5.2 Polar-optical phonons: Frohlich interaction	5.2 Các phonon quang phân cực: tương tác Frohlich

	checked
One of the most important carrier-phonon scattering mechanisms in semiconductors occurs when charge carriers interact with the electric polarization, P(r), produced by the relative displacement of positive and negative ions. In low-defect polar semiconductors such as GaAs, InP, and GaN, carrier scattering in polar semiconductors at room temperature is dominated by this polar-optical-phonon (POP) scattering mechanism. The POP-carrier interaction is referred to as the Frohlich interaction, after H. Frohlich, who formulated the first qualitatively correct formal description. In this book, the potential energy associated with the Frohlich interaction will be denoted by #r(r). Clearly the polarization P associated with polar-optical phonons and the potential energy associated with the Frohlich interaction, #r(r), are related by	Một trong những cơ chế tán xạ hạt tải điện-phonon quan trọng nhất trong bán dẫn xuất hiện khi các hạt tải điện tương tác với lưỡng cực điện, P(r), hình thành do chuyển động tương đối của các ion dương và âm. Trong các bán dẫn phân cực khuyết tật thấp chẳng hạn như GaAs, InP, và GaN, tán xạ hạt tải điện ở nhiệt độ phòng chủ yếu do cơ chế tán xạ phonon quang phân cực (POP) này chi phối. Tương tác POP-hạt tải điện được gọi là tương tác Frohlich, theo tên của Frohlich, người đầu tiên đã mô tả hiện tượng này một cách chính xác về mặt định tính. Trong sách này, chúng ta sẽ kí hiệu thế năng ứng với tương tác Frohlich là #r(r). Rõ ràng, độ phân cực P gắn với các phonon quang phân cực và thế năng gắn với tương tác Frohlich, #r(r) liên hệ với nhau qua công thức
Consider the case of a polar crystal with two atoms per unit cell, such as GaAs. Clearly, the dominant contribution to P(r) results from the phonon modes in which the normal distance between the planes of positive and negative charge varies. Such modes are obviously the LO modes since in the case of	Xét trường hợp tinh thể phân cực với hai nguyên tử trên một ô đơn vị, chẳng hạn như GaAs. Đóng góp chủ yếu vào P(r) là các mode phonon trong đó khoảng cách (vuông góc) giữa các mặt phẳng điện tích dương và âm thay đổi. Hiển nhiên, những mode như thế là các mode LO bởi vì trong trường

LO modes eq, j is parallel to q. However, TO phonons produce displacements of the planes of charge such that they remain at fixed distances from each other; that is, the charge planes ‘slide’ by each other but the normal distance between planes of opposite charge does not change. So, TO modes make negligible contributions to P(r). For TO phonons, eq, j ' q — 0. Accordingly,	hợp các mode LO eq, j song song với q. Tuy nhiên, các phonon TO tạo ra sự dịch chuyển của các mặt phẳng điện tích sao cho chúng vẫn cách nhau khoảng cách cố định; tức là, các mặt phẳng điện tích “trượt” so với nhau nhưng khoảng cách (vuông góc) giữa các mặt phẳng điện tích đối diện không thay đổi. Vì vậy, các mode TO đóng góp không đáng kể vào P(r). Đối với các phonon TO, ……..Do đó,
5.3 Acoustic phonons and deformation-potential interaction The deformation-potential interaction arises from local changes in the crystal’s energy bands arising from the lattice distortion created by a phonon. The deformation- potential interaction, introduced by Bardeen and Shockley, is one of the most important interactions in modern semiconductor devices and it has its origin in the displacements caused by phonons. Indeed, the displacements associated with a phonon set up a strain field in the crystal. In the simple case of a one-dimensional lattice, the energy of the conduction band, Ec, or the energy of the valence band, Ev, will change by an amount Ec,v — Ec,v(a) — Ec,v(a + u), (5.35)	[redacted]

where a is the lattice constant and u is the displacement produced by the phonon mode. Since a » u, it follows that

A Ec,v(a) — (dEc,v(a)/da)u• (5.36)

Thus the phonon displacement field u produces a local change in the band energy; the energy associated with the change is known as the deformation potential and it represents one of the major scattering mechanisms in non-polar semiconductors. Indeed, the deformation-potential interaction is a dominant source of electron energy loss in silicon-based electronic devices. The three-dimensional generalization of AEc,v is

A Ec,v(a) — (dEc,v(a)/dV)AV, (5.37)

where V is a volume element and AV is the change in the volume element due to the phonon field. For an isotropic medium AV/ V — V ■ u and the last expression becomes,

AEc,v(a) — V(dEc,v(a)/dV)V ■ u, (5.38)

which is usually written as

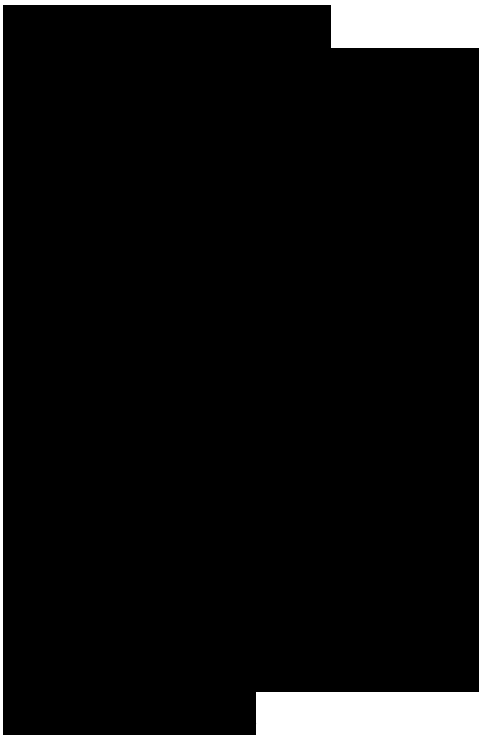
Hdcefv — AEc,v(a) — E1,vV ■ u (5.39)

The superscripts on H^f and E^ are necessary since the deformation potential for electrons is different from that for holes. Chapter 9 provides a discussion of the case where the

medium is not assumed to be isotropic.

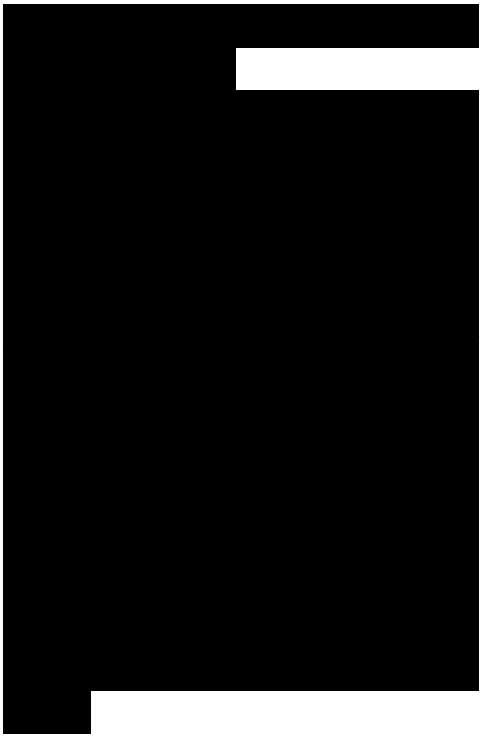
5.4 Piezoelectric interaction

The piezoelectric interaction occurs in all polar crystals lacking an inversion symmetry. In the general case, the application of an external strain to a piezoelectric crystal will produce a macroscopic polarization as a result of the displacements of ions. Thus an acoustic phonon mode will drive a macroscopic polarization in a piezoelectric crystal. In rectangular coordinates, the polarization created by the piezoelectric interaction in cubic crystals, including zincblende crystals, may be written as



