Interaction of electrons with the confined LO phonons of a free-standing GaAs quantum wire

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A continuum model is employed to describe the allowed longitudinal-optical phonons of a cylindrical free-standing GaAs wire. The electron-phonon interaction Hamiltonian is then obtained and used to calculate intrasubband transitions in the extreme quantum limit. The scattering rate is predicted to be markedly reduced compared with the bulk value, and compared with the value expected when the wire is not free standing. This result is due to the lack of LO interface modes in the free-standing situation.

I. INTRODUCTION

Recent developments in microfabrication techniques have led to carrier confinement in two spatial directions resulting in quasi-one-dimensional (Q1D) behavior and leading to a wealth of interesting physics.[1-4] As a consequence of their possible applications in microelectronic devices, the transport properties of these systems have received a great deal of attention since Sakaki[5] predicted an enhanced mobility due to remote impurity scattering. The interaction of the electrons with longitudinal-optical phonons has been investigated by various workers,[6,7] where the phonons were assumed to be bulkline and phonon confinement effects ignored. This is an oversimplification; indeed in the corresponding two-dimensional system (e.g., GaAs/$Al_xGa_{1-x}As$ quantum well) it has been point out by various investigators that phonon confinement effects lead to important modifications in the transport properties, with both guided and interface modes contributing to electron energy relaxation.[8-10] Furthermore, the recent fabrication by Hasko and co-workers[11] of free-standing single-crystal GaAs wires has made the need to discuss phonon confinement more pressing. Their wires have a triangular cross section (although we will assume circular cross section for mathematical simplicity) with widths of around 0.25 μm. At the moment, for various reasons, this seems to be about the minimum width attainable.

In this paper we investigate the allowed LO-phonon modes of a free-standing GaAs wire. The resultant electron-phonon interaction is derived anticipating future developments in microfabrication techniques that could lead to devices in which truly Q1D carriers interact with these novel LO modes at high temperatures. It is well known that in higher dimensions LO-phonon emission is the dominant mechanism responsible for electron energy (and often momentum) relaxation at high temperatures. The outline of the paper is as follows: In Sec. II we describe the guided LO modes of a cylindrical GaAs wire using a continuum approach and show that interface modes do not occur. The electron-phonon interaction Hamiltonian is derived in Sec. III where it is applied to intrasubband transitions. Finally, Sec. IV contains our comments and conclusions.

II. THE LO MODES OF A FREE-STANDING GaAs WIRE

We consider a single cylindrical wire of radius R and length L (assumed large) surrounded by vacuum. As practical radii are typically large (i.e., many atomic spacings) we may employ the dispersive hydrodynamic model developed by Babiker[12] and applied to the LO phonons of a GaAs/$Al_xGa_{1-x}As$ quantum well. This model reasonably assumes a dispersion for the bulk 3D phonons of the form

$$\omega^2=\omega_{LO}^2-\beta^2Q^2 , \tag{1}$$

where Q is the bulk phonon wave vector, ω_{LO} the zone-center LO-phonon frequency (5.55×10^{13} s^{-1} for GaAs), and β the velocity parameter (4.73×10^3 $m\,s^{-1}$ for GaAs). This model describes the phonons well if the wave vector is small (i.e., for phonons with frequencies close to ω_{LO}), which of course is the important regime for the electron-phonon coupling as the Fröhlich interaction is enhanced at low-phonon wave vectors. For larger wave vectors (shorter wavelengths) this approximation breaks down. The situation is fine for the Q2D, system as the existence criterion for guided modes is rather restrictive; the allowed frequencies having to lie between the two constituent bulk values which, for the GaAs/$Al_xGa_{1-x}As$ system, are very close together.[12] In the case of a free-standing GaAs wire, within this continuum approximation we will see that the existence criterion is relaxed with the allowed frequencies lying between 0 and ω_{LO}. Nevertheless, we show in Sec. II that, again, as with the 3D and Q2D system it is only the modes with small wave vectors (i.e., frequencies close to ω_{LO}) that give the dominant contributing to electron energy relaxation. These modes are well described by a continuum model.

