where $d = 20$ Å, polar coupling induces an inelastic current comparable to the elastic current. As can be seen, deformation-potential coupling has much smaller effects than polar coupling. The reason is that the PO coupling is much stronger than the DP coupling. We may neglect the contribution from DP coupling in comparison to that from PO coupling. Effects of both coupling increase as the barrier becomes wider, due to the exponential enhancement in the right wave function ψ_r. For the thick barrier case where $d = 40$ Å, polar coupling even gives rise to an inelastic current which is a thousand times as large as the elastic one.

In Fig. 2, we plot the upper limit of the ratio of the resonant current, which occurs at $V_a = 0.3$ V, to the current at $V_a = 0.4$ V, which occurs off resonance, versus barrier thickness. The dotted line is obtained with Tsu-Esaki model,[12] which includes only elastic process. In that case, the ratio shown here is equal to the peak-to-valley ratio of the J-V curve. The solid line is obtained with inelastic tunneling included. The peak current is mostly due to the elastic tunneling, since, at resonance, the elastic current is much larger than the inelastic current. The current off resonance is largely due to the inelastic tunneling, since the inelastic current is much larger than the elastic current, as shown in Fig. 2. The ratios shown by the two curves are comparable for thin barrier cases. However, as the barrier becomes thicker, the solid curve only varies slowly, since both J_{peak} and $J_{\text{"valley"}}$ have same exponential dependence. For barrier thickness equal to 40 Å, magnitudes of the two ratios differ by 7 in the natural log scale. The theory with the inelastic process included predicts a much smaller value of ratio for thick barrier cases.

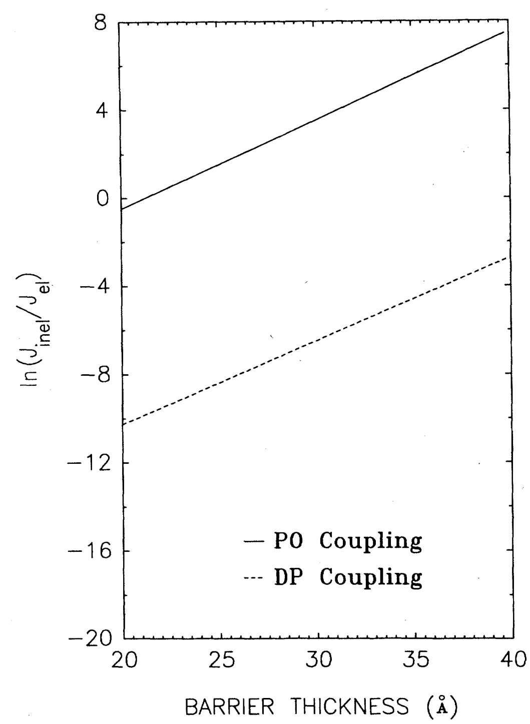

FIG. 1. The lower limit of $J_{\text{inel}}/J_{\text{el}}$; $E_1 \approx 150$ meV with respect to the conduction-band edge of the GaAs well.