7.1 Dielectric continuum model of phonons

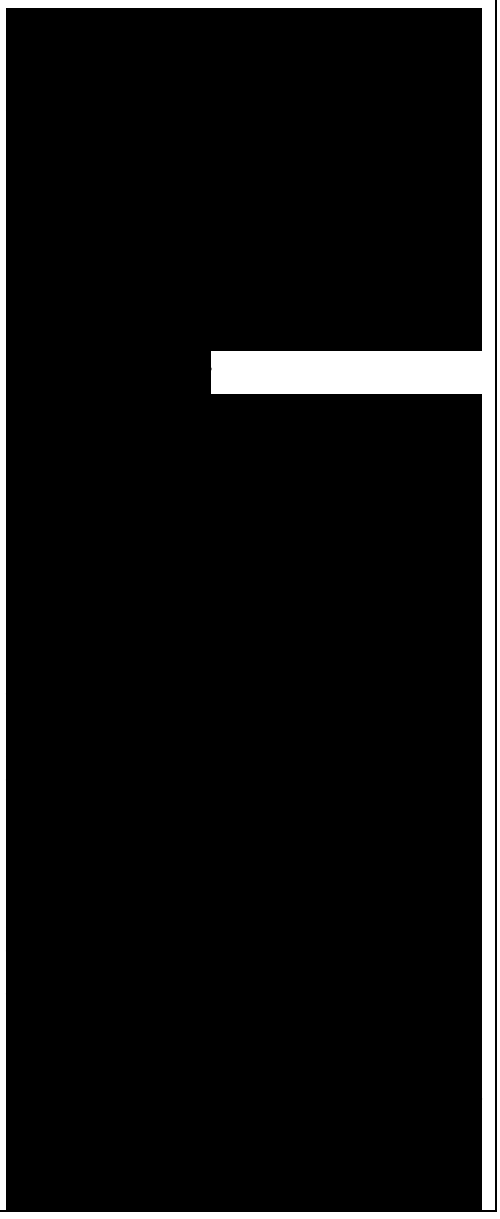
The dielectric continuum model of optical phonons in polar materials is based on the concept that the associated lattice vibrations produce an electric polarization P(r) that is describable in terms of the equations of electrostatics for a medium of dielectric constant e(rn). The volume of the structure is assumed to be L3 (-L/2 < x, y, z < +L/2) with periodic boundary conditions. The potential $(r) associated with P(r) is given by (Kim and Stroscio, 1990)



for a ternary polar material

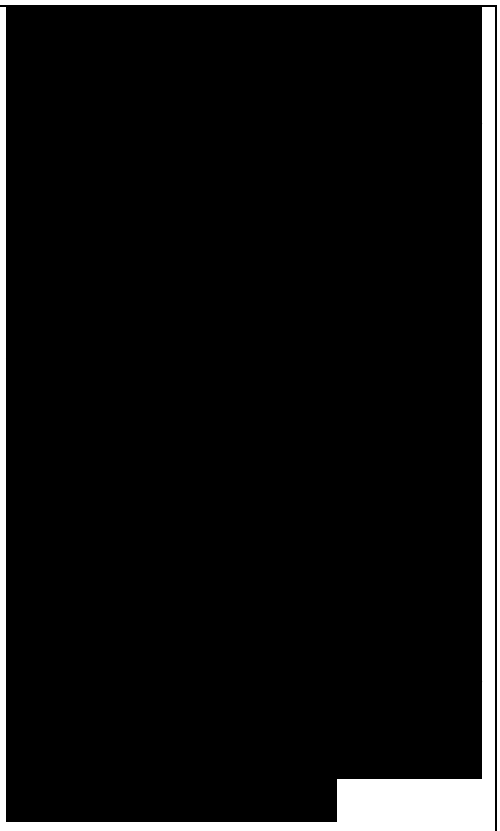
AyB\—yC, where the subscript a denotes frequencies associated with the dipole pairs AC and the subscript b denotes frequencies associated with the dipole pairs BC. As in subsection 2.3.1, the displacement field is related to the fields E(r) and P(r) through the driven oscillator equation and through the effective charge, e* : for a binary medium n,

An alternative and useful form of these equations for the case of a binary material results straightforwardly from the relations of Appendix A. Indeed, it is shown in Appendix A, equations (A.8) and (A.9), for a diatomic polar material that



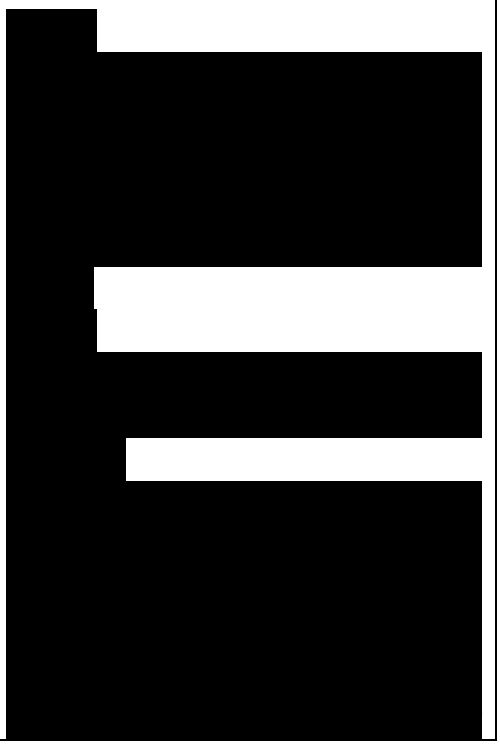
In the first equation it has been assumed that u has a general form for the time dependence and may not be simply sinusoidal in o. As will become evident, this pair of equations is well suited as the basis for an alternative method for performing the calculations of subsection 7.3.1. Moreover, it provides a convenient starting point for the derivation of the macroscopic equations describing optical phonons in polar uniaxial materials (Loudon, 1964). Uniaxial materials such as the hexagonal wurtzite structures GaN, AlN, and Gax Ali-x N have relatively

wide bandgaps and are suited for high-temperature electronics and short-wavelength optoelectronic devices. Loudon (1964) introduced a useful model for describing the macroscopic equations of a uniaxial polar crystal by introducing one dielectric constant associated with the direction parallel to the c-axis, ey, and another dielectric constant associated with the direction perpendicular to the c-axis, e±. In Loudon's model a separate set of Huang-Born equations is necessary for the phonon mode displacements parallel to the c-axis, uy, and perpendicular to it, uT. For a medium denoted by n it then follows straightforwardly that



and

(7.12)



Of course, in Loudon's model these six equations must be supplemented by the following three equations of electrostatics for the case where there is no free charge:

(7.13)

where z and p are the unit vectors in the \| and ± directions respectively.

In the first and third of this set of nine equations, it has been assumed that uT,n and iiy,n have a general form of the dependence and may not be simply sinusoidal in M; the

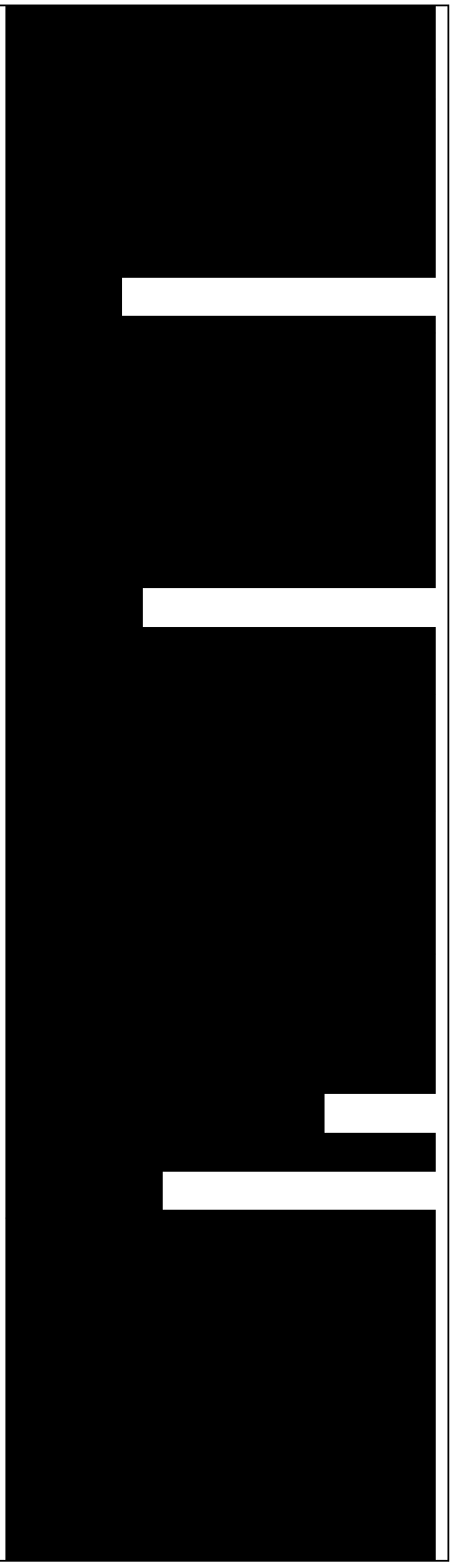
assumption of sinusoidal time dependence made in Appendix A was not necessary and simply by replacing -«2u by u it is straightforward to rederive the results of Appendix A without assuming a sinusoidal time dependence.

