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LETTER TO THE EDITOR

Macroscopic behaviour of longitudinal optical phonons in a AlAs/GaAs/AlAs quantum well

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Abstract. Calculation of longitudinal optical (LO) mode potential functions and dispersion curves are made for a AlAs/GaAs/AlAs quantum well using a macroscopic model. The interface boundary conditions employed are continuity of potential and normal components of both electric flux density and relative ionic displacement. In the non-dispersive limit the model yields unique potential functions of two types: confined modes and interface modes. The confined mode potential functions are almost identical to those calculated for a microscopic model by Huang and Zhu. The interface modes are identical to those predicted by both the microscopic model and the dielectric continuum model. The introduction of bulk dispersion in GaAs produces modes which are hybrids of the confined and interface phonons.

Microscopic models of the behaviour of optical phonons in semiconductor heterostructures necessarily involve extensive numerical calculations [1–8]. A simple macroscopic model giving analytical results close to those of microscopic models would be useful in studies of the interaction of phonons with electrons and light. A natural starting point is the dielectric continuum model (DCM) based on the bulk phenomenological equations of Born and Huang [11]. The modes predicted are like those of Fuchs and Kliever [10]. They have antinodes in the normal component of the GaAs displacement at the interfaces in a AlAs/GaAs/AlAs quantum well, which is contrary to the results of microscopic calculations [7,8]. A hydrodynamic model [12,13] has been proposed to avoid this difficulty. However, a hydrodynamic approach is not generally valid in the systems under discussion [9] and it leads to other contradictions to the microscopic calculations [14].

In this letter we describe a simple modification of the dielectric continuum model (the MDCM) which yields results almost identical to those predicted by the microscopic model of Huang and Zhu [1,2] in the dispersionless limit. We describe the model below and discuss the results obtained from it later both in the non-dispersive limit and when finite dispersion is introduced in the GaAs.

We use the phenomenological equations of Born and Huang [11] modified to include parabolic bulk dispersion [12]. In electrostatic units the equations for LO phonons are:

$$\ddot{\boldsymbol{w}} = -\omega_{\mathrm{T}}^2 \boldsymbol{w} + \left(\frac{\varepsilon_o - \varepsilon_\infty}{4\pi}\right)^{1/2} \omega_{\mathrm{T}} \boldsymbol{E} - b^2 \nabla^2 \boldsymbol{w} \tag{1}$$

$$\boldsymbol{P} = \left(\frac{\varepsilon_o - \varepsilon_\infty}{4\pi}\right)^{1/2} \omega_{\mathrm{T}} \boldsymbol{w} + \frac{(\varepsilon_\infty - 1)}{4\pi} \boldsymbol{E} \tag{2}$$

where $\boldsymbol{w}$ is the displacement of the positive ions relative to the negative ions multiplied by the square root of the reduced mass per unit volume, $\boldsymbol{P}$ is the dielectric polarization, $\boldsymbol{E}$ is the electric field, ε_o and ε_∞ are the static and the high frequency dielectric constants respectively and ω_{T} is the transverse optical resonant frequency. The parameter b introduces parabolic dispersion. We ignore retardation so that

$$\nabla \times \boldsymbol{E} = 0 \tag{3}$$

and for LO modes in the quantum well structure we may write

$$\boldsymbol{E} = -\nabla V \tag{4}$$

with

$$V = \Phi(z) \mathrm{e}^{\mathrm{i}\boldsymbol{k}_\parallel \boldsymbol{x}_\parallel}. \tag{5}$$

Here z is measured perpendicular to the AlAs/GaAs/AlAs interfaces, $\boldsymbol{x}_\parallel$ lies in the transverse plane and $\boldsymbol{k}_\parallel$ is a wave vector in that plane.

