Guided and interface LO phonons in cylindrical GaAs/$Al_xGa_{1-x}As$ quantum wires

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A dispersive hydrodynamic continuum theory is employed to describe the LO phonons in GaAs/$Al_xGa_{1-x}As$ cylindrical quantum wires. It is demonstrated that a finite number of guided modes exist for a given wire radius, their number being greater than the corresponding slab system due to the reduced symmetry. As for the interface modes, it is shown that a given mode occurs at a *critical* wave vector, although the axially symmetric mode always exists, it having zero critical wave vector. The situation is drastically modified in the case of a free-standing wire. Within the continuum model and with physically plausible boundary conditions, guided modes exist whereas interface modes *do not*. Implications for electron transport are discussed.

I. INTRODUCTION

Recently there has been concerted attention given to electron energy relaxation in semiconductor quantum wells. An important mechanism in these quasi-two-dimensional (Q2D) structures is carrier relaxation via LO-phonon emission. Early calculations assumed a bulk three-dimensional character for the phonons[1,2] although subsequent experimental evidence, mainly inelastic light scattering, suggests that they are confined to the quantum well.[3] Various investigators have incorporated the confinement of the LO modes in discussing transport properties, with particular application to the GaAs/$Al_xGa_{1-x}As$ system. To describe the modes, two continuum theories have been employed; a slab mode approach[4,5] and the dispersive Born-Huang model of Babiker.[6–8] Both predict confined guided modes together with modes localized at the interfaces (interface modes). Unfortunately, they differ markedly in the symmetry of the phonon potential Φ. This difference is crucial for the description of the electron–LO-phonon scattering, where the interaction Hamiltonian is $e\Phi$ (i.e., Fröhlich type). This has been pointed out by Ridley,[9] who employed Babiker's model to evaluate scattering rates in these Q2D devices. The resolution of this conflict lies in experiment and the recent work of Tatham *et al.*[10] suggests that it is in fact the dispersive model of Babiker that yields the correct phonon potential.

Given the apparent usefulness of this model, it is worthwhile applying it to quasi-one-dimensional (Q1D) structures. The system we have in mind consists of a cylindrical GaAs wire embedded in $Al_xGa_{1-x}As$, which was proposed by Infrate *et al.*[11] and is similar to structures fabricated by Gibert *et al.*[2] The interaction of Q1D electrons with phonons has been discussed in these structures with the phonons being bulk three dimensional in character.[13,14] We would expect the interaction to be modified (as indeed is the case in Q2D systems) when confined and interface phonons are involved. Our aim in this paper is to describe the guided and interface LO phonons in these structures. We leave their coupling to electrons for a future paper.

II. THE GUIDED LO MODES

We take as our model system a cylindrical wire of length L (assumed large) and radius R composed of material one embedded in material two. Within the dispersive hydrodynamic model developed by Babiker,[6] it is convenient to work with the modified ionic displacement $\mathbf{u}$ rather than the true ionic displacement $\mathbf{w}$. The two are related via

$$\mathbf{u}=(M_r/V_0)^{1/2}\mathbf{w}=\rho^{1/2}\mathbf{w} , \tag{1}$$

where M_r is the reduced mass, V_0 the volume of the unit cell, and ρ the mass density. This displacement satisfies the following vector Helmholtz equation

$$(\nabla^2+k_i^2)\mathbf{u}^{(i)}=0 \tag{2}$$

with

$$k_i^2=(\omega_i^2-\omega^2)\beta_i^{-2}, \quad i=1,2 . \tag{3}$$

In the above, ω_1 and ω_2 are the zone-center LO-phonon frequencies for material one and two, respectively, with β_1 and β_2 the acoustic velocity parameters.

