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Phonon-assisted tunneling due to localized modes in double-barrier structures

P. J. Turley and S. W. Teitsworth
Department of Physics, Duke University, Durham, North Carolina 27706

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The excess current associated with phonon-assisted tunneling at low temperature in GaAs/AlAs double-barrier resonant-tunneling structures is calculated taking into account localized phonon modes. We find that symmetric interface phonon modes generate the most current in a typical structure, while confined modes in the GaAs well also contribute significantly. Antisymmetric interface modes and confined modes in AlAs barrier layers generate much less current. Numerical results are in unexpectedly close agreement with available experimental data.

GaAs/$Al_xGa_{1-x}As$ double-barrier resonant-tunneling (DBRT) structures have recently been the focus of intensive research, both for their interesting physical properties and their technological potential as a generation of high-speed electronic devices.[1-3] Although a range of theoretical methods successfully predict qualitative features of experimental current-voltage curves in these devices,[4-6] quantitative agreement between theory and experiment is still lacking. In particular, experimental DBRT structures possess an off-resonance "valley" current which is generally much larger than predicted.

This valley current is due to a number of causes, including Γ to X conversion in the barriers,[7,8] alloy and interface scattering,[9] and inelastic scattering by phonons.[10] For polar semiconductors such as GaAs and AlAs, electrons couple strongly to longitudinal-optical (LO) phonons, and in DBRT structures this coupling causes phonon-assisted tunneling which manifests itself in current-voltage characteristics as satellite peaks that appear for applied voltages above the main resonant-tunneling peaks.[11-13] Although calculations of the excess current due to phonon-assisted tunneling have been performed,[10,14,15] they generally use bulk phonon modes and do not take into account the localized nature of LO phonon modes.[16] In this paper, we calculate the current due to phonon-assisted tunneling in the presence of these localized modes for a DBRT structure consisting of a GaAs well sandwiched between two AlAs barriers.

For voltages above the resonant-tunneling peak a small portion of the emitter electronic wave function extends through the first AlAs barrier into the GaAs well region.[4] This wave function can therefore couple with the quasibound resonant state through emission of a LO phonon. Because the device is biased above resonance, the resonant state is lower in energy than the emitter conduction-band edge, so that every electron dropping into the resonant state tunnels through the collector barrier giving rise to current. This unidirectional process is shown in Fig. 1.

Using the effective-mass approximation and assuming that the potential varies in the z direction only, we write the initial and final electronic states associated with phonon emission as

$$\begin{aligned}\Psi_i(\mathbf{r})&=\frac{e^{i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel}}{\sqrt{A}}\varphi_i(z)\,,\\ \Psi_f(\mathbf{r})&=\frac{e^{i\mathbf{k}'_\parallel\cdot\mathbf{r}_\parallel}}{\sqrt{A}}\varphi_f(z)\,,\end{aligned}\tag{1}$$

where A is the cross-sectional area of the entire structure, and $\mathbf{r}_\parallel$ and $\mathbf{k}_\parallel$ are, respectively, the position and wave vector projected onto the plane of the interfaces. The energies of these states are given by

$$E_i=\frac{\hbar^2k_\parallel^2}{2m^*}+E_z$$

and

$$E_f=\frac{\hbar^2k_\parallel'^2}{2m^*}+E_{zf}\,,$$

where E_z is the electron energy in the z direction. The z dependent parts of the wave functions $\varphi_i(z)$ and $\varphi_f(z)$ are determined by a one-dimensional Schrödinger equation with effective potential $U(z)$ (shown in Fig. 1), and are normalizable with respect to the total length of the DBRT structure including the emitter and collector regions. For phonon-assisted tunneling processes, φ_i is taken as a plane-wave state impinging on the DBRT struc-

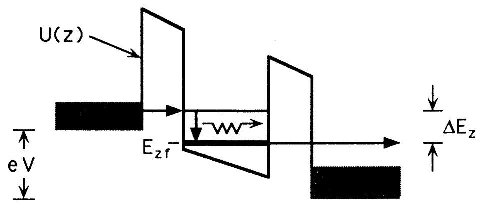

FIG. 1. Schematic illustration of the phonon-assisted tunneling process in a DBRT structure. $U(z)$ denotes the effective one-dimensional potential, E_{zf} is the energy of the quasibound resonant state, and ΔE_z is the electron-energy loss in the z direction. Shaded regions denote reservoirs of electrons in collector and emitter regions while arrows indicate movement of the tunneling electron.

ture from the left-hand (emitter) side, and φ_f is taken as the quasibound resonant state wave function with energy E_{zf}.

