Effects of inelastic electron-phonon scattering on the resonant tunneling in double-barrier structure

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The Breit–Wigner formula is exploited to calculate the tunneling transmission probability affected by longitudinal optical phonon scattering in multiple quantum wells composed of $Ga_{1-x}Al_xAs$ compounds. A quantitative result shows that the resonance electron energy and the integrated total transmission probability through the potential barriers are not changed, while the transmission peak is reduced and the linewidth is broadened.

I. INTRODUCTION

The first theoretical description of multibarrier quantum-well tunneling was proposed by Tsu and Esaki.[1] In their approach, the applied electric field was assumed to appear only at interfaces, implying a flat band within the well, and no difference of effective mass existed between wells and barriers. An improvement of the theory had been attempted by Brennan *et al.*[2] based on effective mass approximation which constitutes a more realistic treatment of spatial dependence of effective mass and band edges, a recognition of the special dynamical role played by transverse energy as a consequence of the difference in itinerant two-dimensional carrier motion from layer to layer; and a direct numerical calculation of the wave function instead of using the plane waves or WKB approximation. Recently, Vassell and Lee[3] showed a theoretical result by implementing an exact solution of a one-electron Schrödinger equation. In their model, the external electric field was assumed to be constant throughout the multibarrier quantum-well structure. By using the transfer matrix method, the transmissivity of this structure was determined as functions of incident electron energies.

All of the above theoretical studies of electron tunneling in multibarrier quantum wells supposed that the incident electron energy was constant without considering the inelastic scattering during propagating sequences. This seems to be unrealistic for the multibarrier quantum-well structures where strong electron-phonon coupling is manifest.

The effect of inelastic scattering processes on resonant tunneling in one dimension had been considered by Stone *et al.*[4] To make the argument quantitatively, they employed a formalism analogous to that used to derive the Breit–Wigner formula as being familiar to nuclear physicists in the derivation of scattering cross section near resonance when several decay modes (elastic and inelastic) are presented.

Here, we intend to show the influence of the inelastic scattering process produced by polar optical phonons on the resonant tunneling of double-barrier quantum-well structures. We first calculate the transmission coefficient of resonant tunneling following the same approach Brennan *et al.* had exploited in conjunction with the Breit–Wigner scattering formula. The schematic diagram of the device employed in this work is shown in Fig. 1.

II. THEORY

Stone *et al.*[4] gave a detailed derivation of transmission coefficient for a symmetric scattering potential. When the elastic and inelastic modes are both presented, the total transmission coefficient near resonance can be written as

$$T = |t_e|^2 + |t_i|^2 = \frac{\frac{1}{4}\Gamma_e\Gamma}{(E-E_r)^2 + (\frac{1}{2}\Gamma)^2}, \quad (1)$$

where E is the electron's energy, E_r is the resonance energy, Γ_e is the elastic scattering width, and $\Gamma = \Gamma_e + \Gamma_i$ is the total scattering width with Γ_i being determined by the inelastic scattering potential. However, this result is inappropriate to the case of double-barrier quantum-well structures under biasing since the scattering potential is asymmetric. This can be clearly inspected by considering pure elastic scattering. On putting $\Gamma_i = 0$, from Eq. (1) we find that when the incident electron energy aligns with the resonant energy of the subbands in multiple quantum wells, the transmission coefficient is maximum and equal to unity. This is true only when the scattering potential is symmetric. Since the symmetry will be destroyed by bias, the probability of resonance tunneling may be much

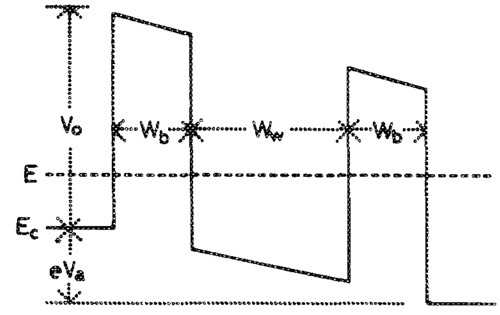

FIG. 1. Schematic diagram for the double-barrier quantum-well structure with potential barrier of V_0, barrier width of W_b, and well width of W_w at bias of V_a.

smaller than unity, especially at low incident electron energies. To amend this discrepancy, Eq. (1), which is employed in symmetric potential wells, is modified by introducing a prefactor $T_{\max}$, and consequently

$$T=T_{\max}\frac{\frac{1}{4}\Gamma_e\Gamma}{(E-E_r)^2+(\frac{1}{2}\Gamma)^2}, \tag{2}$$

where $T_{\max}$ is the resonance peak for asymmetric wells when the incident energy is equal to E_r for elastic mode only.

