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LETTER TO THE EDITOR

Effects of finite well depth on polar optical phonon scattering rates in cylindrical quantum well wires

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Abstract. An investigation of the effects of a finite confining potential on the sub-band energies and electron–bulk-polar-optical-phonon scattering rates is presented within the effective-mass approximation for quasi-one-dimensional cylindrical quantum wires. Numerical results are given for the GaAs/AlGaAs system where a lowering of both the confined energies and electron–bulk-polar-optical-phonon scattering rates with respect to the widely used infinite-confining-potential approximation is found.

Since the prediction [1] that quasi-one-dimensional (1D) semiconductor systems could be of importance in high-speed-device applications, and their subsequent fabrication [2–5], there has been a great deal of interest in their transport properties. All of the major mechanisms that lead to electron energy relaxation—ionised impurity scattering [1, 6], acoustic phonon scattering [7] and polar optical phonon scattering [8–10] (the dominant mechanism in the technologically important III–V structures at high temperatures)—have been investigated theoretically. The various investigations start by assuming that the carriers are *totally* confined which then implies a corresponding sub-band energy. This is an oversimplification for the GaAs/AlGaAs system where a realistic potential well is needed for a complete description. Indeed, the inclusion of a finite well height was shown to be of importance in certain transport phenomena in the corresponding quasi-two-dimensional (2D) quantum well structure [11].

In this Letter we investigate the effect of a finite potential well on both the sub-band energies and the polar optical phonon scattering rates for cylindrical GaAs wires. Here we restrict attention to the interaction of electrons with bulk phonon modes, leaving the interaction with confined modes to be described in a later paper.

We begin with a description of the confined electron states. The system we have in mind is that proposed by Iafrate and co-workers [12] and is similar to the recently fabricated structures of Cibert and co-workers [4] in which the carriers are confined via a built-in local change in the crystal potential of the material. It consists of a cylindrical wire of length L_z (assumed large) and radius R composed of material 1 embedded in host material 2. The carriers are free to move along the axis of the cylinder (the z axis in cylindrical coordinates (ρ, φ, z)), whereas their motion in the radial direction is quan-

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tised. In the approximation of an infinite potential well (IPW) confining the carriers, the normalised effective-mass wavefunction is given by [2]

$$\psi(\rho, \varphi, z) = J_n(k_{n,l}\rho)\, e^{in\varphi} e^{ik_z z}/V_{1D}^{1/2} J_{n+1}(k_{n,l}R) \tag{1}$$

with corresponding energy

$$E = (\hbar^2/2m^*)(k_z^2 + k_{n,l}^2). \tag{2}$$

Here m^* is the electron effective mass, k_z the wavevector in the z direction, $k_{n,l}$ is related to the lth root of the Bessel function $J_n(k_{n,l}R)$ and V_{1D} is the volume of the wire. For applications to the $GaAs/Al_xGa_{1-x}As$ system this approximation is rather crude as has been remarked on for 2D quantum well systems. We now analyse the effect of a finite potential well (FPW), of depth V_0, on the 1D electron states.

The effective-mass wavefunction for the confined state that has the correct behaviour on the axis of the cylinder and at a radial distance greater than R is

$$\psi(\rho, \varphi, z) = \begin{cases} A_n J_n(k_1\rho)\, e^{in\varphi} e^{ik_z z} & \rho < R \\ B_n K_n(\kappa_2\rho)\, e^{in\varphi} e^{ik_z z} & \rho > R. \end{cases} \tag{3}$$