The above set of nine equations provides a convenient basis for describing carrier-optical-phonon scattering in wurtzite crystals. Indeed, using the relations for the displacement perpendicular (parallel) to the c-axis,

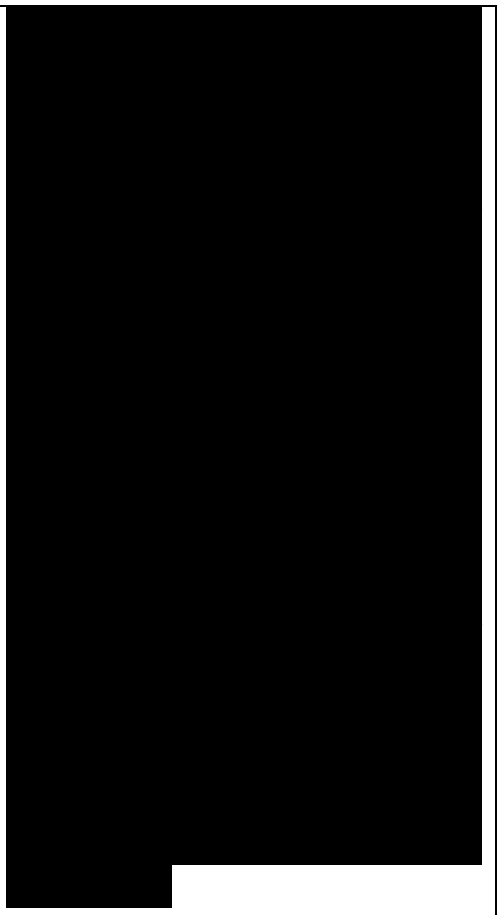
In the isotropic case, e(rn)T = e(«)y and this result must reduce to the expression, (5.34), obtained in Section 5.2 for the interaction Hamiltonian describing the carrier-LO-phonon interactions. Indeed, since the general form of the Lyddane-Sachs-Teller relation implies that the Hamiltonian for the uniaxial case reduces to (5.34) upon taking e(rn)T = e(«)\| and Mq = MLO.

7.2 Elastic continuum model of phonons

As will become clear, the elastic continuum model of acoustic phonons provides an adequate description of acoustic phonons for nanostructures having confined dimensions of about two atomic monolayers. A simple and illustrative application of the elastic



continuum model is found in the case of a longitudinal acoustic mode propagating in a quasi-one-dimensional structure. Consider an element dx located along this structure between x and x +dx. Let u(x, t) be the elastic displacement at x along the axis of the one-dimensional structure; that is, u (x, t) describes the uniform longitudinal displacement of the element dx. In the elastic continuum model the dynamics of the mass-containing element, dx, are described in terms of Newton's laws. Indeed, defining the strain as e = du/dx and the stress, T(x), as the force per unit area in the quasi-one-dimensional structure of area A, it follows from Hooke's law that



T = Ye, (7.23)

where Y is a proportionality constant known as Young's modulus. The force equation describing the dynamics of the element dx of density p(x) is given by

Seeking solutions of this one-dimensional wave equation of the form u(x) =

% el (qx Mt), where q = 2n/\ and M is the angular frequency of the wave, it follows that the dispersion relation for the longitudinal acoustic (LA) mode is pm2 = Yq2 or m = viq, where vi = Y/p. The

longitudinal sound speed, vi, has typical values (3-5) x 105 cm s 1 and for p = 4 g cm 3 it follows that Y must have an order of magnitude of 1012 g cm s-2.

The three-dimensional generalization of these results may be accomplished through the replacements (Auld, 1973) u(x) ^ u(x, y, z) = (u, v, w) and T = Ye ^ T = c : S with T\ = djSj. In this generalization, Young's modulus is replaced by a 6 x 6 matrix of elastic constants Cij; T is replaced by a six-component object Ti; e is replaced by a six-component object Sj. For the cubic, zincblende, and wurtzite crystals the most general form of the stress-strain relation, Tij = cijklSkl, where i, j, l, k run over x, y, z, may be represented by Ti = cij Sj. In this last result,

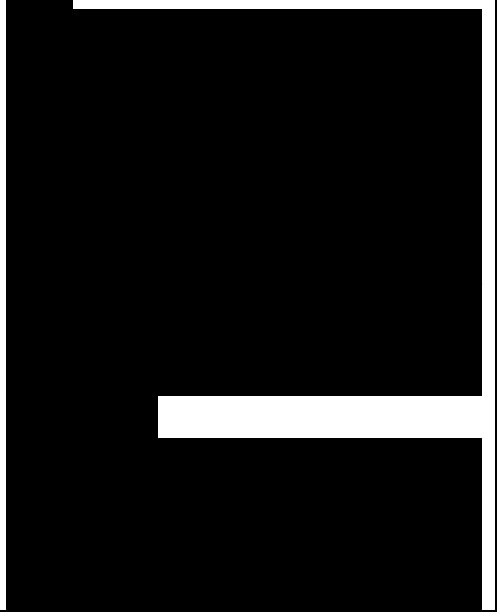
For the elastic energy to be single valued cij = Cji, and it follows that only 21 distinct elements are necessary to define the 6 x 6 matrix cij. Nanostructures of widespread interest in modern electronics and optoelectronics are generally fabricated from zincblende and wiirtzite crystals. For cubic crystals, including zincblende crystals, the matrix cij is of the form and

for wurtzite crystals cij is of the form

For a cubic medium such as the zincblende crystal, only three independent elastic constants, c11, c1q, and c44, are needed to specify all the cij. For an isotropic cubic medium c1q = c11 — 2c44, and only two constants X and i are necessary to define the ci

The constants X and i are known as Lame's constants. Thus, in the cubic case three independent constants replace Y: c11, which relates the compressive stress to the strain along the same direction, [100]; c44, which relates the shear stress and the strain in the same direction; and c1q, which relates the compressive stress in one direction and the strain in another direction. For the isotropic case, it follows that

Two alternative forms of the three-dimensional force equations are encountered frequently in the literature. The first of these is derived by writing the components of u(x, y, z) = (ui, u2, u3) as ua, a = 1, 2, 3; it then follows that the three force equations may be rewritten as

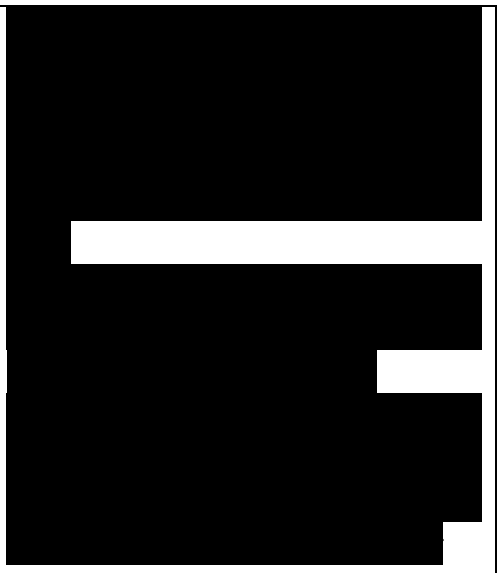


In these equations, the subscripts a and fi run over 1, 2, 3 (corresponding to x, y, z). A repeated index in a term implies