It is convenient to work with a modified ionic displacement **u** rather than the true ionic displacement field **w**; the two are related via

$$\mathbf{u}=(\bar{M}/V_0)^{1/2}\mathbf{w} \ . \tag{2}$$

Here $\bar{M}$ is the reduced mass and V_0 the volume of the unit cell. This displacement satisfies the following wave equation:[12]

$$[\nabla^2+(\omega_{\rm LO}^2-\omega^2)\beta^{-2}]\mathbf{u}=0, \quad r\le R \ , \tag{3}$$

The solution of the above which is regular on the axis of the cylinder[13] and satisfies the condition that the pressure is zero at the surface (equivalent to $\nabla\cdot\mathbf{u}|_{r=R}=0$) is in cylindrical coordinates (r,φ,z)

$$\begin{aligned} u_z &= C_{mn}e^{im\varphi}e^{iq_z z}J_m(q_{mn}r) \ , \\ u_\varphi &= (m/q_z r)u_z \ , \\ u_r &= -i(q_{mn}/q_z)C_{mn}e^{im\varphi}e^{iq_z z}J_m'(q_{mn}r) \ . \end{aligned} \tag{4}$$

Note that applying the condition that the pressure be zero at the surface eliminates the possibility of LO interface modes. In (4) m is an integer, differentiation is with respect to the argument of the Bessel function, and we have used the fact that the modes are purely longitudinal (i.e., $\nabla\times\mathbf{u}=0$). Also C_{mn} is the mode amplitude, q_z the wave vector along the axis of the wire and q_{mn} is related to the nth zero (x_{mn}) of the Bessel function $J_m(x)$ by $q_{mn}R=x_{mn}$.

The frequency of a mode labeled (m,n) is easily determined from the boundary condition, we find

$$\omega_{\rm mn}^2=\omega_{\rm LO}^2-\beta^2(q_{mn}^2+q_z^2) \ . \tag{5}$$

This is precisely the same form as the 3D and 2D case. Now for a given radius this theory predicts a large though finite number of modes, the only restriction being (with $q_z=0$ for simplicity)

$$x_{mn}\le\omega_{\rm LO}R/\beta \tag{6}$$

to ensure real frequencies. As was previously discussed, it is only the small wave-vector modes that the theory describes well. We will restrict our interest to the so-called extreme quantum limit, in which the electrons occupy the lowest subband. In Sec. III we demonstrate that for scattering within this band only the $(0,n)$ modes are allowed and of these only the first few make any real contribution to the scattering rate. In fact the (0,1) mode often dominates with the interaction reduced by at least an order of magnitude as the mode index n increases by 1. It is of course, precisely these modes that the theory applies to (note $\omega_{01}\simeq\omega_{\rm LO}$).

Before considering in detail the electron-phonon interaction, it is worth justifying the boundary conditions employed. Within the spirit of a hydrodynamic approximation, and given that the wire is surrounded simply by vacuum, the vanishing of the pressure at the surface is reasonable. Indeed, from (4) the only nonvanishing component of the phonon field is the radial component. This is analogous to ripples on the surface of a liquid; again the pressure is zero at the surface with no restriction on the normal component of displacement. It is also consistent with the well-known Fuchs and Kliewer[14] guided modes for an *isolated* ionic slab that also have antinodes at the surface. The situation is strikingly modified if the ionic slab is surrounded, not, as here by vacuum, but with another material (e.g., the GaAs/Al_xGa_{1-x}As system). In this case, the guided modes have near nodes at the interface and LO-interface modes become allowed[10] that leads to a modification of the electron-phonon interaction. The analogous GaAs wire embedded in Al_xGa_{1-x}As has also been investigated by us.[15]

III. THE ELECTRON-PHONON INTERACTION

To obtain the electron-phonon interaction we follow the quantization procedure used by Ridley[10] to derive the interaction Hamiltonian for an ionic slab. The mode amplitudes may be determined by relating the total energy in the cavity to that of an equivalent harmonic oscillator. Thus

$$\tfrac{1}{2}\omega_{mn}^2\frac{\bar{M}}{V_0}\int_V \mathbf{w}^*\cdot\mathbf{w}\,dV=\tfrac{1}{2}\omega_{mn}^2\bar{M}\chi_{mn}^2 \ , \tag{7}$$

whence

$$\chi_{mn}^2=\frac{1}{\bar{M}}\int_V \mathbf{u}^*\cdot\mathbf{u}\,dV \ , \tag{8}$$