Here K_n is a modified Bessel function of the third kind and

$$k_1 = [(2m_1^*/\hbar^2)E - k_z^2]^{1/2} \tag{4}$$

$$\kappa_2 = [(2m_2^*/\hbar^2)(V_0 - E) + k_z^2]^{1/2} \tag{5}$$

with E the electron energy, and m_1^* (m_2^*) the electron effective mass in medium 1 (2). The normalisation factors A_n and B_n are given by

$$A_n = (K_n(\kappa_2 R)/V_{1D}^{1/2})(J_n^2(k_1R)K_{n+1}(\kappa_2 R)K_{n-1}(\kappa_2 R) - K_n^2(\kappa_2 R)J_{n+1}(k_1 R)J_{n-1}(k_1 R))^{-1/2} \tag{6}$$

$$B_n = (J_n(k_1R)/K_n(\kappa_2 R))\, A_n = a_n A_n. \tag{7}$$

We now apply the standard effective-mass boundary conditions [13] at $\rho = R$, which leads to the following transcendental equation satisfied by the electron energy:

$$J_n(k_1R)K_n'(\kappa_2 R) - (m_2^* k_1/m_1^* \kappa_2)J_n'(k_1R)K_n(\kappa_2 R) = 0. \tag{8}$$

Figure 1 compares the variation of the bound levels with wire radius using the IPW approximation (2), and those obtained from the solution of (8). The system considered is a GaAs wire surrounded by $Ga_{0.7}Al_{0.3}As$ for which the corresponding parameters are $V_0 = 190$ meV, $m_1^* = 5.73 \times 10^{-32}$ kg and $m_2^* = 1.4\, m_1^*$. Only the $n = 0$ levels are shown, and for convenience we take $k_z = 0$. It is seen that the IPW approximation overestimates the energy, and for a radius of 50 Å this discrepancy is in fact quite appreciable. This situation is similar to that found in studies of 2D quantum wells [11]. The effect of a FPW on the electron–polar-optical-phonon scattering rates will be considered shortly, but it is worth noting that although the lowest bound state corresponds to $n = 0$, the next bound level is an $n = 1$ state. This is analogous to the

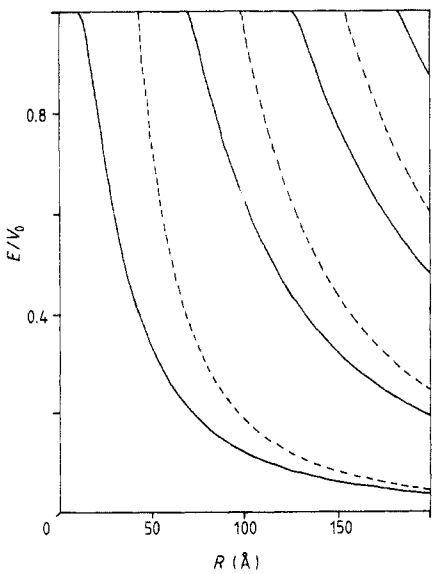

Figure 1. The variation in the $n = 0$ bound-state energies with the quantum wire radius. The broken curves correspond to the IPW approximation, whilst the full curves are derived from the finite-potential results (see the text for the assumed values of the parameters).

symmetric and antisymmetric states found in 2D systems [14]. In fact from (8) the value of R at which a confined level appears, for a given n ($\neq 0$), satisfies

$$nJ_n(yR)[1-(m_1^*/m_2^*)^{3/2}]-yRJ_{n-1}(yR)=0 \tag{9}$$

with

$$y=(2m_1^*V_0/\hbar^2)^{1/2}. \tag{10}$$

It so happens that the first $n = 1$ sub-band, obtained via equation (9), appears at a radius of 40 Å for the situation depicted in figure 1.