We find from (1), (2) and (3) that Maxwell's equation $\nabla \cdot \boldsymbol{D} = 0$ leads in each material to the fourth-order differential equation

$$b^2(\Phi^{(4)} - k_\parallel^2 \Phi'') + (\omega_{\mathrm{L}}^2 - \omega^2 - b^2 k_\parallel^2)(\Phi'' - k_\parallel^2 \Phi) = 0 \tag{6}$$

in which $\omega_{\mathrm{L}} = (\varepsilon_o/\varepsilon_\infty)^{1/2}\omega_{\mathrm{T}}$. It follows that

$$\Phi = A\mathrm{e}^{\mathrm{i}nz} + B\mathrm{e}^{-\mathrm{i}nz} + C\mathrm{e}^{k_\parallel z} + D\mathrm{e}^{-k_\parallel z} \tag{7}$$

where

$$n^2 = \frac{\omega_{\mathrm{L}}^2 - \omega^2 - b^2 k_\parallel^2}{b^2}. \tag{8}$$

Equation (8) is equivalent to the bulk dispersion relation for LO phonons: $\omega^2 = \omega_{\mathrm{L}}^2 - b^2(k_\parallel^2 + n^2)$. The coefficients A, B, C, D and n in (7) remain to be determined by the interface boundary conditions.

We confine our attention to modes with frequencies close to ω_{L} for GaAs. Then the effect of dispersion in the AlAs is unimportant and we set $b = 0$ in AlAs region. We also set $A = B = 0$ there because propagating modes are not possible without dispersion. Finally we keep Φ finite as $z \to \pm\infty$ by putting $C = 0$ in the right-hand AlAs region (in which $z \to +\infty$) and $D = 0$ in the left-hand AlAs region. Six coefficients remain to be determined. We determine them by using the boundary conditions of the DCM (Φ and D_z continuous at each interface) to which we add a further boundary condition: w_z also continuous at each interface [6].

It is convenient to measure z from the middle of the quantum well because the system is symmetrical about the plane $z = 0$. Consequently we find modes for which $\Phi(z)$ is even (even modes) and modes for which $\Phi(z)$ is odd (odd modes). The matching conditions and determinental consistency conditions are easily derived in both cases. Let d be the half-width for the GaAs layer. Then the consistency conditions for even and odd modes are respectively

$$n \tan(nd)\alpha = k_\parallel \tanh(k_\parallel d) \frac{\varepsilon_2 a_1 - \varepsilon_1 a_2}{\varepsilon_1 + \varepsilon_2 \tanh(k_\parallel d)} \tag{9}$$

and

$$n\cot(nd)\alpha = -k_{\|}\coth(k_{\|}d)\frac{\varepsilon_2 a_1 - \varepsilon_1 a_2}{\varepsilon_1 + \varepsilon_2\coth(k_{\|}d)} \tag{10}$$

where n is given by (8) in the GaAs layer with $b \neq 0$. In these equations

$$\varepsilon_j = \varepsilon_{\infty j}\frac{w_{\mathrm{L}j}^2 - \omega^2}{\omega_{\mathrm{T}j}^2 - w^2} \tag{11}$$

$$a_j = \left(\frac{\varepsilon_{oj} - \varepsilon_{\infty j}}{4\pi}\right)^{1/2}\frac{w_{\mathrm{T}j}}{\omega_{\mathrm{T}j}^2 - \omega^2} \tag{12}$$

$$\alpha = \left(\frac{\varepsilon_{o2} - \varepsilon_{\infty 2}}{4\pi}\right)^{1/2}\frac{\omega_{\mathrm{T}2}}{\omega_{\mathrm{T}2}^2 - \omega^2 - b^2k^2} \tag{13}$$

with $j = 1, 2$ denoting AlAs and GaAs respectively.

The solutions of (9) and (10) as a function of $k_{\|}$ give the dispersion relation for each mode. Once this is obtained the coefficients in (7) and $\Phi(z)$ can be determined.