where χ_{mn} is the coordinate of the simple harmonic oscillator equivalent to the mode labeled (m,n). The integration over the volume is outlined in the appendix and we find

$$C_{mn}=\left[\frac{\bar{M}}{V}\right]^{1/2}\frac{q_z}{J_{m+1}(x_{mn})}\frac{1}{(q_z^2+q_{mn}^2)^{1/2}}\chi_{mn} \ , \tag{9}$$

with V the volume of the wire. The potential is related to the ionic displacement via

$$\nabla\Phi=\frac{e^*}{V_0\epsilon_0}\mathbf{w}=\frac{e^*}{(V_0^{1/2}\bar{M}^{1/2}\epsilon_0)}\mathbf{u} \ , \tag{10}$$

with e^* the Callen effective charge. It follows from (4), (9), and (10) that the total potential is

$$\Phi=-\frac{e^*}{\epsilon_0(V_0V)^{1/2}}\sum_{q_z,q_{mn}}\left[\frac{ie^{iq_z z}e^{im\phi}J_m(q_{mn}r)\chi_{mn}}{J_{m+1}(x_{mn})(q_z^2+q_{mn}^2)^{1/2}}+\text{c.c.}\right] . \tag{11}$$

The electron-phonon interaction Hamiltonian is then

$$\hat{H}_{\rm int}=-e\Phi \tag{12}$$

and has the desired Fröhlich form being inversely proportional to the phonon wave number.

We are now in a position to evaluate the scattering rate. We assume that we are in the extreme quantum limit in which the carriers occupy the lowest subband and scattering is within this band. The generalization to intersubband scattering is fairly straightforward but will not be discussed in this paper.

Within the spirit of the effective-mass and parabolic-band approximation, the Q1D electron wave function is

$$\psi=J_0(k_{01}r)e^{ik_z z}[V_e^{1/2}J_1(x_{01})]^{-1} \ , \tag{13}$$

where k_z is the wave number along the axis of the cylinder and $k_{01}R_e = x_{01}$. We assume that the electrons occupy a cylindrical volume V_e of radius R_e which is less than the volume occupied by the phonons, see Fig. 1. This is indeed the case in practice as the conducting channel is less than the dimensions of the wire due to carrier depletion into the crystal from the surface.[11] The total energy is simply

$$E_T = E + \frac{\hbar^2}{2m^*}k_{01}^2 , \tag{14}$$

with E the kinetic energy along the wire ($=\hbar^2 k_z^2/2m^*$) and m^* is the carrier effective mass.

The scattering rate for the emission of a guided mode (m,n) is given by

$$W_{mn} = \frac{2\pi}{\hbar}\int |\langle k_z^f, N(\omega_{mn})+1|\hat{H}_{\text{int}}|N(\omega_{mn}), k_z^i\rangle|^2 \times \delta(E_T^f - E_T^i + \hbar\omega_{mn})dS_f , \tag{15}$$

where the integration is over all final states and $i(f)$ denotes initial (final) energy, $N(\omega_{mn})$ is the Bose-Einstein factor at the mode frequency. The evaluation of the matrix element is straightforward and leads to the usual conservation of crystal momentum along the axis of the wire. Further, as we are dealing with carriers in the lowest subband it also implies, via the ϕ integration, that the electrons may only interact with $(0,n)$-type guided modes. The total scattering rate, W, assuming only emission possible is given by

$$W = \frac{4W_0}{J_1^4(x_{01})}\sum_{q_{0n}} \frac{|I_n|^2 \zeta_{0n}\bar{R}^2}{(E/\hbar\omega_{\text{LO}} - \zeta_{0n})^{1/2} J_1^2(q_{0n}R)} \times [F_n(Q_{z,n}^+) + F_n(Q_{z,n}^-)] , \tag{16}$$

where we have used the result

$$W_0 = \frac{e^2}{4\pi\hbar\epsilon_0}\left(\frac{2m^*\omega_{\text{LO}}}{\hbar}\right)^{1/2}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s}\right) \tag{17}$$

and $\epsilon_{\infty(s)}$ is the high- (low-) frequency dielectric constant; ($W_0 \sim 7.74\times 10^{12}$ s^{-1} for GaAs). The integral I_n and the function F_n are