We solve this equation in cylindrical coordinates (r,ϕ,z). The solutions involve Bessel functions of various kinds, and it is straightforward to show that the guided mode solution (oscillatory behavior within the wire and decay outside) is, in vectorial notation (u_r,u_ϕ,u_z),

$$\mathbf{u}^{(1)}=A_1^{(n)}e^{in\phi}e^{iq_z z}\left[\frac{-iq_1}{q_z}J_n'(q_1 r),\ \frac{n}{q_z r}J_n(q_1 r),\ J_n(q_1 r)\right],\quad r\le R ; \tag{4}$$

$$\mathbf{u}^{(2)} = A_2^{(n)} e^{in\phi} e^{iq_z z} \left[\frac{-i|q_2|}{q_z} K_n'(|q_2|r), \frac{n}{q_z r} K_n(|q_2|r), K_n(|q_2|r) \right], \quad r > R . \tag{5}$$

In the above, $A_1^{(n)}$ and $A_2^{(n)}$ are mode amplitudes, n is an integer, q_z the phonon wave vector along the axis of the cylinder, $J_n(x)$ a Bessel function of the first kind, $K_n(x)$ a modified Bessel function of the third kind, and differentiation is with respect to their arguments. To obtain this solution we made use of the fact that the modes are purely longitudinal (i.e., $\nabla \times \mathbf{u}^{(i)} = \mathbf{0}$). Also the radial wave vectors are given by

$$q_i^2 = -|q_i|^2 = k_i^2 - q_z^2, \quad i = 1,2 . \tag{6}$$

The mode frequencies are determined by applying the hydrodynamic boundary conditions at the interface. These are continuity of normal velocity,

$$\rho_2^{-1/2} u_r^{(2)}|_{r=R} = \rho_1^{-1/2} u_r^{(1)}|_{r=R} , \tag{7}$$

and continuity of pressure,

$$\beta_2^2 \rho_2^{1/2} \nabla \cdot \mathbf{u}^{(2)}|_{r=R} = \beta_1^2 \rho_1^{1/2} \nabla \cdot \mathbf{u}^{(1)}|_{r=R} . \tag{8}$$

The above boundary conditions are just those employed by Babiker[6] and may be deduced from general energy and momentum flow arguments. Together with (4) and (5) they lead to the following transcendental equation for the mode frequencies:

$$\bar{\rho}(\omega_1^2 - \omega^2)|q_2| K_n'(|q_2|R) J_n(q_1 R) - (\omega_2^2 - \omega^2) q_1 J_n'(q_1 R) K_n(|q_2|R) = 0 , \tag{9}$$

where $\bar{\rho} = \rho_1/\rho_2$. The guided mode frequencies must satisfy the following inequality:

$$\omega_2^2 - \beta_2^2 q_z^2 < \omega^2 < \omega_1^2 - \beta_1^2 q_z^2 . \tag{10}$$

Figure 1 illustrates the allowed $n=0$ modes as a function of wire radius (with $q_z = 0$ for simplicity) with parameters appropriate for the $GaAs/Al_{0.3}Ga_{0.7}As$ system[6] ($\omega_1 = 292.8\ \mathrm{cm}^{-1}$, $\omega_2 = 0.95\omega_1$, $\beta_1 = 4.73 \times 10^3\ \mathrm{m\,s}^{-1}$, $\beta_2 = 1.06\beta_1$, $\bar{\rho} = 1.11$). For a 50-Å radius there are six allowed $n=0$ modes. Of course there are other allowed modes corresponding to various choices of n for this radius. In fact with the help of McMahon's expansion[15] of the zeros of $J_n(x)$, it may be deduced from (9) that for a wire of radius R (in Å) the number N of allowed guided modes of type n for this particular structure is

$$N = \left\lfloor \frac{0.363R}{\pi} - \frac{1}{2}n + \frac{1}{4} \right\rfloor , \tag{11}$$

(the "floor"), where $\lfloor \cdots \rfloor$ stands for the largest integer equal to or less than the argument. For a wire of radius 50 Å there are 36 allowed guided modes, this compares with 11 for a 100-Å-wide slab.[6] The increase in the number of modes is due to the lower symmetry associated with the cylindrical geometry. Of course, electrons that may only scatter within the lowest subband (i.e., electrons confined to thin wires) can only interact with modes of