When the double-barrier structure is under bias, $T_{\max}$, Γ_e, and E_r can be determined by the Airy function approximation. For the potential structure as shown in Fig. 1, the Schrödinger equation in the direction normal to the surface is

$$-\frac{\hbar^2}{2}\frac{\delta}{\delta x}\frac{1}{m^*(x)}\frac{\delta}{\delta x}\phi(x)+V(x)\phi(x)=E_x\phi(x) \tag{3}$$

where $m^*(x)$ is the effective mass which varies through wells and barriers. It seems reasonable to assume that the potential is linearly graded in the structure such that

$$\begin{aligned} V(x)&=V_0-eV_a x/L \text{ in barrier regions}\\ &=-eV_a x/L \text{ in well regions,}\end{aligned} \tag{4}$$

where V_0 is the barrier height, V_a is the applied bias, and L is the total width of the barriers and wells. With a change of variables, Eq. (3) becomes

$$\frac{\delta^2}{\delta\xi^2}\phi(\xi)+\xi\phi(\xi)=0, \tag{5}$$

where

$$\xi=(2m^*eV_a/L\hbar^2)^{1/3}(x-\eta)$$

and

$$\eta=(V_0-E_x)L/eV_a.$$

The solutions of Eq. (5) can be expressed by a linear combination of Airy functions and its complimentary functions, such as

$$\phi(\xi)=C_i^+A_i(-\xi)+C_i^-B_i(-\xi),\ \text{for } 0\leqslant x\leqslant L, \tag{6}$$

where

$$A_i(\xi)=\frac{1}{\pi}\int_0^\infty \cos(\xi\zeta+\zeta^3/3)d\zeta$$

and

$$B_i(\xi)=\frac{1}{\pi}\int_0^\infty [\exp(\xi\zeta-\zeta^3/3)+\sin(\xi\zeta+\zeta^3/3)]d\zeta.$$

This form of wave function is implemented in the barrier and well regions. On the outward ohmic contact faces the wave functions can be simply expressed as a linear combination of incident and reflected plane waves such as

$$\phi(x)=Ie^{ikx}+re^{-ikx},\quad x<0$$

$$=I'e^{-ik'x}+te^{ik'x},\quad x>L, \tag{7}$$

where $k=\sqrt{2m^*E_x/\hbar^2}$ and

$k'=\sqrt{2m^*(E_x+eV_a)/\hbar^2}$.

In applying the boundary conditions at each interface to obtain the transfer matrix, we have assumed that the effective mass in barrier and well regions is different. Accordingly,

$$\frac{1}{m_w^*}\frac{\delta}{\delta x}\phi_w(x)\bigg|_{x_0}=\frac{1}{m_b^*}\frac{\delta}{\delta x}\phi_b(x)\bigg|_{x_0}, \tag{8}$$

Here, we use m_w^* and m_b^* to denote the effective masses in the well and barrier region, respectively. Defining the two matrices,

$$S_w=\begin{bmatrix} A_i(-\xi) & B_i(-\xi)\\ \frac{1}{m_w^*}A_i'(-\xi) & \frac{1}{m_w^*}B_i'(-\xi)\end{bmatrix},$$

$$S_b=\begin{bmatrix} A_i(-\xi) & B_i(-\xi)\\ \frac{1}{m_b^*}A_i'(-\xi) & \frac{1}{m_b^*}B_i'(-\xi)\end{bmatrix}, \tag{9}$$

$$\begin{aligned}\begin{bmatrix} I\\ r\end{bmatrix}&=\begin{bmatrix} 1 & 1\\ \frac{ik}{m_w^*} & \frac{-ik}{m_w^*}\end{bmatrix}S_b[\xi(x=0)]S_b^{-1}[\xi(x=x_1)]\\ &\times S_w[\xi(x=x_1)]S_w^{-1}[\xi(x=x_2)]\\ &\times S_b[\xi(x=x_2)]S_b^{-1}[\xi(x=L)]\\ &\times\begin{bmatrix} 1 & 1\\ \frac{ik'}{m_w^*} & \frac{-ik'}{m_w^*}\end{bmatrix}\begin{bmatrix} t\\ I'\end{bmatrix}=\frac{1}{2}\begin{bmatrix} M_{11} & M_{12}\\ M_{21} & M_{22}\end{bmatrix}\begin{bmatrix} t\\ I'\end{bmatrix}.\end{aligned} \tag{10}$$