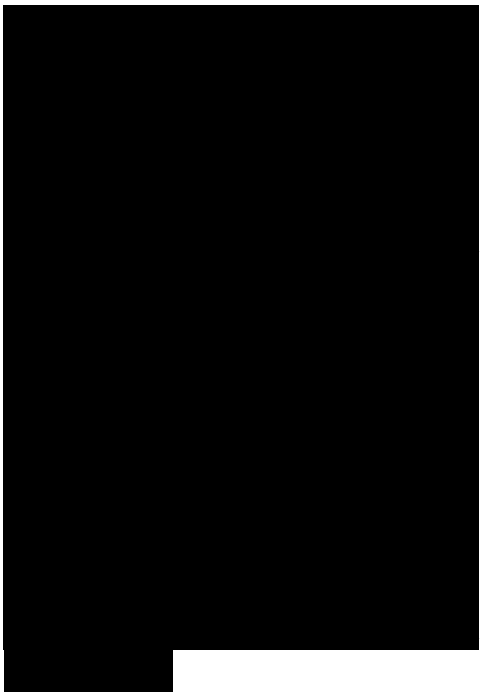
summation. Sap is the Kronecker delta function. In a second alternative form the three force equations are written straightforwardly as the single vector equation

Here, ct and ci are the transverse and longitudinal sound speeds and we have

In physical acoustics the solutions for the displacement fields are frequently specified in terms of two potential functions, a scalar potential $ and a vector



The scalar potential $ corresponds to the ‘irrotational’ part of the solution and the vector potential corresponds to any remaining ‘rotational’ fields. In the literature the irrotational solutions are also referred to as the longitudinal, compressional, or dilatational solutions. Moreover, seismologists frequently refer to these solutions as P waves. Likewise, the rotational vector-potential solutions based on are identified as transverse, shear, distortional, or equivoluminal solutions. In seismology these solutions are commonly identified as S waves.



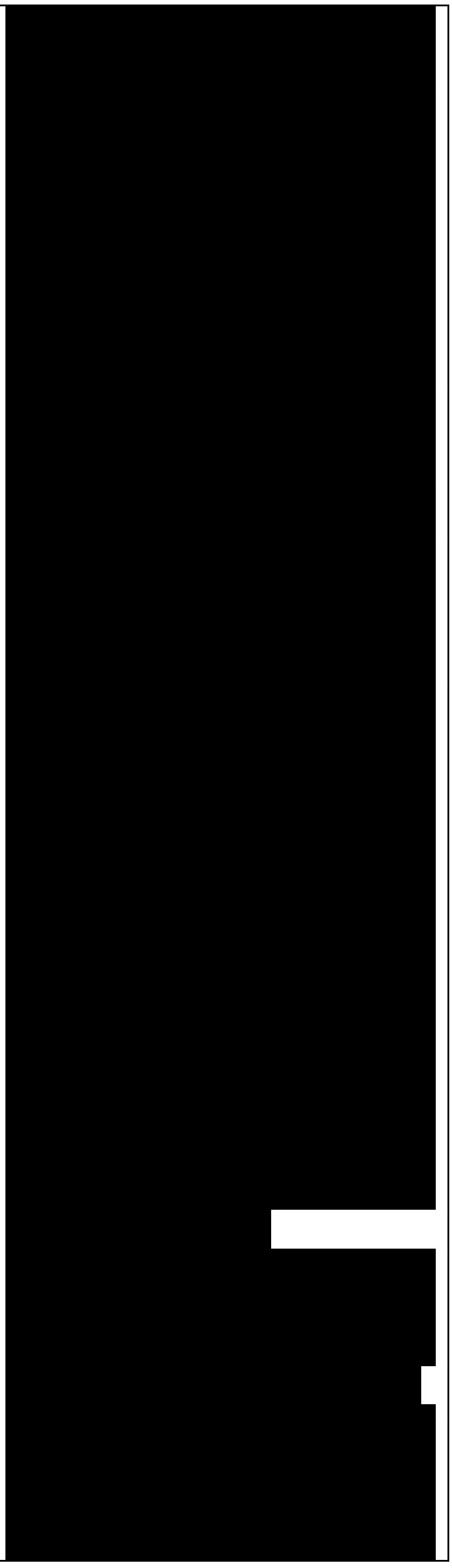
7.3 Optical modes in dimensionally confined structures

The dielectric continuum model has been applied to describe the properties of dimensionally

confined optical phonons in many electronic and optoelectronics devices fabricated from semiconductor nanostructures. These include quantum wells, superlattices, quantum wires, and quantum dots. To illustrate the basic features of the dielectric continuum model of optical phonons, the case of confinement in just one dimension - as in a quantum well or superlattice - is considered first. In addition, the dielectric continuum model will be compared with other continuum models, including the hydrodynamic model and the reformulated dielectric continuum model. These models predict different sets of confined optical phonon modes but each model predicts the same carrier-phonon scattering rate as long as it includes a complete set of orthogonal phonon modes (Nash, 1992). Following a comparison of these models, a microscopic treatment of confined phonon modes will be discussed.

7.3.1 Dielectric continuum model for slab modes: normalization of interface modes

The dielectric continuum model predicts a set of confined optical phonon modes commonly referred to as the slab modes.



These slab modes may be determined by applying the dielectric continuum model and by imposing electrostatic boundary conditions at each heterointerface. The normal-mode frequencies and orthogonal confined phonon modes are obtained through the simultaneous solution of the equations arising from the dielectric continuum model, subject to the boundary conditions that the potential, $ (r) and the normal component of D(r) are continuous at each heterointerface. Taking the heterointerfaces to be normal to the z-direction, the electrostatic potential (r) in the region Ri — (zi, n+1) and its two-dimensional Fourier transform (q, z) are related by

(7.42)

Following the concepts of Section 5.1, the mode normalization condition requires that the energy of a phonon of mode q is h rnq; for the case of a single interface at z — 0 separating two layers n and m, this condition is

(7.44)

To illustrate the normalization procedure, let us consider one of the classes of optical phonon modes existing for this one-heterointerface structure. The wave equations for the fields of relevance here admit both

oscillating and exponential solutions. In particular, let us consider the solutions having an exponential character. For these modes, known as the interface (IF) modes, we take. where q is the unit vector specifying the direction of q = (qx, qy). Let material n be a binary layer filling the space z > 0, region i, and material m be a ternary layer filling the space z < 0, region 2, as illustrated in Figure 7.i. Then, for the right-hand medium, material i, using the notation of Appendix B, it follows that

For material 2, there are two driven-oscillator equations, one for the AC pair, denoted by a, and one for the BC pair, denoted by b:

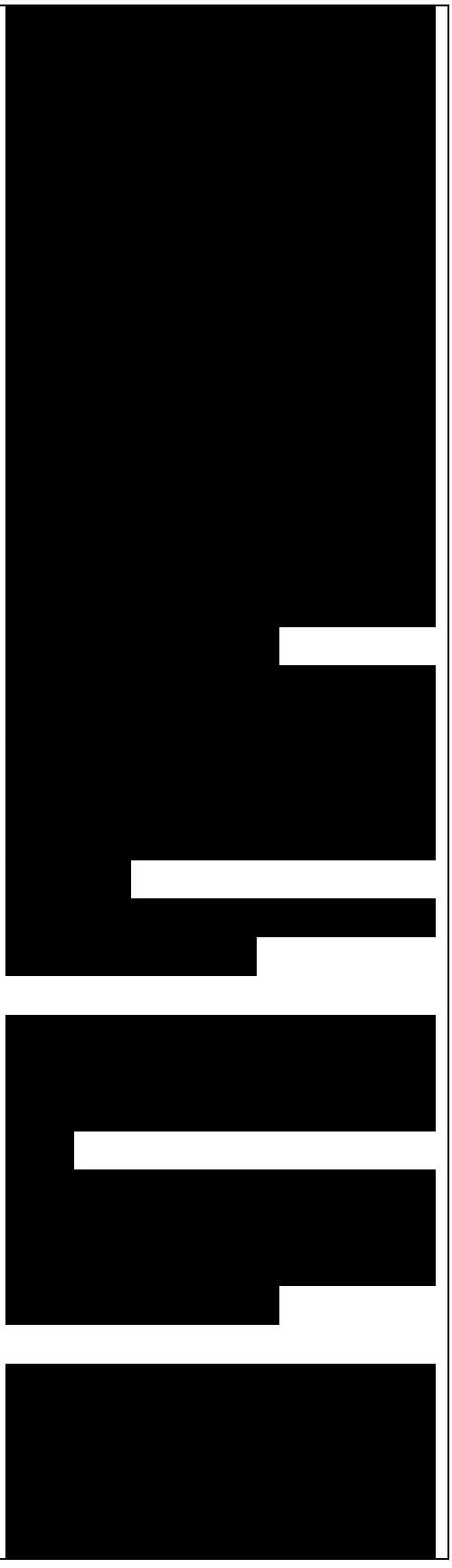
and the electric polarization in the virtual-crystal approximation is