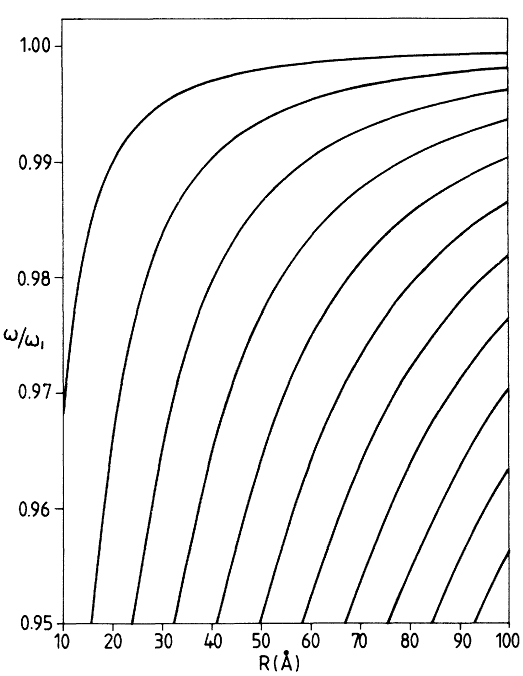

FIG. 1. Mode frequencies as a function of wire radius for $n=0$. See text for the assumed value of the parameters.

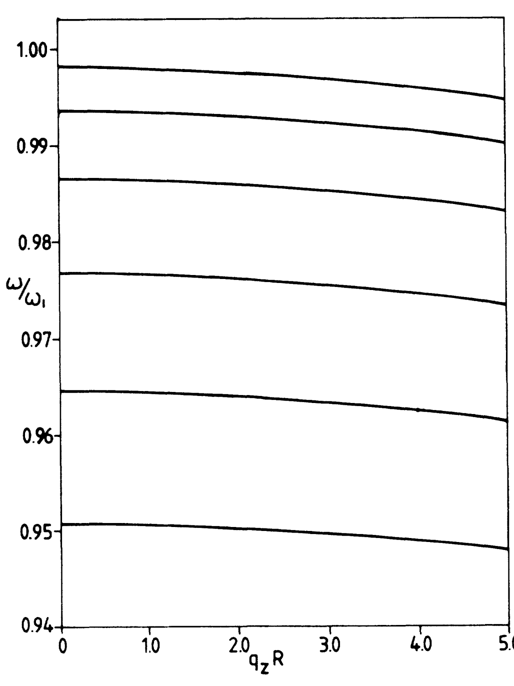

FIG. 2. Dispersion of the allowed $n=0$ guided modes for a 50-Å wire radius.

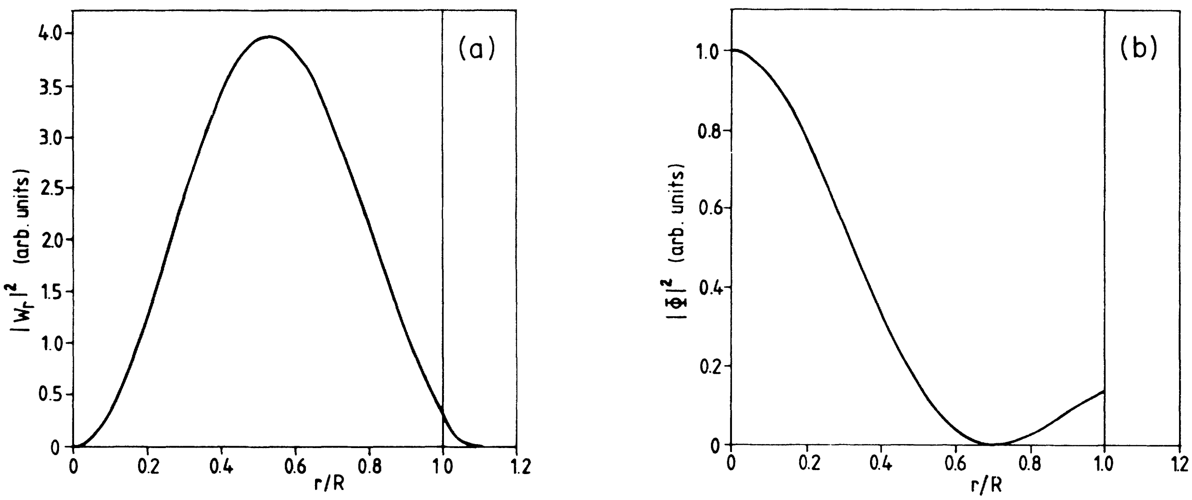

FIG. 3. (a) Variation in the radial component of the displacement and (b) its associated potential for the highest frequency $n=0$ guided mode of a 50-Å wire ($q_zR=2.0$).