The total transmission coefficient is defined as the ratio of the transmitted flux to the incident flux as

$$T=(t^*t)k'/[(I^*I)k].$$

By using the result of Eq. (10) with $I'=0$, it becomes

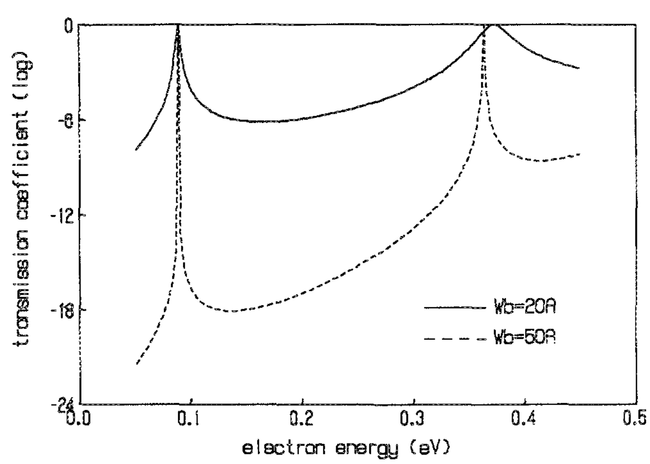

FIG. 2. Logarithm plot of elastic transmission coefficient vs incident electron energy for a double-barrier quantum-well structure.

TABLE I. The calculated first resonant energy E_r, elastic scattering width, and transmission peak at various barrier widths.

	$W_b = 20$ Å	$W_b = 50$ Å
E_{r1}	0.088 9 eV	0.0895 eV
Γ_{el}	0.002 62eV	0.6×10^{-5} eV
T_{max}	0.997 5	0.9931
E_{r2}	0.373 eV	0.363 eV
Γ_{e2}	0.373 eV	0.000 58 eV
T_{max}	0.999 7	0.9963

$$T = 4k'/k|M_{11}|^2. \tag{11}$$

This equation is the exact solution for transmission coefficient without involving any scattering process. With the inclusion of phonon scattering, Eq. (11) is a good approximation to evaluate T_{max} as shown in Eq. (2).

Before using Eq. (2) to derive the total transmission coefficient, we must first decide the magnitude of Γ_i. To include the effect of inelastic scattering, we had assumed that the scattering potential has an imaginary part, $\Gamma_i/2$. Since the materials composing the quantum wells are polar semiconductors, the inelastic scattering is mainly contributed by the interaction of electrons with optical phonons. In this work, we are interested in the scattering with incident electron energies being near the resonance. In this case, the transmission coefficient is large, and the localized nature of the electron wave function in the incident direction can be neglected. Since the electron wave function outside the double-barrier structure is assumed to be plane waves, we may simplify our problem by exploiting the 3D optical-phonon transition matrix, which implies[5]

$$|H_{\mathbf{k}\pm\mathbf{q},\mathbf{k}}| = \left(\frac{|e|N_u e_c}{\kappa_0 q}\right)\left(\frac{(N_q + \frac{1}{2} \mp \frac{1}{2})\hbar}{2M\omega}\right)^{1/2}, \tag{12}$$

where N_u is the number of lattice cell per unit volume, M is the reduced mass, e_c is the so-called Callen effective charge, and N_q is the Bose–Einstein distribution. The Einstein model is used to approximate the density of states of the optical phonon spectrum.[6] In Eq. (12) the positive and negative signs correspond to the phonon-absorption and -emission processes respectively. Thus, the inelastic scattering matrix is calculated by

$$\frac{\Gamma_i}{2} = \int_{q_l}^{q_u} |H_{\mathbf{k}+\mathbf{q},\mathbf{k}}| D(\mathbf{q}) d^3q + \int_{q'_l}^{q'_u} |H_{\mathbf{k}-\mathbf{q},\mathbf{k}}| D(\mathbf{q}) d^3q, \tag{13}$$

where $D(\mathbf{q})$ is the density of states and $d^3q = q^2 \sin\theta\, d\theta\, d\phi\, dq$. The upper and lower limits of the integration are decided by the laws of conservation of momentum and energy, and yield