With these expressions for u1(q, z) and uq a(b)(q, z), the normalization condition, with n — 1 and m — 2, yields

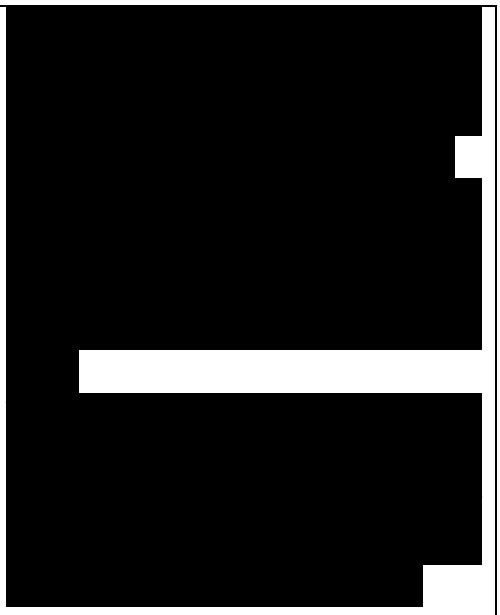
where the integral in the first term has been performed using

and the second and third integrals have been performed using

Thus the normalization constant c is determined. It is convenient to rewrite this expression using conditions derived by Wendler (1985). These conditions are



discussed in Appendix B. The conditions that are useful at this point in our derivation are



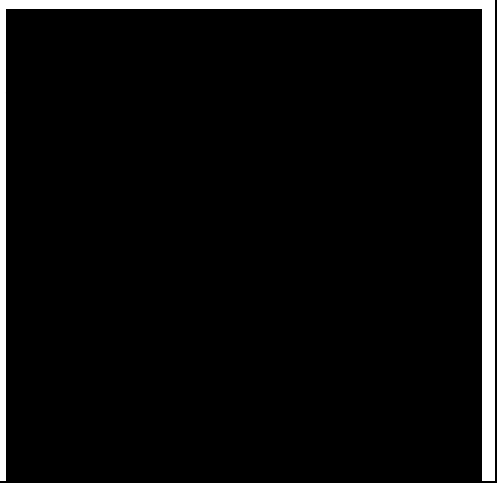
Here the subscript n represents either material 1 or material 2. In these relations, the plasma frequency squared, «2lasma n, is given by

As may be verified algebraically, the Lyddane-Sachs-Teller relations of subsection 2.3.3 are satisfied by these frequencies (Wendler, 1985).

With these results of Wendler, a straightforward but lengthy derivation yields

where, as discussed previously,

Finally, multiplying $(r) by — e and introducing aq and aq, according to the procedure described in Section 5.1, the interaction Hamiltonian for the interface (IF) optical phonon mode may be written as (Kim and Stroscio, 1990)



where eq, j and eq j of equation (6.2) have been taken as unit vectors in the longitudinal direction, since the IF phonon modes considered here are longitudinal optical (LO) phonons. The dispersion relation for this optical phonon mode is given from the requirement that the normal components of the electric

displacement field be continuous at z = 0, that is, 62(G)E2,Z |z=0 = 61 (G)Ei,z |z=0. From this condition, it follows immediately that the frequencies of the IF optical phonons must satisfy 61(G) + 62(G) = 0.

This result is similar to that for a bulk semiconductor, where the optical phonon frequencies must satisfy 6 (G) = 0. Moreover, since this is the condition necessary for the propagation of any longitudinal electromagnetic disturbance, it was expected that the frequencies of longitudinal optical phonons should satisfy this dispersion relation.

7.3.2 Electron—phonon interaction for slab modes

Here, it is instructive to consider an earlier - and intuitively very appealing - theory of electron-phonon interactions in a dielectric slab given by Licari and Evrard (1977). In this theory, a single dielectric slab of infinite extent in the x- and y-directions is situated with its faces at —a and +a and with its surface bounded by a vacuum in the regions with |z| > a. Within this dielectric slab V- D — 0, where,

as usual, D(r) = e(;)E(r) = E(r) + 4nP(r); 6(G) is the dielectric constant of the slab and P(r) is

the electric polarization associated with the optical phonons in the slab. Defining a scalar potential through E(r) = —V0(r) and, since the system is translationally invariant in the xy-plane, taking 0(r) to be of the form 0(r) = 0(z) elqH'p, where p = (x, y) and qy = (qx, qy), it follows that

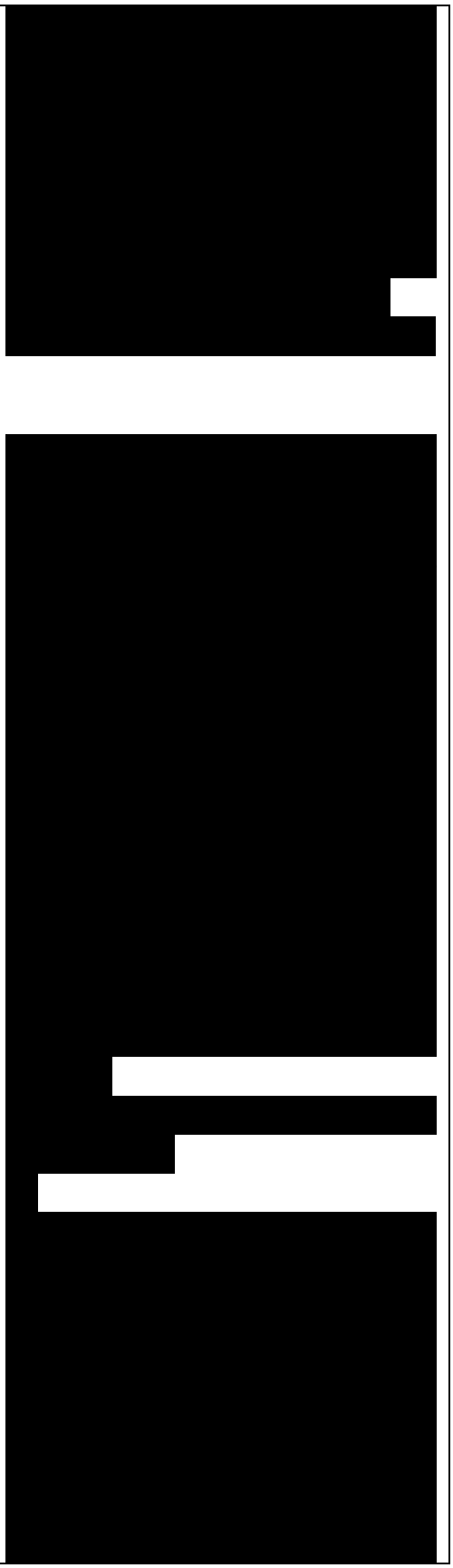
6(G) (1°, — q2) t(z) = 0 (7.61)

where q2 = qX + q2 This equation is satisfied when 6(G) = 0 or when (d2/d2z — q\\)0(z) = 0. As shown previously, from the general form of 6(G) - as given for example in Appendix A - and the Lydanne-Sachs-Teller relation, the condition 6(G) = 0 is satisfied for a single-material system when G = glo. In this case an arbitrary function, 0(z), is a solution of the wave equation; Licari and Evrard took this solution (as did Fuchs and Kliewer, 1965, and Kliewer and Fuchs, 1966a, b) to be of the form