$$I_n = \int_0^1 y J_0(x_{0n}\bar{R}y) J_0^2(x_{01}y)dy , \tag{18}$$

$$F_n(Q_{2,7}^{\pm}) = \left[\left(Q_{z,n}^{\pm}\right)^2 + x_{0n}^2\bar{R}^2\right]^{-1} , \tag{19}$$

with $\bar{R} = R_e/R$, $\zeta_{0n} = \omega_{0n}/\omega_{\text{LO}}$, and

$$Q_{z,n}^{\pm} = \left(\frac{2m^*\omega_{\text{LO}}}{\hbar}\right)^{1/2} \times R_e[(E/\hbar\omega_{\text{LO}})^{1/2} \pm (E/\hbar\omega_{\text{LO}} - \zeta_{0n})^{1/2}] , \tag{20}$$

where $+(-)$ designates forward (backward) scattering.

In the limit $R \to \infty$, in which case q_{0n} becomes a continuous variable, (16) reduces to the case of a wire of radius R_e interacting with the bulk 3D phonons of GaAs (Ref. 7) as it should. It is found numerically that only the first few terms in (16) are of any importance with (0,1) often the most dominant. This is true away from any phonon energies where the scattering rate is seen to diverge. This is due to the singularity in the 1D density of states and of course occurs also in the study of Q1D electrons coupled to bulk 3D phonons; the singularity here being at the *single*-phonon energy $\hbar\omega_{\text{LO}}$. In practice there will always be damping in the system and, for fairly large radii, it is anticipated that any peaked structure in the rate for electron energies less than $\hbar\omega_{01}$ would be smoothed out leading to a gradual rise to its value at $\hbar\omega_{01}$. This novel prediction is due entirely to the discrete nature of the LO-phonon spectrum. A quantitative investigation regarding the implications of this result is now underway.

Figure 2 illustrates the variation in the scattering rate

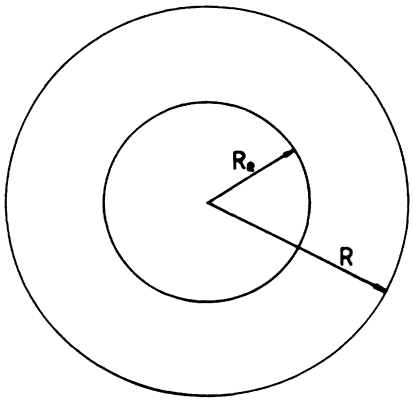

FIG. 1. Geometry of the system depicting the conducting channel of radius R_e contained within the wire of radius R.

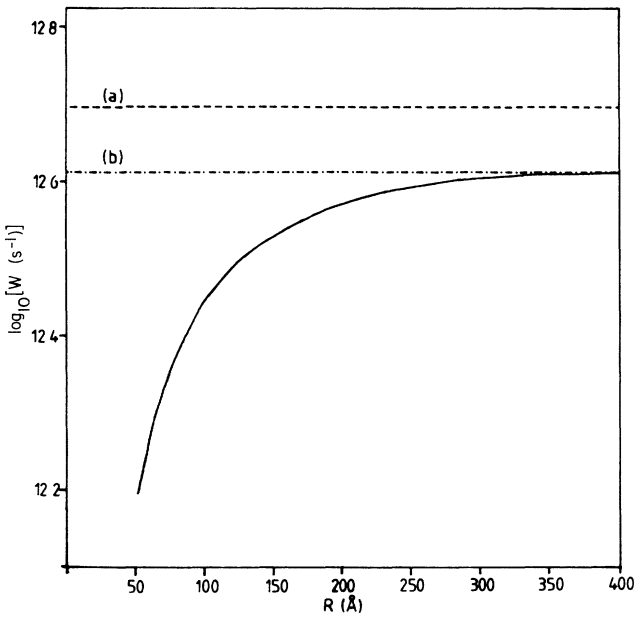

FIG. 2. The scattering rate as a function of wire radius (solid curve). The dashed line labeled (a) corresponds to the bulk result, whilst (b) that of Q1D electrons interacting with bulk phonons, as deduced from Constantinou and Ridley (Ref. 7). (See text for the assumed value of the parameters.)