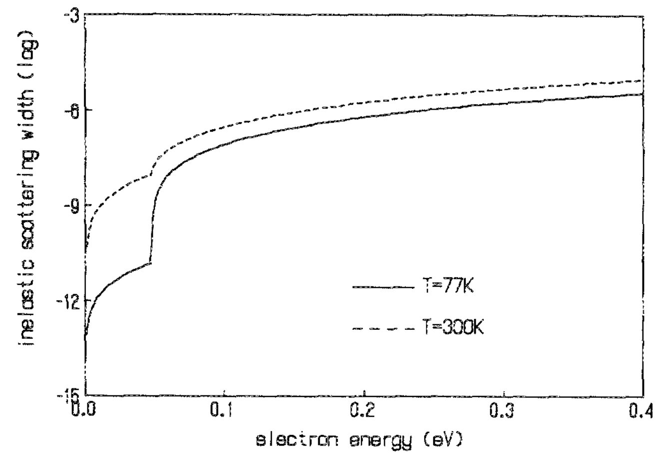

FIG. 3. Log plot of inelastic scattering with AlAs-type polar LO phonons in $Al_{0.5}Ga_{0.5}As$ material at various temperatures.

$$\frac{\Gamma_i}{2} = \frac{V}{4\pi^2}\left(\frac{|e|N_u e_c}{\kappa_0}\right)\left(\frac{N_q\hbar}{2M\omega}\right)\Big(\big([(a+1)k]^2 - [(a-1)k]^2 + e^{\hbar\omega/2k_BT}\{[(1+b)k]^2 - [(1-b)k]^2\}\big)\Big), \tag{14}$$

where k is the electron wave vector, $\hbar\omega$ is the optical phonon energy, and $a = \sqrt{1+\hbar\omega/E}$, $b = \mathrm{Re}(\sqrt{1-\hbar\omega/E})$. Γ_i, Γ_e, E_r, and T_{max} can be readily calculated by exploiting the Airy functions. When these values are substituted into Eq. (2), we can obtain the total transmission coefficient near resonance region. This result will be compared with the case obtained from the numerical simulation merely concerning elastic scattering.

III. DISCUSSION AND RESULTS

A series of calculations of transmission coefficient for a double-barrier quantum well between two ohmic contact regions will be illustrated. The material of the cover layers and the well region is GaAs, while that of the barrier layers is $Al_{0.5}Ga_{0.5}As$. The conduction-band offset, i.e., potential barrier height, is about 0.5 eV. The effective electron mass is 0.067 m_e and 0.1085 m_e for GaAs and $Al_{0.5}Ga_{0.5}As$, respectively.[7] In this simulation, the transmission coefficient for constant electron energy without suffering scattering is comparable with the results obtained by Vassell *et al.*[3] Figure 2 gives the results for the structures with a well width of 50 Å while the barrier widths are 50 and 20 Å, respectively, under a bias of 0.01 V. From these results, we can obtain the resonant energy E_r, the resonance peak T_{max}, and the resonance width Γ_e with the detailed data as shown in Table I. Obviously, the width of potential barrier and the magnitude of resonance energy vastly affect the magnitude of Γ_e.

Since the difference of relative displacement of positive and negative ions for the transverse mode is zero, only the longitudinal mode of polar optical phonon scattering is considered. The longitudinal polar optical phonon energy in GaAs is 36.25 meV. In ternary compound $Al_{0.5}Ga_{0.5}As$, there are two types of polar optical phonons with phonon