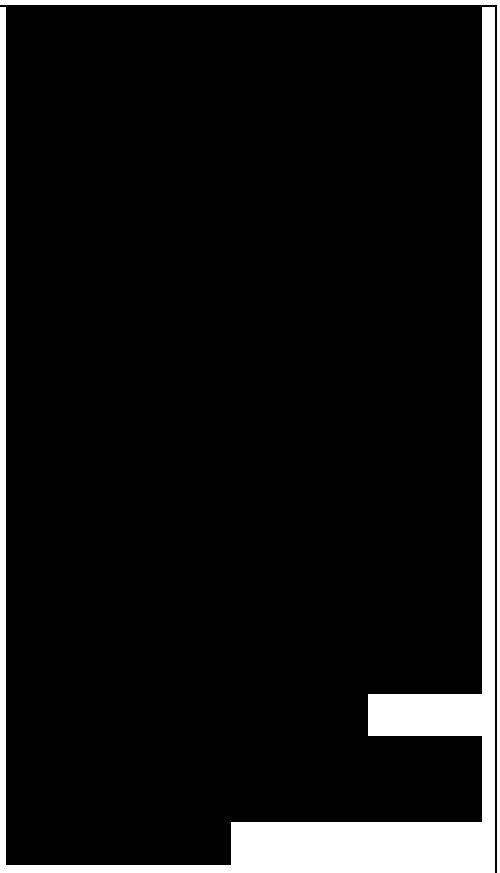
0(z) = ^($i sin qzz + 02 cos qzz), (7.62)

qz

inside the slab i.e., in the range (—a, +a). Outside the slab, where 6 = 1, the solutions have the form 0(z) = 0±exp(±^j~q2+~q2z), where the positive sign applies for z < — a and the negative sign applies for z > +a. The constants 0i, 02, 0+, and 0— are determined by the

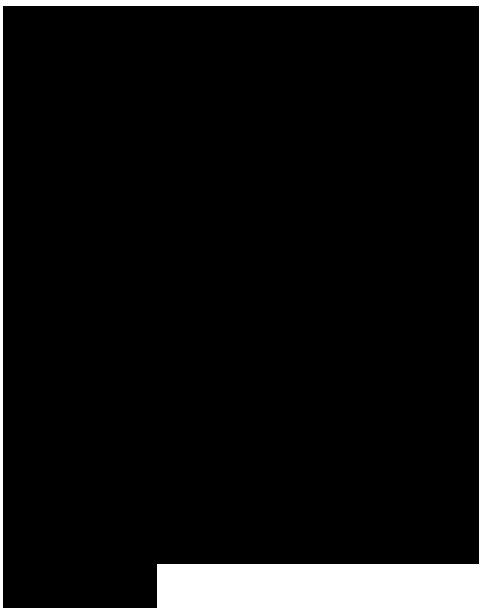


usual boundary conditions that the tangential component of E and the normal component of D are continuous at z = ±a. From these conditions it is seen that 0± = 0 and it is thus clear that for this mode 0(z), E(r), and D(r) are zero in the regions surrounding the slab; in particular 0 (z) vanishes at the surfaces of the layer, where z = ±a. For z in the range (—a, +a), the boundary conditions may be satisfied by taking either 01 = 0 or 02 = 0, so that there are two solutions corresponding to the two polarization vectors:

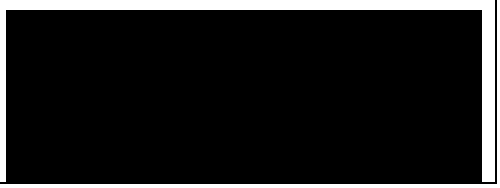


where z is the unit vector in the z-direction. Of course, V- D(r) = 0 implies that

V 20(r) = - V-E(r) = +4n V-P(r). These standing modes are now widely known as the confined optical phonon modes in a slab. They exist for m running from i to some maximum number N2a; the values of m must terminate at N2a, the number of unit cells in thickness 2a, since the continuum model adopted here must fail when the number of half-wavelengths in 2a becomes equal to or greater than the number of unit cells in the same thickness.

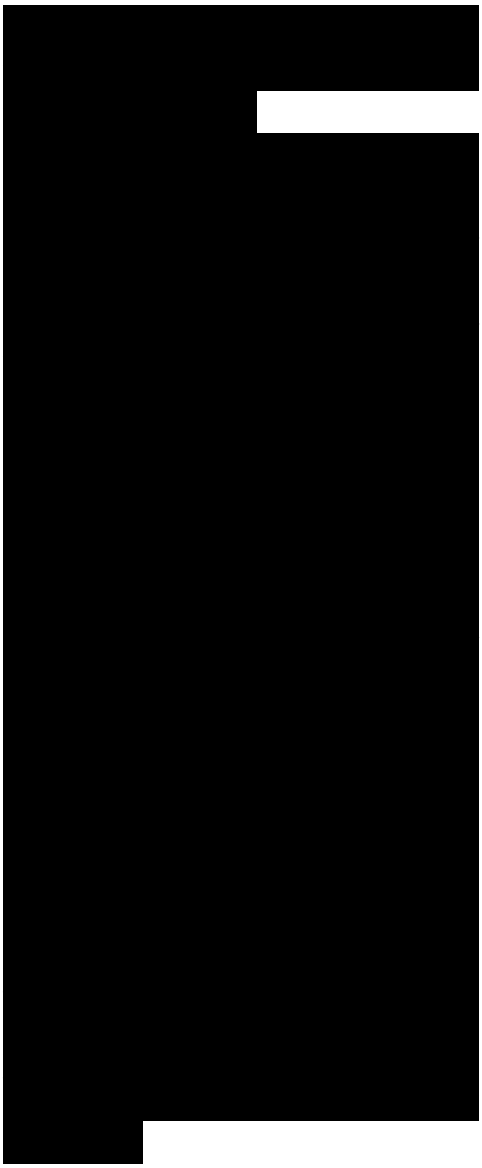


where qy is the unit two-dimensional wavevector. These last two modes describe the so-called IF optical phonon modes



in the polar semiconductor slab of thickness 2a. The boundary conditions imply that the frequencies for these modes are solutions of

where the plus sign corresponds to the even mode, the minus sign to the odd mode.



As pointed out by Licari and Evrard (1977), this continuum model is capable of predicting both the confined LO phonons and the interface IF optical phonons because for both of these modes there exists a polarization charge density. In particular, both p — —V • P, the volume charge density, and a ’ — —P • n, the surface charge density, contribute to the confined LO modes; here, n is the unit vector normal to the surface and pointing into the vacuum. For the IF modes, only a' makes a contribution. Clearly, in this model the polarization charge acts as the source of the fields associated with these phonon modes. Transverse modes are not predicted by this continuum approach since for such modes V P — 0 and P • n — 0.

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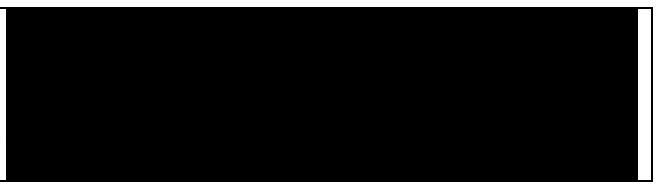
Licari and Evrard (1977) used this model to study the effects of electronic polarizability on the phonon modes and they derive conditions for the slab



which are equivalent to Wendler's conditions for the two-layer system described in Appendix B. Licari and Evrard also used their model to construct the normalized polarization eigenvectors and frequencies for the phonon modes of the dielectric slab. Moreover, they constructed the Hamiltonian for the electron-polar-optical-phonon interaction and showed that the correct harmonic oscillator energy is recovered when the eigenvectors of the slab are used to evaluate the Hamiltonian; in particular, it can be shown that the normal modes are consistent with the harmonic oscillator energy of Section 5.1. Finally, Licari and Evrard presented a very enlightening physical derivation of the electron-phonon interaction Hamiltonian for a slab by applying boundary conditions to the electron-phonon interaction Hamiltonian for a bulk semiconductor. Specifically, starting with expression for the bulk Frohlich interaction, which we take as the expression (5.34) derived in Section 5.2,