We are now in a position to discuss the main investigation of this Letter, namely the effect of the finite potential on the electron–polar-optical-phonon scattering rates. The Fröhlich interaction Hamiltonian describing an electron interacting with bulk-like polar optical phonons is

$$\hat{H}_{\text{int}}=\sum_q\left[\left(\frac{C}{q}\right)e^{iq\cdot r}a_q+\text{HC}\right]. \tag{11}$$

In the above, a_q is the annihilation operator for optical phonons of wavevector q and

$$C=i[(2\pi/V_c)e^2\hbar\omega(1/\varepsilon_\infty-1/\varepsilon_0)]^{1/2}. \tag{12}$$

Here V_c is the crystal volume, ω is the zone-centre polar optical phonon frequency (we ignore dispersion), and ε_∞ and ε_0 are the high-frequency and static dielectric constants of the medium. It is convenient to express the interaction Hamiltonian in cylindrical coordinates, and this is accomplished on noting that [15]

$$e^{\pm iq\cdot r}=e^{\pm i(q_z)z}\left(J_0(q_\perp\rho)+2\sum_j(\pm i)^jJ_j(q_\perp\rho)\cos(j\varphi)\right) \tag{13}$$

with $q_\perp$ the projection of the phonon wavevector on the x–y plane and q_z the wavevector

in the z direction. The probability of an electron making a transition from a state k_z to k_z' by emitting or absorbing a polar mode is given by Fermi's Golden Rule

$$W^{(e)}_{(a)}(k_z', k_z) = (2\pi/\hbar)\,|M^{(e)}_{(a)}|^2\,\delta(E(k_z') - E(k_z) \pm \hbar\omega) \tag{14}$$

where $E(k_z) = \hbar^2 k_z^2/2m_1^*$ and

$$M^{(e)}_{(a)} = \langle k_z', N(\omega) \pm 1|\hat{H}_{\text{int}}|k_z, N(\omega)\rangle. \tag{15}$$

In the above, $N(\omega)$ is the Bose–Einstein factor and e (a) denotes emission (absorption) of a mode. We now assume that only the lowest sub-band is populated—the so-called extreme quantum limit. This is often the most important regime for transport phenomena, although the theory may readily be extended to yield inter-sub-band scattering rates. The matrix elements may now be evaluated using the $n = 0$ wavefunction (3) and the transformed Hamiltonian, and hence the transition probabilities. The scattering rates are then obtained by integrating the transition probabilities over all final electron states. Here we simply quote the final results for the scattering rates. For emission we find

$$\frac{1}{\tau_e(E)} = \frac{2A_0'^4(N(\omega)+1)}{\tau_0(E/\hbar\omega - 1)^{1/2}}\,[I(q^+_{z,e}(E)) + I(q^-_{z,e}(E))] \tag{16}$$

with $A_0' = V_{1D}^{1/2}A_0$, and where τ_0^{-1} is a characteristic scattering rate given by

$$\tau_0^{-1} = (e^2/\hbar)(2m_1^*\,\omega/\hbar)^{1/2}(1/\varepsilon_\infty - 1/\varepsilon_0) \tag{17}$$

and the phonon wavevector is

$$q^\pm_{z,e}(E) = (2m_1^*\,\omega/\hbar)^{1/2}[(E/\hbar\omega)^{1/2} \pm (E/\hbar\omega - 1)^{1/2}] \tag{18}$$

where $+\,(-)$ designates forward (backward) scattering. For absorption the rate is similarly expressible as

$$\frac{1}{\tau_a(E)} = \frac{2A_0'^4 N(\omega)}{\tau_0(E/\hbar\omega + 1)^{1/2}}\,[I(q^+_{z,a}(E)) + I(q^-_{z,a}(E))] \tag{19}$$

and

$$q^\pm_{z,a}(E) = (2m_1^*\,\omega/\hbar)^{1/2}[-(E/\hbar\omega)^{1/2} \pm (E/\hbar\omega + 1)^{1/2}]. \tag{20}$$

The function $I(q_z)$ is the following integral:

$$I(q_z) = \int_0^\infty \frac{q_\perp |F_1(q_\perp) + a_0^2 F_2(q_\perp)|^2}{q_\perp^2 + q_z^2}\,\mathrm{d}q_\perp \tag{21}$$

and

$$F_1(q_\perp) = \int_0^1 xJ_0^2(k_1 Rx)J_0(q_\perp Rx)\,\mathrm{d}x \tag{22}$$

$$F_2(q_\perp) = \int_1^\infty xK_0^2(\kappa_2 Rx)J_0(q_\perp Rx)\,\mathrm{d}x. \tag{23}$$

A simplification has arisen in the intermediate steps from considering only the lowest sub-band, namely that the term involving a summation over the index j in (13) gives zero contribution to the rates.