The scattering rate due to phonon emission is then given by Fermi's golden rule

$$W(i\rightarrow f)=\frac{2\pi}{\hbar}|\langle f|H_{e\text{-ph}}|i\rangle|^2\delta(E_i-E_f-\hbar\omega_0)\ , \qquad (2)$$

where the Hamiltonian $H_{e\text{-ph}}$ describes the interaction between electrons and the electrostatic potential set up by optical phonons in a polar semiconductor; $\hbar\omega_0$ denotes the LO phonon energy, ~36 meV for GaAs and ~50 meV for AlAs.[16] The *total* initial state $|i\rangle$ has one electron in state Ψ_i with no phonons, while the *total* final state consists of one electron in the state Ψ_f plus one emitted phonon.

While the exact form of the electron-phonon Hamiltonian $H_{e\text{-ph}}$ for localized phonon modes in GaAs/AlAs DBRT structures is not known, numerous models have been advanced.[18-22] The most widely accepted of these is the dielectric continuum model, which approximates the different semiconductor layers by uniform slabs of material with each slab assumed to have the dielectric properties of the same material in bulk.[16] Within the dielectric continuum picture two types of localized phonon modes that exist for DBRT structures: (1) *confined modes* which give rise to electrostatic potentials that are strictly localized in either a barrier or well layer and vanish at the interfaces, and (2) *interface modes* —also known as surface optical modes—which give rise to potentials that are largest at the interfaces and decay into the device layers.

The electron-phonon (Fröhlich) Hamiltonian for confined modes in a layer of thickness d can be written[16]

$$H_n^{\text{con}}=\sum_{\mathbf{q}_\parallel}\frac{\gamma}{\sqrt{Ad}}\frac{e^{i\mathbf{q}_\parallel\cdot\mathbf{r}_\parallel}}{[q_\parallel^2+(n\pi/d)^2]^{1/2}}\times\sin\left[\frac{n\pi}{d}z\right][a_n(\mathbf{q}_\parallel)+a_n^\dagger(-\mathbf{q}_\parallel)]\ , \qquad (3)$$

where z is measured from the right-hand side of the confining region and γ is a coupling constant (from Ref. 16 we estimate $\gamma^2=0.098$ eV^2 Å for GaAs layers and $\gamma^2=0.208$ eV^2 Å for AlAs layers). Here $\mathbf{q}_\parallel$ is the component of the phonon wave vector parallel to the interfaces, and $a_n^\dagger(\mathbf{q}_\parallel)$ and $a_n(\mathbf{q}_\parallel)$ are creation and annihilation operators for confined phonons; the mode number $n=1,2,3\ldots$, gives the number of phonon half-wavelengths which "fit" into the confining layer in the z direction.

Inserting the Hamiltonian into Eq. (2) and integrating over all final states which have z components of electron energy equal to the resonant value E_{zf} yields the phonon emission rate $W_{\text{con}}(\mathbf{k};n,V)$ which depends on the applied voltage V. The excess current density associated with phonon-assisted tunneling via a single confined mode with mode number n is then calculated using[4]

$$J_n^{\text{con}}=\frac{1}{A}\int eW_{\text{con}}(\mathbf{k};n,V)g_e(\mathbf{k})f_e(E(\mathbf{k}))d\mathbf{k}\ , \qquad (4)$$

where $f_e(E(\mathbf{k}))$ is the Fermi distribution of electrons in the emitter and $g_e(\mathbf{k})=2[AL_e/(2\pi)^3]$ is the density of electron states in the emitter (L_e is the emitter length).