as a function of the wire radius. The carrier energy is fixed at $5\hbar\omega_{LO}$, with the conducting channel radius held at 50 Å, which prohibits intersubband events. It is seen that the rate approaches the Q1D bulk phonon result fairly quickly. On the otherhand, for small wire radii (<200 Å) there is quite a marked decrease in the scattering rate. For a wire radius of 50 Å (equal to the channel radius) the rate has fallen by 60% as compared with the Q1D bulk phonon value and to 70% of the well-known result for 3D electrons interacting with bulk 3D phonons.[16] A reduction of about the same order is also obtained in the case of a free-standing slab.[17]

IV. COMMENTS AND CONCLUSIONS

In this paper we consider for the first time the interaction of guided LO phonons with Q1D carriers in free-standing GaAs wires. The phonon modes are described by a dispersive hydrodynamic model[12] valid for wire dimensions much larger than the interatomic spacing, and the boundary condition employed is seen to lead to results consistent with those of an *isolated* ionic slab.[14] The number of allowed guided modes is found to be large due to the general reduction in the symmetry and a loosening of the existence criteria compared to the investigations for a symmetric heterojunction.[12]

The electron-phonon interaction is then derived using an intuitive quantization procedure and applied to scattering within the lowest band. The radius of the conducting channel is assumed to be small, prohibiting any intersubband events (the so-called extreme quantum limit). It is found that the rate can be markedly reduced if the wires are very thin. These are beyond the capabilities of present microfabrication techniques. Nevertheless, given the remarkable advances in microfabrication techniques over recent years, we envisage that the technology will be developed to produce free-standing GaAs wires thin enough so that Q1D effects become important above subliquid helium temperatures. The formalism may of course be extended, given the generality of the interaction Hamiltonian obtained, to include intersubband events. The predicted intrasubband rate for guided mode emission is found to be greater than half an order of magnitude less than that of bulk phonon emission.

The effects of surface modes on electron energy relaxation have been ignored in the present formalism, which has dealt with purely longitudinal modes that have no surface counterpart and are simply standing modes of the system. The surface modes associated with these free-standing structures are polaritonlike modes that are transverse in character.[18] The interaction of electrons with these surface modes is now under investigation and the results will be published in the future. Nevertheless, it is anticipated that any effects will restrict themselves to thin wires and for larger radii, (keeping the channel radius small of course), will be negligible. This is one advantage of containing the electrons electrostatically to a thin 1D channel over the 1D and 2D GaAs/$Al_xGa_{1-x}As$ systems in which interface modes are always present. Intersubband events are also ruled out in this system.

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APPENDIX

The z and ϕ integrations of the volume integral are straightforward. The integral over the radial coordinate is the following:

$$I_r=\int_0^R r\left[J_m^2(q_{mn}r)\left[1+\frac{m^2}{q_z^2r^2}\right]+\left[\frac{q_{mn}}{q_z}\right]^2[J_m'(q_{mn}r)]^2\right]dr\ . \tag{A1}$$

When the recurrence relation is employed for the derivative the integral is then the sum of four integrals, viz.

$$I_r=\sum_{i=1}^{4} I_r^{(i)}\ , \tag{A2}$$

where

$$I_r^{(1)}=\int_0^R rJ_m^2(q_{mn}r)dr=\tfrac{1}{2}R^2J_{m+1}^2(x_{mn})\ , \tag{A3}$$

$$I_r^{(2)}=\left[\frac{q_{mn}}{q_z}\right]^2\int_0^R rJ_{m+1}^2(q_{mn}r)dr=\frac{q_{mn}^2R^2}{2q_z^2}J_{m+1}^2(x_{mn})\ , \tag{A4}$$

$$I_r^{(3)}=\frac{2m^2}{q_z^2}\int_0^R r^{-1}J_m^2(q_{mn}r)dr=\frac{2m}{q_z^2}\sum_{k=1}^{\infty}J_{m+k}^2(x_{mn})\ , \tag{A5}$$

$$I_r^{(4)}=\frac{-2q_{mn}m}{q_z^2}\int_0^R J_{m+1}(q_{mn}r)J_m(q_{mn}r)dr\ , \tag{A6}$$

$$I_r^{(4)}=-\frac{2m}{q_z^2}\sum_{k=1}^{\infty}J_{m+k}^2(x_{mn})=-I_r^{(3)}\ . \tag{A7}$$

All the above integrals may be found in any standard text on Bessel functions, e.g., Ref. 19. The result of Eq. (9) follows easily.

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