$n=0$ symmetry. This is because, within the effective-mass approximation, the electron wave function has $n=0$ symmetry leading to a δ function on the index n when integrations over ϕ are performed. Figure 2 depicts the $n=0$ mode dispersion. It is seen that they are only slightly dispersive, which is consistent with what is found for the slab.

The LO-phonon potential Φ is related to the ionic displacement via

$$\nabla\Phi=\frac{e^*}{V_0\epsilon_0}\mathbf{w}=\kappa\mathbf{u} \tag{12a}$$

with e^* the Callen effective charge. The above together with (4) and (5) gives

$$\Phi=\begin{cases}(\kappa/q_zi)A_1^{(n)}J_n(q_1r)e^{in\phi}e^{iq_zz}, & r\le R\\ (\kappa/q_zi)A_2^{(n)}K_n(|q_2|r)e^{in\phi}e^{iq_zz}, & r>R\ .\end{cases} \tag{12b}$$

This implies that for $n=0$, Φ is proportional to Bessel functions of type $n=0$, whereas from (4) and (5) the radial component w_r has $n=1$ behavior. Figure 3(a) shows the radial variation of w_r for the highest frequency $n=0$ mode. Note that it is practically confined within the wire with a near node at the boundary and zero displacement on the axis. In the slab case the corresponding mode is again practically confined within the layer with near nodes at the surfaces, but here the maximum displacement occurs at the layer midpoint. In Fig. 3(b) we illustrate the potential associated with this mode, noting that this is practically zero outside of the wire due predominantly to the large value of $|q_2|R$ (~ 17). A quantum theory of these modes follows from (12).[9]

III. THE INTERFACE MODES

We seek solutions to the vector Helmholtz equation (2) that are purely longitudinal ($\nabla\times\mathbf{u}^{(i)}=\mathbf{0}$) and decay on either side of the interface. Such solutions do indeed exist and are of the form

$$\mathbf{u}^{(1)}=B_1^{(n)}e^{in\phi}e^{iq_zz}\left[\frac{-i|q_1|}{q_z}I_n'(|q_1|r),\ \frac{n}{q_zr}I_n(|q_1|r),\ I_n(|q_1|r)\right],\quad r\le R\ ; \tag{13}$$

$$\mathbf{u}^{(2)}=B_2^{(n)}e^{in\phi}e^{iq_zz}\left[\frac{-i|q_2|}{q_z}K_n'(|q_2|r),\ \frac{n}{q_zr}K_n(|q_2|r),\ K_n(|q_2|r)\right],\quad r>R\ . \tag{14}$$

Again, $B_1^{(n)}$ and $B_2^{(n)}$ are mode amplitudes and here $I_n(x)$ is the modified Bessel function of the first kind. On application of the hydrodynamic boundary conditions (7) and (8) we find that the mode frequencies satisfy the following equation:

$$\bar{\rho}(\omega_1^2-\omega^2)|q_2|K_n'(|q_2|R)I_n(|q_1|R)-(\omega_2^2-\omega^2)|q_1|I_n'(|q_1|R)K_n(|q_2|R)=0 \tag{15}$$

with the interface mode frequencies satisfying the condition

$$\omega^2>\omega_1^2-\beta_1^2q_z^2\ . \tag{16}$$

Figure 4 depicts the interface LO-phonon dispersion for a wire of radius 50 Å. The bold solid curve is the solution of $|q_1|=0$, namely,

$$\omega^2=\omega_1^2-\beta_1^2q_z^2\ . \tag{17}$$

This is simply the dispersion curve for "bulk" LO modes in GaAs and the various branches ($n=0,1,2,3,\ldots,$) emerge from this "bulk" curve. Analogous behavior is