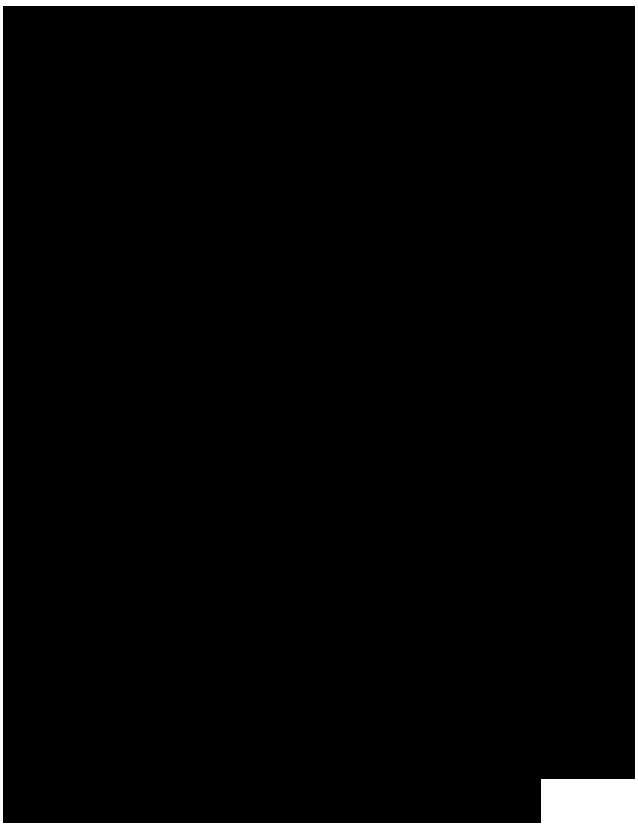
Licari and Evrard took q = (qy, qz) and split the sum over q into a sum over qy and a sum over qz

Then, using el9 = cos 9 + i sin 9 to write e±iqzz in terms of sines and cosines,

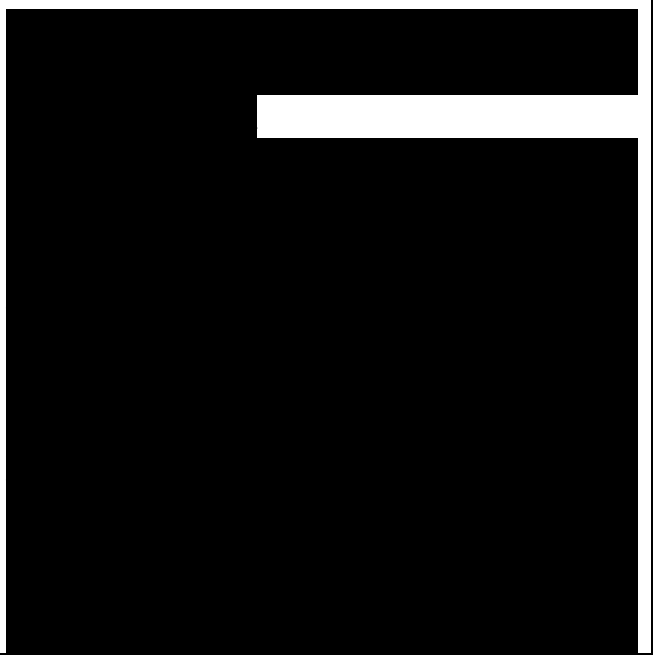
The operators a+ (—qy) and a— (—qy) are given by taking the adjoints. These operators describe phonons which propagate as plane waves in the x- and y-directions but as standing modes in the z-direction. Indeed, since qz =

mn/2a the Frohlich Hamiltonian for the two-dimensional slab takes the form

This Hamiltonian vanishes for z — ±a, as it must since the Frohlich interaction Hamiltonian is given by — e$, as explained in Section 5.2, and since $(±a) — 0 for the potential describing the fields associated with phonon modes in the dielectric slab. This heuristic derivation makes manifest the fact that the confined phonon modes in the slab located between —a and +a are standing modes with an integer number of half-wavelengths confined within the slab. This Hamiltonian does not contain the contributions of the IF optical phonons in the slab since it satisfies only the boundary conditions for the confined optical phonon modes at z — ±a, namely HFr(a) — —e^(±a) — 0. As shown by Licari and Evrard (1977), the Frohlich interaction Hamiltonian for the IF optical phonon modes in the dielectric slab is



7.3.4 Transfer matrix model for multi-heterointerface structures



Yu et al. (1997) derived a very useful set of normalization conditions for heterostructures containing multiple parallel heterointerfaces separating different semiconductor layers. These normalization conditions are essential for examining the optical phonon bandstructure in superlattices and they provide the basis for relatively straightforward calculations of the normalization factors for heterostructures containing just a few

heterointerfaces. Since translational invariance holds in the two-dimensional planes parallel to the heterointerfaces, the electrostatic potential describing the carrier-optical-phonon interaction in each region R; = (z;, z;+0 is denoted by $; (r) and is taken to be of the form

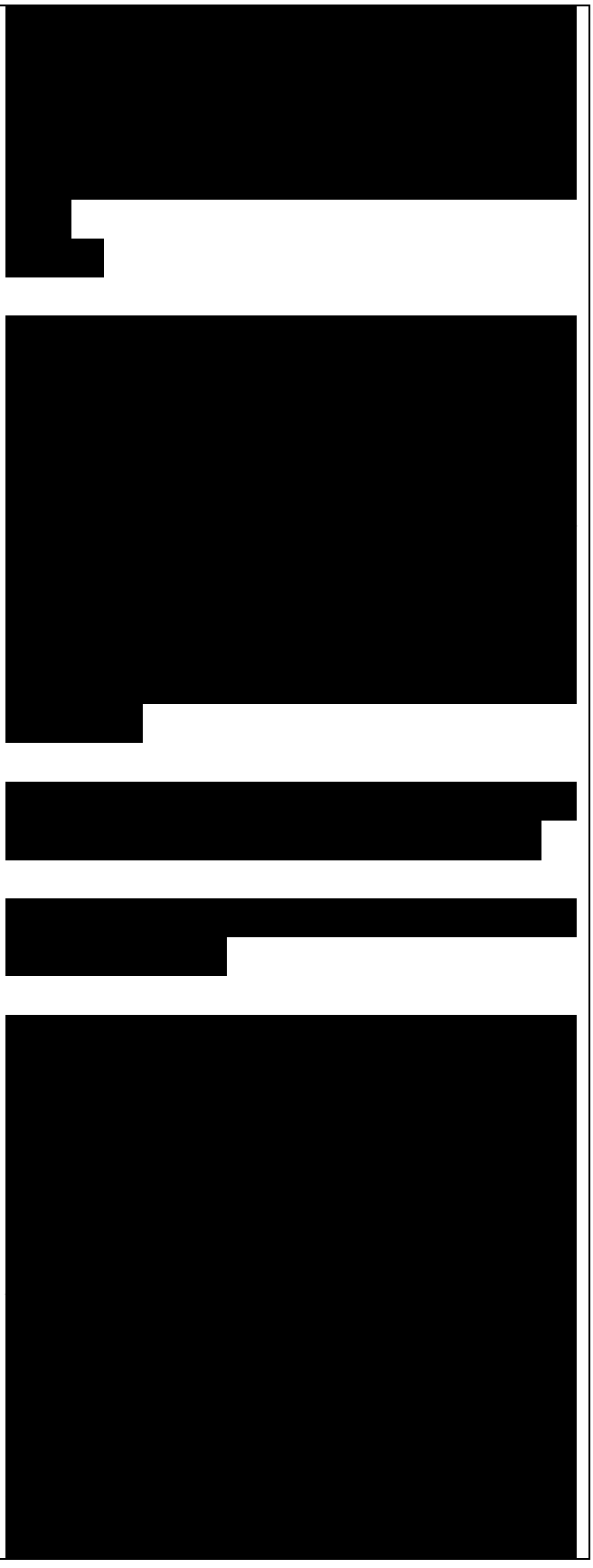
(7.101)

where the z-axis is taken to be normal to the heterointerfaces and where, as usual, p = (x, y) and q denote the position and wavevector in two dimensions. c;- and c; + are the relative amplitudes of the exponentially decaying and growing potentials, respectively, in layer i; as will become clear, these relative amplitudes are related through a transfer matrix. Figure 7.5 depicts a generic potential &; (z) for regions Ro, Ri,... , R„.