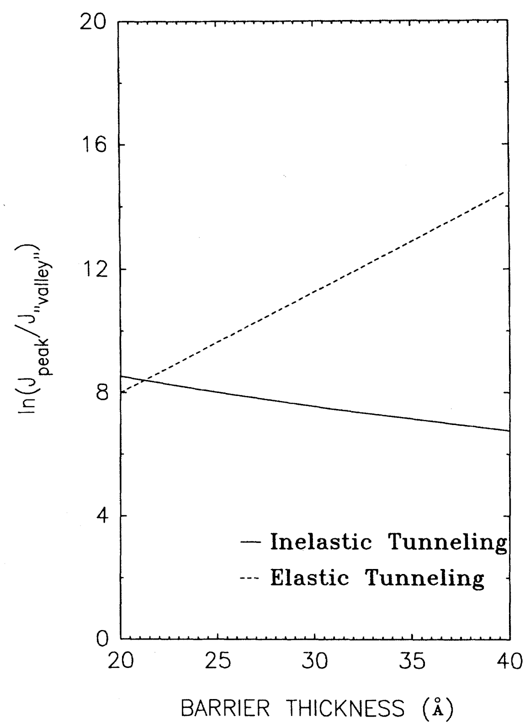

FIG. 2. The upper bound of $J_{\text{peak}}/J_{\text{"valley"}}$, the ratio of the peak current at $V_a = 0.3$ V (at resonance, the peak in the current-voltage curve) to the current at $V_a = 0.4$ V (off resonance, the valley in the case of elastic transport but not necessarily in the case with inelastic processes) vs barrier thickness with and without the inelastic part of the current included for biased symmetric structures with a well width of 50 Å, and $E_f = 50$ meV.

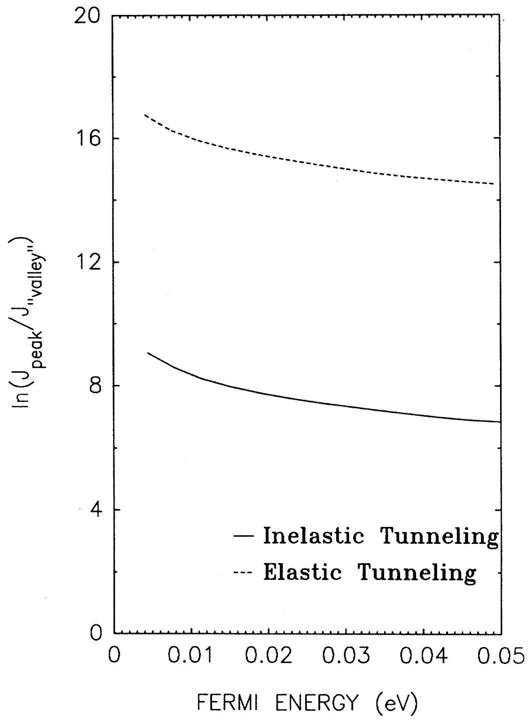

FIG. 3. The upper bound of $J_{\text{peak}}/J_{\text{``valley''}}$, the ratio of the peak current at $V_a=0.3$ V (at resonance, the peak in the current-voltage case) to the current at $V_a=0.4$ V (off resonance, the valley in the case of elastic transport but not necessarily in the case with inelastic processes) vs Fermi energy for the symmetric structure with a barrier thickness of 40 Å and a well width of 50 Å.

In Fig. 3, the upper bound of the ratio is shown versus Fermi energy for the symmetric structure with $d=40$ Å and $w=50$ Å. The solid curve includes contribution from the inelastic process and the dashed curve includes only contribution from the elastic process. The curves are shown for the region from $E_f=5$ meV to $E_f=50$ meV corresponding to dopant density from $10^{17}/\text{cm}^3$ to $10^{18}/\text{cm}^3$ currently used in the tunneling experiments. We see that both curves behave similarly as the Fermi energy changes. The difference between them is maintained through the Fermi energy range of interest. This shows the importance of the inelastic process for both low and high doping cases.

In summary, the inclusion of the inelastic tunneling in the theory for double-barrier structures is very important. We have studied specifically the inelastic tunneling induced by phonons. Two types of coupling have been considered. The PO coupling is much stronger than the deformation-potential coupling, and hence the current induced by PO coupling is much larger than that by DP coupling. Because of similar reasons, we expect the effect of piezoelectric (PE) coupling also to be negibile in comparison to that of PO coupling.

The electron-phonon interaction induces a channel through which the electron can tunnel much more readily than through the elastic channel. With the excitation of a barrier phonon, the electron can utilize the quasibound level to tunnel through the barrier. The *inelastic resonant tunneling* enhances the current off resonance by orders of magnitude. The effects are best reflected in the big difference between the magnitudes of current ratios which are predicted, with and without inclusion of electron-phonon coupling, in the simple model of Tsu and Esaki.[2] We expect the inclusion of inelastic processes to be important in any refined theory such as the self-consistent analysis of Ohnishi[5] or Frensley's transport approach.[7] Other mechanisms such as impurity scattering could also be critical to current transport in a double-barrier structure.

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