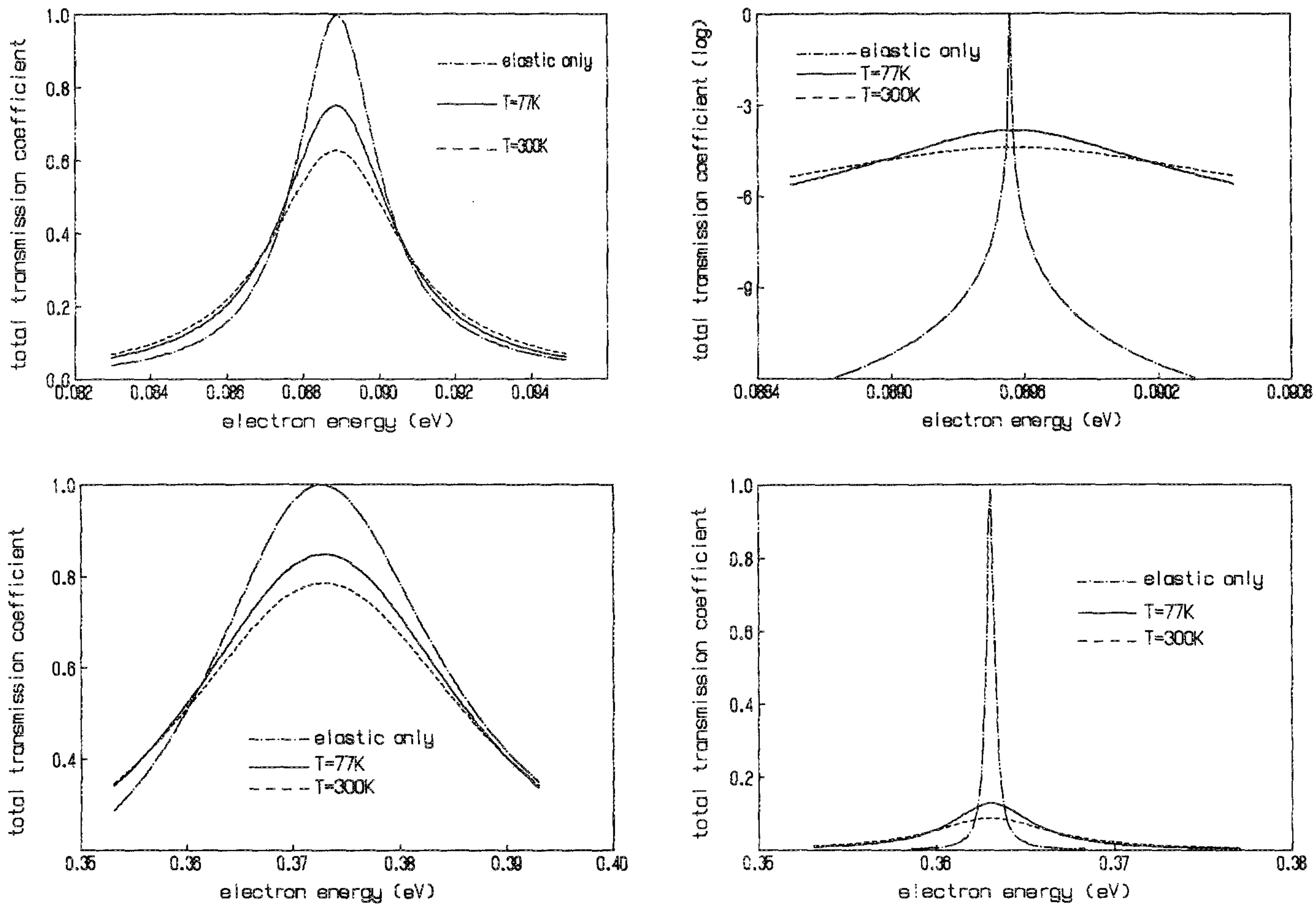

FIG. 4. A comparison of the elastic and total transmission coefficients for double-barrier quantum wells at temperatures of 77 and 300 K. The barrier height is 0.5 eV, well width is 50 Å, and bias is 0.01 V. (a),(b) are the results near the first and second resonance peaks for a barrier width of 20 Å. (c),(d) are the results for a barrier width of 50 Å.

energies being 33.42 and 48.19 meV for GaAs and AlAs-like phonons, respectively. From the experimental data of Goldman *et al.*,[8] we can expect that the AlAs-like polar optical phonon is the dominant factor that guides electron motion by inelastic scattering. The basic characteristics about this phonon spectrum can be obtained from Ref. 7. The inelastic scattering width for different electron energy at different temperature is shown in Fig. 3. The total transmission coefficient with various conditions of barrier and well widths at two specified temperatures are shown in Fig. 4 and arranged in Table II. These figures clearly show that inelastic scattering lowers the resonant peak and broadens the full width at half maximum. These phenomena significantly increase with the lattice temperature and especially when the barrier width is reduced. This is a result observed directly from Eq. (2). The inelastic scattering effect becomes observable when the inelastic scattering width is greater than or equal to the intrinsic (elastic) resonance ($\Gamma_i \geqslant \Gamma_e$).

TABLE II. The elastic and inelastic scattering width, at different barrier widths, renonant energy levels, and temperatures.

	Γ_e(meV)		Γ_i(meV)	
	$W_b = 20$ Å	$W_b = 50$ Å	$T = 77$ K	$T = 300$ K
$E_{r1} \cong 89$ meV	2.65	0.005	0.7	1.285
$E_{r2} \cong 368$ meV	27.35	0.55	2.785	4.285

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