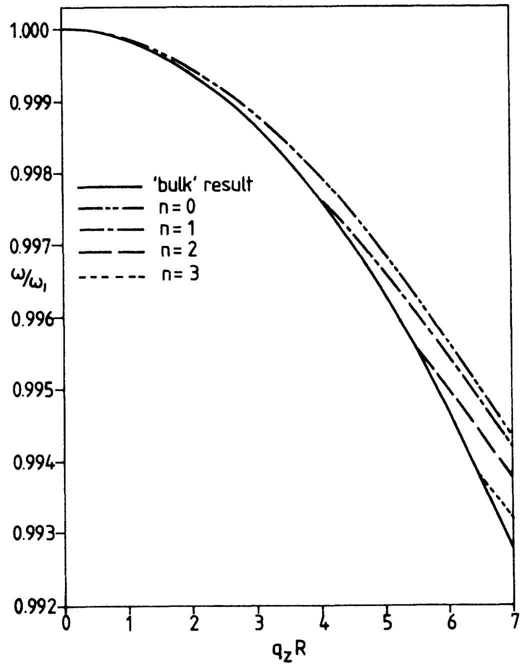

FIG. 4. Interface mode dispersion curves for a 50-Å wire. The bold solid curve corresponds to the "bulk" result (17). Note that the various interface modes (here corresponding to $n=0,1,2,3$) emerge from this curve.

observed for other surface modes; for example, surface phonon polaritons emerge from the "light line" at some critical wave vector (see, e.g., Cottam and Tilley[16] for a slab and Ruppin[17] for a cylinder). The critical wave vector q_z^*, at which an LO-interface mode of type n appears, satisfies the following quadratic equation:

$$(\bar{\rho}-\gamma+n^2)q_z^{*4}+\gamma q_0^2 q_z^{*2}-n^2(q_0^2/\bar{\beta}^2)^2=0 \tag{18}$$

with $\bar{\beta}=\beta_1/\beta_2$ and

$$\gamma=\bar{\rho}\bar{\beta}^2+2n^2 , \tag{19}$$

$$q_0^2=(\omega_1^2-\omega_2^2)/\beta_2^2 . \tag{20}$$

Equation (18) may be deduced from (15) in the limit $|q_1|\rightarrow 0$ and on noting that $|q_2|R$ is large (again typically ~ 17). It is interesting that $q_z^*=0$ for the axially symmetric ($n=0$) interface mode, this is readily deduced from (18).

The radial component of the $n=0$ interface mode is shown in Fig. 5(a). Again as with the guided mode most of the energy is confined within the well with a rapid decay outside the wire. The potential associated with this mode is depicted in Fig. 5(b). It is practically constant inside the well and zero outside. The fact that there is little variation of the potential within the wire (even when q_z is varied) is consistent with a constant scattering rate (independent of in-plane wave vector) predicted for interface mode scattering in the Q2D system.[9] The units for Figs. 3 and 5 are unrelated, the mode amplitudes may only be compared after a quantization procedure is carried out.

IV. FREE-STANDING WIRE

We briefly consider the LO modes of a free-standing GaAs wire. These types of structures have recently been fabricated by Hasko *et al.*[18] Since the wire is surrounded simply by vacuum, the correct boundary condition within our hydrodynamic approximation is the vanishing of the pressure at the interface. This is consistent with the vanishing of both energy and momentum flow at the boundary. The solution of (2) is then

$$\mathbf{u}=C^{(n)}e^{in\phi}e^{iq_z z}\left[\frac{-iq_{nm}}{q_z}J_n'(q_{nm}r)\,,\right.$$
$$\left.\frac{n}{q_z r}J_n(q_{nm}r),\,J_n(q_{nm}r)\right] , \tag{21}$$