The values of the parameters of bulk GaAs and AlAs used in our calculations are taken from reference [15]. We set $d = 50$ Å and begin by discussing the non-dispersive limit when $b \to 0$. There are two possibilities allowed by equations (9) and (10). In the first case n remains finite, then we see from (8) that $\omega \to \omega_{\mathrm{L}2}$ and from (11) that $\varepsilon_2 \to 0$. Hence (9) and (10) reduce to

$$n\tan(nd) = -k_{\|}\tanh(k_{\|}d) \tag{14}$$

$$n\cot(nd) = k_{\|}\tanh(k_{\|}d) \tag{15}$$

which determine n uniquely. The corresponding potential functions are shown by solids lines in figure 1(a) for $k_{\|}d = 0.05\pi$ and in figure 1(b) for $k_{\|}d = 0.5\pi$. The dashed lines show the results obtained in the microscopic calculations of Huang and Zhu [2]. When the microscopic model curves are omitted it is because they are indistinguishable from the results of our macroscopic model on the scale of the graphs. The dotted lines show a rough analytical fit to the microscopic results which are described in [2]. We see that the model used here provides an almost perfect fit to the microscopic results. These modes with finite n were first proposed by Dharssi [16] without recourse to the limiting procedure used here. The argument was open to the objection that the propagating modes are infinitely degenerate when there is no dispersion so that there is no reason to take just two propagating waves in (7). This difficulty is removed by first including dispersion so that n is uniquely defined and then letting $b \to 0$ so as to simplify the results. We see that all the modes are confined to the GaAs layer. Moreover, it is easy to verify that $\partial\Phi/\partial z$ (and hence w_z) vanishes at the interfaces as well as Φ. The values of n when $k_{\|} \to 0$ may be determined from (14) and (15). They are $n = m\pi/2d$ with $m = 2, 4, 6, \ldots$ for the even modes and $m \sim 3, 5, 7, \ldots$ for the odd modes. Huang and Zhu obtain the same results and give exact values of m in the odd case [2].

The second possibility when $b \to 0$ is that n diverges, because $\omega \to \omega_{\mathrm{L}2}$. When $\omega > \omega_{\mathrm{L}2}$ we see from (8) that n becomes purely imaginary as well as having a

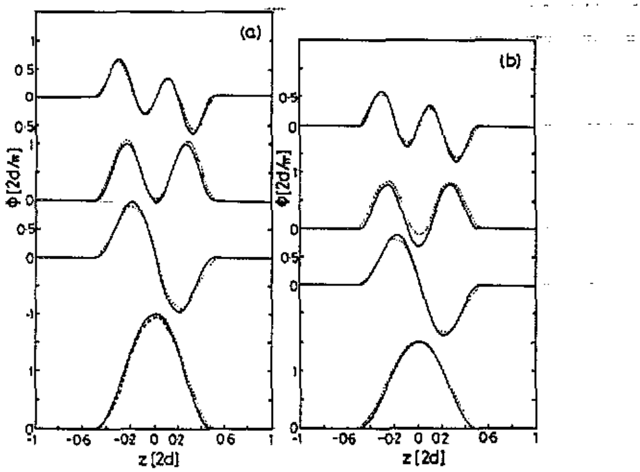

Figure 1. The potential functions for (a) $k_{\|}d = 0.05\pi$ and (b) $k_{\|}d = 0.5\pi$ predicted by (i) the MDCM in the dispersionless limit (full lines); (ii) Huang and Zhu's microscopic model in the dispersionless limit (dashed lines) and (iii) Huang and Zhu's macroscopic model (dotted lines).

magnitude which approaches infinity. Consequently the left-hand sides of (9) and (10) both diverge so that the dispersion relations reduce to

$$\varepsilon_1 + \varepsilon_2 \tanh(k_{\|}d) = 0 \tag{16}$$

$$\varepsilon_1 + \varepsilon_2 \coth(k_{\|}d) = 0. \tag{17}$$

These are just the dispersion relations of the interface modes of the DCM which Huang and Zhu find are reproduced by their microscopic calculations in the non-dispersive limit [2]. Our model fails to yield (16) and (17) when $w < w_{\mathrm{L}}$ because n remains real. The reason is that the assumption of parabolic bulk dispersion is misleading in this case. Equations (16) and (17) are recovered when a bulk dispersion relation which is more realistic for large wave vectors is introduced.