We have found that the emission rate $W_{\text{con}}(\mathbf{k};n,V)$ has a strong dependence on k_z, but only weakly depends on $\mathbf{k}_\parallel$ above a threshold value determined by energy conservation considerations. Thus, we can approximate the dependence on $\mathbf{k}_\parallel$ by a step function, i.e., $W_{\text{con}}(\mathbf{k};n,V)=0$ below threshold, and $W_{\text{con}}(\mathbf{k};n,V)=W_{\text{con}}(E_z;n,V)$ above threshold. Equation (4) is then easily integrated over $\mathbf{k}_\parallel$ to yield,

$$J_n^{\text{con}}=\frac{emk_BTL_e}{2\pi^2\hbar^3}\int_0^\infty\frac{W_{\text{con}}(E_z;n,V)}{v_z}\ln\{1+\exp[(E_F-E_z-E_{\min})/k_BT]\}dE_z\ , \qquad (5)$$

where $v_z=(2E_z/m^*)^{1/2}$, E_F is the electron Fermi level in the emitter, and $E_{\min}=\hbar\omega_0-\Delta E_z$ for $\Delta E_z<\hbar\omega_0$ while $E_{\min}=0$ for $\Delta E_z>\hbar\omega_0$ (here $\Delta E_z=E_z-E_{zf}$ is the electron-energy loss in the z direction). Equation (5) is analogous to the Tsu-Esaki formula[1] for the current due to standard resonant tunneling.

To calculate the phonon-assisted tunneling current due to *interface modes* we note that, within the dielectric continuum model, there are eight sets of distinct interface modes for a double barrier structure. In the long-wavelength limit (i.e., $q_\parallel d\ll 1$, where d is the width of the well layer), four of these modes behave like bulk transverse-optical (TO) phonon modes and only weakly couple to the electrons. The remaining four interface modes behave like bulk LO phonons and can therefore couple strongly to electrons; these consist of two sets of antisymmetric modes and two sets of symmetric modes. One set of symmetric modes are localized around the inner heterointerfaces (i.e., the two barrier-well interfaces) and have the energy of bulk AlAs LO phonons. The other set of symmetric modes are concentrated about the outer interfaces (i.e., the emitter-barrier and barrier-collector layers) and have bulk GaAs LO phonon energies.[23]

The electron-phonon Hamiltonian for the *inner* symmetric interface phonons can be approximated as[16]

$$H_{\text{sym}}=\sum_{\mathbf{q}_\parallel}\left[\frac{\hbar\omega_s e^2\beta}{2\epsilon_0 A}\right]^{1/2}\frac{e^{i\mathbf{q}_\parallel\cdot\mathbf{r}_\parallel}}{\sqrt{2q_\parallel}}f_s(q_\parallel,z)\times[b(\mathbf{q}_\parallel)+b^\dagger(-\mathbf{q}_\parallel)]\ , \qquad (6)$$

where $b(\mathbf{q}_\parallel)$ and $b^\dagger(\mathbf{q}_\parallel)$ are creation and annihilation operators for symmetric interface phonons, $\hbar\omega_s$ is the energy per phonon ~ 50.1 meV, and we estimate $\beta = 0.335$ from Ref. 16. The function $f_s(q_\parallel, z)$ is proportional to the electrostatic potential generated by these phonons and, when z is measured from the center of the GaAs well, is given by[16]

$$f_s(q_\parallel, z) = \begin{cases} e^{q_\parallel(z+d/2)}, & z \le -d/2 \\ \cosh(q_\parallel z)/\cosh(q_\parallel d/2), & |z| \le d/2 \\ e^{-q_\parallel(z-d/2)}, & z \ge d/2. \end{cases} \quad (7)$$

Note that $f_s(q_\parallel, z)$ is spatially symmetric with respect to the GaAs well center at $z = 0$, and achieves a maximum value of 1 at the inner heterointerfaces interfaces (i.e., $z = \pm d/2$) while decaying exponentially into the device layers with characteristic length $1/q_\parallel$.

This Hamiltonian is inserted into Eq. (2) and summed over final states to obtain the symmetric interface phonon emission rate and the current is calculated using a formula similar to Eq. (5). The current due to antisymmetric interface modes is calculated in a completely analogous manner.

Numerical results were obtained for a DBRT structure with a 60-Å GaAs well sandwiched between two 30-Å AlAs barriers, and an emitter Fermi level of $E_F = 20$ meV. Dielectric and electronic properties of AlAs and GaAs used in the calculations were taken from Refs. 4 and 16, and the wave functions $\varphi_i(z)$ and $\varphi_f(z)$ were numerically calculated by a standard transfer-matrix method.[4,17]