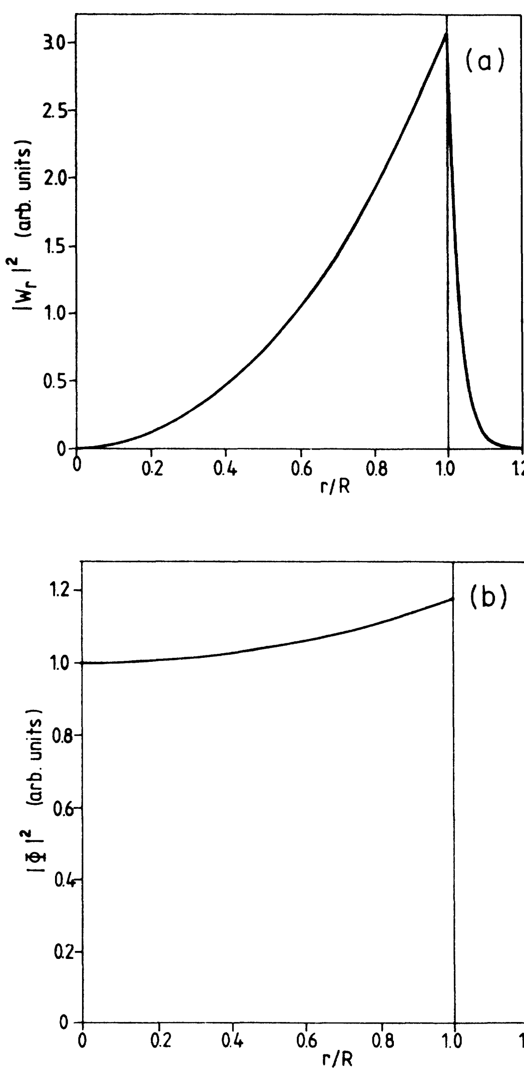

FIG. 5. Variation in the radial component of the displacement (a) and its associated potential (b) for the $n=0$ interface mode of a 50-Å wire ($q_z R=2.0$). The units are not related to those of Fig. 3.

where $C^{(n)}$ is the mode amplitude and q_{nm} is related to the mth zero (x_{nm}) of the Bessel function $J_n(x)$ via $q_{nm}R = x_{nm}$. The dispersion relation is then simply

$$\omega_{nm}^2 = \omega_1^2 - \beta_1^2(q_z^2 + q_{nm}^2) \ . \tag{22}$$

Note that the potential is zero at the interface in this case since $\Phi \sim J_n(q_{nm}r)$. The important point is that purely longitudinal interface modes (i.e., modes with vanishing curl) are not present. The reason is straightforward. The phonon wave functions for a "possible" interface mode would involve Bessel functions of type $I_n(q_r r)$ completely analogous to (13), where q_r is some radial wave vector. The dispersion relation would then follow from the vanishing of the pressure at the boundary that leads to $I_n(q_r R)=0$. This has no solutions for $n=0$ and the unphysical solution $q_r=0$ for n greater than zero.[15] The lack of LO-interface modes in these structures has important consequences for electron transport. Interface modes dominate energy relaxation in thin quantum wells[9] and their absence in these novel free-standing structures leads to a dramatic reduction in the scattering rate (see Constantinou and Ridley[19] for a more detailed discussion of these modes and their coupling to electrons). The surface excitations that are allowed are polaritons that are *transverse* solutions of Maxwell's equations (i.e., have vanishing divergence) and are hybrid TO-phonon-photon modes.[17] The interaction of these surface polaritons with electrons is now under investigation, but it is known that in the bulk the TO part of the mode contributes to the usual deformation-potential scattering only in the case of holes and not at all for electrons in a Γ minimum, whereas the electromagnetic part interacts only *very* weakly with the carriers.[20]

V. CONCLUSIONS

In this paper we have applied the hydrodynamic model of Babiker to describe both guided and interface LO phonons in typical GaAs/Al_xGa_{1-x}As cylindrical quantum wires. This type of model is valid for small wave vectors which, of course, is the regime in which the Fröhlich interaction is enhanced. Indeed our aim was to provide a detailed description of the allowed modes with a view to coupling these to the carriers in a later paper.

A finite number of guided modes is predicted for a given wire radius. This number is greater than that found for the equivalent slab system due to the reduced symmetry. As for the interface modes, we demonstrate that they exist only if the wave vector is greater than some critical wave vector where the mode emerges from the "bulk" result. The axially symmetric mode ($n=0$) always exists as it has zero critical wave vector. This is the analogue of the odd (with respect to reflection in the midpoint) slab interface mode, which is mainly responsible for intrasubband scattering.[9] The situation is drastically modified in the case of free-standing wires. Here it is demonstrated that although LO-guided modes are allowed, interface LO modes are not. This leads to a marked reduction in the scattering rate for thin wires.[19]

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