We see from the above discussion that there is a clear distinction between interface and confined modes in the dispersionless limit. We turn now to the case when the GaAs dispersion is kept finite and show that the modes are hybrids having both interface and confined phonon character.

Figure 2(a) shows the dispersion curves for even modes which are the solutions of equation (9). The potential functions are presented in figure 3(a) for $k_{\|}d = 0.05\pi$ and figure 3(b) for $k_{\|}d = 0.5\pi$. At high frequencies the even modes have dispersion curves which are parabolic (figure 2(a)) and potential functions which are confined (figure 3). The potential functions do not differ significantly from those shown in figure 1 for the dispersionless limit. On the other hand, we see in figure 2(a) that for modes with a frequency approaching $(\omega_{\mathrm{L2}} + \omega_{\mathrm{T2}})/2$ the parabolic dispersion is distorted. The distortion is due to the interface admixture which increases with $k_{\|}$ because the dispersion curve comes closer to that for the even interface phonon (dashed curve in figure 2(a)) when $k_{\|}d = 0.5\pi$. This behaviour is particularly clear for the last mode in figure (2(a)). Another result of the increase of the interface admixture with $k_{\|}$ is that for $k_{\|}d = 0.5\pi$ the modes after the sixth leak into the AlAs (see figure 3(b)), which does not happen when $k_{\|}d = 0.05\pi$. Finally, we note that in

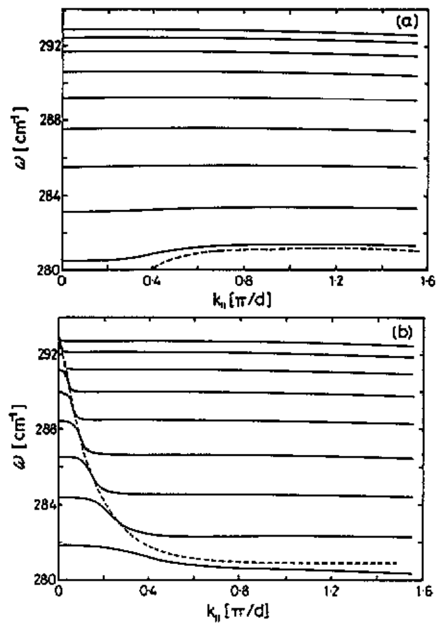

Figure 2. The dispersion curves (full lines) for (a) even modes and (b) odd modes. The dashed curves are the dispersion curves for the corresponding interface phonons in the DCM.

the long wavelength limit $k_{\|} \to 0$ equation (9) gives $n = m\pi/2d$, $m = 2, 4, 6, \ldots$ in agreement with the theory in the dispersionless limit.

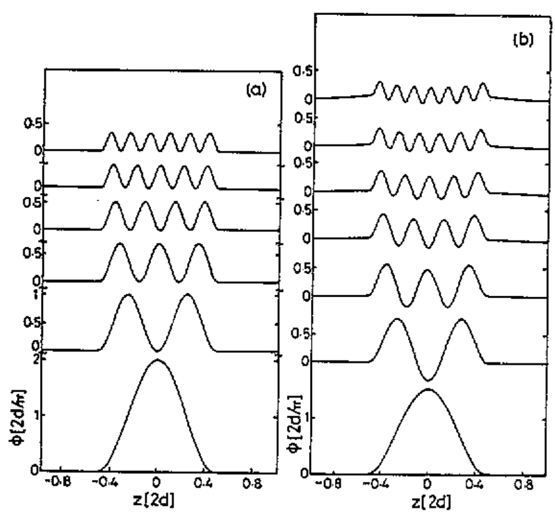

Figure 3. The potential functions for even modes for (a) $k_{\|}d = 0.05\pi$ and (b) $k_{\|}d = 0.5\pi$.