Plots of the phonon emission rate *W per electron* are shown in Fig. 2. To obtain these rates, the initial electronic state has been normalized so that there is precisely one electron in the DBRT structure. Curve 1 shows the emission rate (averaged over $\mathbf{k}_\parallel$) for the $n = 1$ confined mode of the GaAs well as a function of ΔE_z for fixed applied voltage $V = 210$ mV. As expected, W peaks at 36 meV, the energy of confined phonons in the GaAs well. At this energy the electron-energy loss is entirely in the z direction, and the emitted phonon has vanishing $q_\parallel$. For $\Delta E_z > 36$ meV the electron gains energy in the parallel direction, and for $\Delta E_z < 36$ meV the electron loses energy in the parallel direction. Curve 2 plots the emission rate W vs ΔE_z for the symmetric interface mode at the same applied voltage. In this case, the emission rate peaks very sharply at 50.1 meV, the energy of AlAs LO phonons. The sharpness of the peak in curve 2 is due to the divergence of the interface Hamiltonian Eq. (6) as $q_\parallel \to 0$.[24] Although the symmetric interface mode has AlAs phonon energies, it is *not* spatially localized in the barrier region.

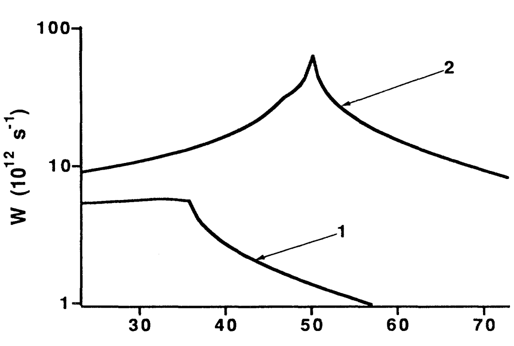

FIG. 2. Curve 1: the phonon emission rate W for the $n = 1$ confined mode in the GaAs well as a function of ΔE_z and fixed voltage $V = 210$ mV for an AlAs/GaAs/AlAs structure with 30-Å barriers and a 60-Å well. Curve 2: Emission rate for the inner symmetric interface modes with $V = 210$ mV.

Numerical calculations of the current density J versus applied voltage V using Eq. (5) and temperature $T = 4$ K are shown in Fig. 3. The largest contribution to the phonon-assisted tunneling peak comes from the symmetric interface modes. This occurs because the symmetric interface modes extend over the entire structure and the resulting matrix element integral implicit in Eq. (2) is large. The antisymmetric modes also extend over the entire structure, but since electronic states are both roughly symmetric with respect to the GaAs well center,[4] this mode will not couple them strongly. The current due to confined well modes is somewhat smaller than the symmetric mode current, but much larger than the confined barrier mode currents. This occurs because the resonant state electronic wave function is much larger in the well region and thus the matrix element integral is much larger for the well than for the barrier.[4]

The characteristic widths of the resonant and phonon-assisted current peaks in Fig. 3 are essentially determined by the emitter Fermi level E_F, and for larger E_F values the peaks will blend together. Conversely, the effective emitter Fermi level should be made as small as possible in order to achieve maximum resolution of satellite peaks caused by distinct phonon modes. We have found that other DBRT structures give qualitatively similar results to Fig. 3 with the current contribution of confined well

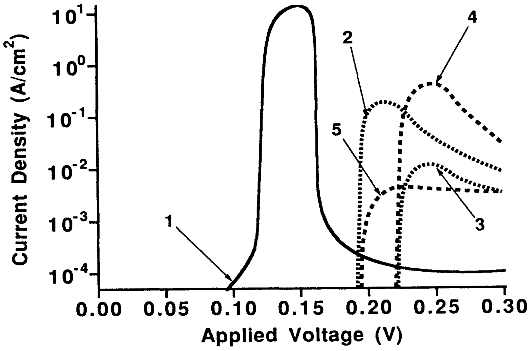

FIG. 3. Resonant and phonon-assisted tunneling currents in an AlAs/GaAs/AlAs structure with a 60-Å well and 30-Å barriers. Curve 1 is the resonant-tunneling current, and curves 2–5 are the phonon-assisted tunneling currents due to (2) the $n = 1$ confined modes in the GaAs well, (3) the $n = 1$ confined modes in the left-hand AlAs barrier, (4) the inner symmetric interface modes, and (5) the inner antisymmetric interface modes.

modes relative to symmetric interface modes *increasing* in wider structures, while symmetric interface modes are predicted to dominate electron-phonon interactions in narrower DBRT structures.