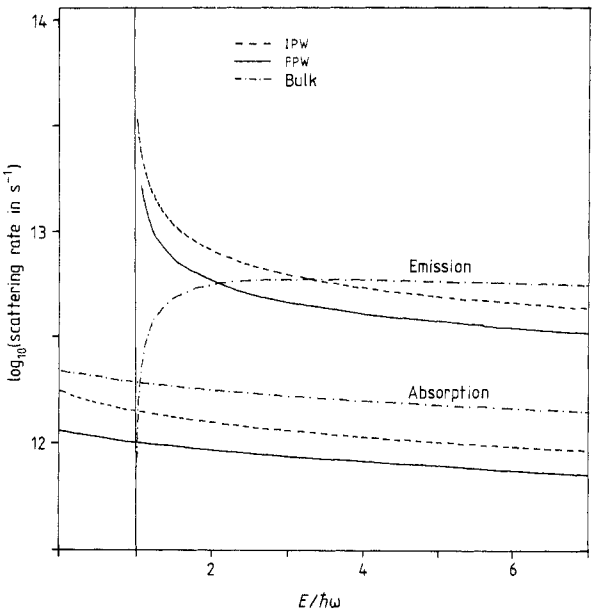

Figure 2. The variation in phonon emission and absorption rates with electron energy for a GaAs/AlGaAs quantum wire at a temperature of 300 K. Also depicted are the corresponding curves for the IPW approximation and the bulk 3D case. The additional parameters used are $\hbar\omega = 36.6$ meV, $\varepsilon_\infty = 10.9$ and $\varepsilon_0 = 12.9$.

The results for the scattering rates as functions of the initial electron energy are illustrated in figure 2. It is seen that both the 1D emission and 1D absorption rates are reduced by about 25% due to the inclusion of a finite well height as compared with their IPW values. Also illustrated in figure 2 are the bulk 3D results for comparison. The 1D absorption rate lies below the bulk value and is practically uniform throughout the energy range under consideration. On the other hand, the 1D emission rate starts off at high energies below the bulk value, and steadily increases until, close to the phonon energy, emission is greatly enhanced with a singularity at the phonon energy. This singularity is due to the 1D density of states and, as was pointed out by various researchers, will result in strong energy relaxation via phonon emission, although this phenomenon is restricted to a narrow energy interval, in agreement with Leburton's results [9]. In fact our emission rate calculated in the IPW approximation closely corresponds to Leburton's curve marked (2,2) in his paper. This is encouraging since the cross sectional area of his rectangular wire is practically equal to that of our circular wire. This gives credence to the above formalism. We are unable to make a detailed comparison with Leburton's absorption rates as he omitted to include forward scattering [10], although our results agree with his for high electron energies.

In conclusion we have developed an effective-mass theory for electrons in cylindrical quantum well wires incorporating the finite value of the confining potential. The theory, applied to the GaAs/AlGaAs system, predicts a reduction in sub-band energy compared with the values given by an infinite confining potential. The lowering of the energy is found to be quite appreciable for certain values of the radius. The effective-mass eigenfunctions were then employed to calculate electron–bulk-polar-optical-phonon

scattering rates in which a lowering from their corresponding values, assuming an infinite confining potential, is predicted.

Although the theory developed in this paper assumes scattering by bulk 3D phonons, it is anticipated that interface modes will be of importance in transport phenomena. Indeed, corresponding investigations in the analogous 2D structures indicate that these confined modes are of major importance in the electron relaxation process [16, 17]. Investigations of their role in the corresponding quantum wires are now under way.

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