Figure 2(b) shows the dispersion curves for odd modes which are the solutions of equation (10). The potential functions are presented in figure 4(a) for $k_{\|}d = 0.05\pi$ and figure 4(b) for $k_{\|}d = 0.5\pi$. We see by inspection of figure 2(b) that, for large $k_{\|}$,

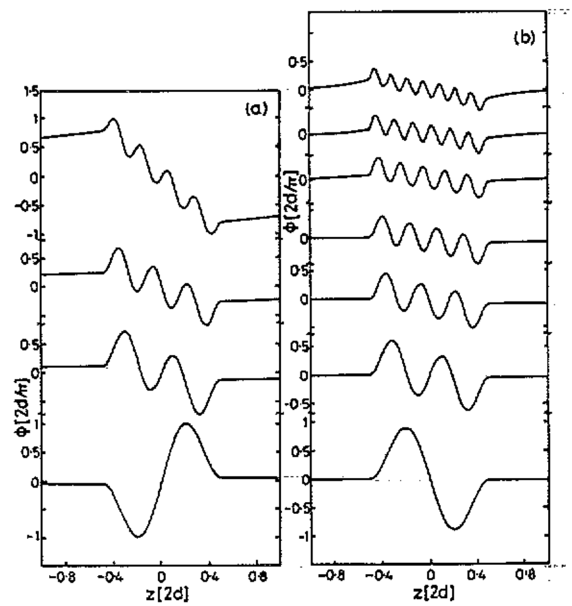

Figure 4. The potential functions for odd modes for (a) $k_{\parallel}d = 0.05\pi$ and (b) $k_{\parallel}d = 0.5\pi$.

the dispersion is again almost parabolic. The corresponding modes (figure 4(b)) are confined and have potential functions close to those predicted in the dispersionless limit. The odd modes with lower frequency, closer to $(\omega_{L2} + \omega_{T2})/2$, begin to leak into the AlAs layers and show stronger interface character. As $k_{\parallel}$ becomes smaller the parabolic dispersion is distorted. The distortion follows the odd interface phonon dispersion curve [10] which is plotted as a dashed line in figure 2(b). The number of modes that acquire interfacial character is larger for $k_{\parallel}d = 0.05\pi$ than for $k_{\parallel}d = 0.5\pi$, because the odd interface phonon is more dispersive for small $k_{\parallel}$. The dispersion curves for the odd modes are almost horizontal straight lines when $k_{\parallel}$ is large because b is rather small in GaAs. If these lines are extrapolated to $k_{\parallel} = 0$ we find points of intersection with the dashed curve for the corresponding interface phonon. Strong admixture of the confined and interface character of the true modes occurs near these points. Moreover, we see that the true dispersion curves bend upwards there and, when $k_{\parallel} \to 0$,they follow the extrapolated dispersion curves for the confined mode with one less node. (In this limit, equation (10) gives $n = m\pi/2d$, $m = 3, 5, 7, \ldots$. We note that m assumes *exactly* odd values and not *approximately* an odd integer as in the dispersionless limit.)

We have ignored retardation throughout our calculations for the following reason. The space scale of the system is set by the width of the GaAs layer which is typically 100 Å. An electromagnetic wave will traverse this distance in the order of 10^{-17}s which is much less than the period (10^{-13}s) of the LO phonons with which we are concerned (see, for example, [18]).

Closer comparison of the predictions for the odd modes when $k_{\parallel}$ is small for the model used here with results for a microscopic model would be very illuminating. We also find strong hybridization for modes with frequencies lying between the two interface phonon curves and microscopic calculations in this region would also be useful.

While this letter was in the course of publication the authors became aware of a calculation by Nash reaching similar conclusions [19]. Ridley has recently discussed optical phonons in a quantum well with infinitely rigid side walls [20].

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