Most published data on phonon-assisted tunneling have been obtained for GaAs/$\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ DBRT devices with Al concentration $x<0.5$ rather than the case of pure AlAs barriers to which the above results most directly apply.[11,12] Using a generalization of the dielectric continuum model to binary-ternary alloy (i.e., GaAs/$\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$) heterostructures by Kim and Stroscio,[25] we have adjusted values of the γ and β coupling constants in our calculations to allow a closer comparison with recent experimental data of Leadbeater *et al.*[13] For their structure II ($x=0.4$ and 58-Å undoped GaAs well) we estimate a satellite peak height of 14.4 μA using no adjustable parameters, while they reported a measured peak height of approximately 10 μA. This close agreement should be compared with a previous calculation of phonon-assisted tunneling currents which used bulk GaAs LO phonon modes and in which predicted and experimental peak heights differed by a *factor* of ~ 250.[10] In order to correctly fit the voltage scale (or, equivalently, the satellite peak line shape), space-charge effects should be treated. Our model can be generalized in a straightforward manner to include such effects.

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[1] R. Tsu and L. Esaki, Appl. Phys. Lett. **22**, 562 (1973).

[2] T. C. L. G. Sollner, W. D. Goodhue, P. E. Tannenwald, C. D. Parker, and D. D. Peck, Appl. Phys. Lett. **43**, 588 (1983).

[3] F. Capasso, K. Mohammed, and A. Y. Cho, IEEE J. Quantum Electron. **QE-22**, 1853 (1986).

[4] P. J. Turley and S. W. Teitsworth, Phys. Rev. B **44**, 3199 (1991).

[5] M. C. Payne, J. Phys. C **19**, 1145 (1986).

[6] W. R. Frensley, Rev. Mod. Phys. **62**, 745 (1990).

[7] E. E. Mendez, W. I. Wang, E. Calleja, and C. E. T. Gonclaves da Silva, Appl. Phys. Lett. **50**, 1263 (1987).

[8] H. C. Lui, Superlatt. Microstruct. **7**, 35 (1990).

[9] D. D. Coon and H. C. Liu, Superlatt. Microstruct. **6**, 409 (1989).

[10] F. Chevoir and B. Vinter, Appl. Phys. Lett. **55**, 1859 (1989).

[11] V. J. Goldman, D. C. Tsui, and J. E. Cunningham, Phys. Rev. B **36**, 7635 (1987).

[12] M. L. Leadbeater, E. S. Alves, L. Eaves, M. Henini, O. H. Hughes, A. Celeste, J. C. Portal, G. Hill, and M. A. Pate, Phys. Rev. B **39**, 3438 (1989).

[13] M. L. Leadbeater, E. S. Alves, L. Eaves, M. Henini, O. H. Hughtes, F. W. Sheard, and G. A. Toombs, Semicond. Sci. Technol. **3**, 1060 (1988).

[14] N. S. Wingreen, K. W. Jacobsen, and J. W. Wilkins, Phys. Rev. Lett. **61**, 1396 (1988).

[15] M. Jonson, Phys. Rev. B **39**, 5924 (1989).

[16] N. Mori and T. Ando, Phys. Rev. B **40**, 6175 (1989).

[17] M. O. Vassell, Johnson Lee, and H. F. Lockwood, J. Appl. Phys. **54**, 5206 (1983).

[18] R. Fuchs and K. L. Kliewer, Phys. Rev. **140**, A2076 (1965).

[19] Michael A. Stroscio, K. W. Kim, Michael A. Littlejohn, and Hsuhung Chuang, Phys. Rev. B **42**, 1488 (1990).

[20] M. Babiker, J. Phys. C **19**, 683 (1986).

[21] B. K. Ridley, Phys. Rev. B **39**, 5282 (1989).

[22] K. Huang and B. Zhu, Phys. Rev. B **38**, 13 377 (1988).

[23] These *outer* symmetric modes are strongly suppressed by electron screening in the emitter and collector layers of the DBRT structures considered here. However, in structures with very low emitter and collector electron densities and narrow barrier layers these modes can produce significant phonon-assisted tunneling.

[24] This phonon emission rate is not truly divergent since polariton coupling of interface modes will occur for very small wave vectors $q_{\parallel}(<3000\ \mathrm{cm}^{-1})$. These polaritons have a negligible effect on the phonon-assisted tunneling current for the narrow DBRT structures considered here.

[25] K. W. Kim and M. A. Stroscio, J. Appl. Phys. **68**, 6289 (1990).