7.6 Continuum model for acoustic modes in dimensionally confined structures

7.6.3 Acoustic phonons in rectangular quantum wires

The classical compressional acoustic modes in free-standing rods with rectangular cross sections have been examined experimentally (Morse, 1948) and theoretically (Morse, 1949, 1950). The solutions obtained by Morse are based on the elastic continuum model as well as on the approximation method of separation of variables. As illustrated previously, these classical elastic continuum solutions provide the basis for describing the compressional - that is, the longitudinal - phonon modes in a nanoscale quantum wire with a



rectangular cross section. For cross-sectional dimensions with aspect ratios of approximately two or greater, Morse (1948, 1949, 1950) found that these solutions provide simple and accurate analytical expressions in agreement with the experimentally observed modes over a wide range of conditions. Consider a free-standing rectangular rod of infinite length in the z-direction with an x-directed height 2a and a width 2d in the y-direction, as shown in Figure 7.18.

Taking the origin of the coordinates in the geometric center of the of the xy-plane, the acoustic mode displacements determined by Morse are given by u(x, y, z) — (u1, v1, w1), where

p is the density of the elastic medium, and the longitudinal and transverse sound speeds are given by

The modes associated with this case are known as the ‘thickness modes’, as designated by Morse, who showed that h — h1 — h2 leads to an adequate description of the experimentally determined modes when d > 2a (Morse, 1948). Using the expressions (7.177) for u, v, and w to evaluate Txx — Tyx — Tzx — 0 at x — ±a, it follows that

(7.180)

The dispersion relation for q2 — 0 is given by the expression resulting from the condition that the determinant of the coefficients vanishes, that is,

tan q2a 4q1q2(h2 + y 2) tan q1a (h2 + y2 — q|)2’

which is similar to the dispersion relation for a free-standing layer

discussed in subsection 7.6.1. For calculating the acoustic phonon frequencies as functions of the wavevector, Y , it is convenient to rewrite this dispersion relation as

where x2 and ty2 are related to q1 and q2 through q1 — (n / a^^JTx^—ty2, q2 — (n/a)^x2 — ty2 and in accordance with mf — cl(y2 + h2 + qf) and mf — ct(y2 +

h2+q|), where e - (ct/ci)2 - (1—2a)/(2 — 2a). Defining 5 - ay/n andrecalling that My - cy, it follows that

(7.183)

The remaining constant A is determined by quantizing the phonon amplitude according to

(7.186)

where MY is the angular frequency of the mode with wavevector y. Performing the indicated integrations, it follows

with

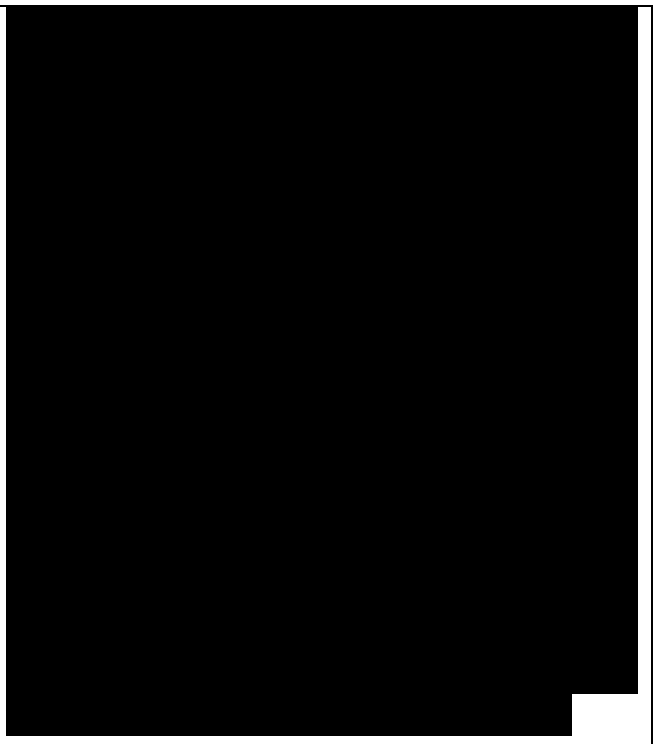
It is convenient to define a new normalization constant BY, through

As discussed by Morse, h must be chosen to satisfy the boundary condition on the stress components at y = ±d, that is, Tyy = Txy = Tzy = 0. This can be accomplished for d > 2a since in this case Txy and Tzy become negligible; with Tyy = 0 this implies that

hd = (n + 1)n, n = 0, 1, 2,... .

The principal propagation mode has no nodal surfaces parallel to the length of the quantum wire; this corresponds to the case n = 0. Morse found close agreement between theory and experiment for a/d = 1/8 and as expected less agreement for a/d = 1/2.

In addition to the ‘thickness modes’ another set of modes was observed experimentally by Morse (1948, 1950). These modes are known as ‘width modes’ and are determined by a procedure used to analyze the ‘thickness modes’. Specifically, Morse took q1 = q2 = q and obtained a set of equations similar to those for u1, u1, and w1 but with x and y interchanged. By imposing the boundary conditions at y = ±d, the ‘width modes’ were found to have a dispersion relation identical in form to that for the ‘thickness modes.’ The dispersion curves for selected acoustic modes are shown in Figure 7.19 for a 28.3 A x 56.6 A GaAs quantum wire and in Figure 7.20 for a 50 A x 200 A GaAs quantum wire.



For carriers at the non-degenerate V point in band a, Ea(k), the deformation-potential interaction Hamiltonian Hof is given in terms of the displacement operator u(r) by
(7.191)

At such a symmetry point, only the irrotational - that is, the longitudinal - components of u(r) contribute to Accordingly, only the the potential 0 contributes to Hdef. Since there are multiple modes for a given value of n, another index, m, is needed to describe the phonon spectrum at each value of Y . For the case of a quantum wire, the quantization of the acoustic phonons may be performed by taking (7.192)

where the components of u(y, x, y) = (u,v,w) were normalized previously over the area 4ad. The deformation

potential is then given by (7.193)
and, upon applying the Fermi golden rule, these combinations lead to conditions enforcing the conservation of energy.

The Hamiltonian is independent of time. In Chapters 8 and 9, such time-independent carrier-phonon Hamiltonians will be used in applying the Fermi golden rule to calculate carrier-phonon scattering rates. The carrier-phonon interaction also has a time dependence of the form eLJY 1, where rnY is the phonon frequency. As will become obvious in Chapters 8 and 9, such time-dependent factors are combined with the time-independent factors of carrier wavefunctions.

7.6.4 Acoustic phonons in cylindrical structures

The acoustic phonons in a cylindrical waveguide and in a cylindrical shell illustrate key features of the confined modes in dimensionally confined structures. The cylindrical waveguide is of obvious practical importance. Furthermore, the cylindrical shell is of interest because it approximates a single-walled buckytube
and also because it resembles the microtubuline structure found in many parts of the human body. As discussed previously in this section and in Section 7.3, the elastic continuum model provides an approximate description of the acoustic phonon modes in such dimensionally confined nanostructures. The force equations for a cylindrical elastic medium may be written as

(7.197)

where the axis of the cylinder is oriented along the z--direction, y is the azimuthal angle, and r is the radial coordinate of the cylindrical structure. As before, the stress tensor T is related to the strain tensor S through the Hooke's law relationship

(7.198)

in this stress-strain relation, k and \x are the Lame constants. Alternatively, these force equations are frequently written in the form

where the elastic stiffness tensor for a particular isotropic medium is expressed as

j = xSijSki + 2^StkSji. (7.200)

These equations are more complicated than their counterparts in rectilinear coordinates, Section 7.2. Indeed, the additional complexity of the force equations in cylindrical coordinates is a direct consequence of the fact that in curvilinear coordinates the basis vectors are coordinate dependent.

Consider the acoustic phonon modes in a cylindrical waveguide of radius a embedded in an elastic medium. Both of these media are taken to be isotropic. From the normalization procedures of Section 5.1, the modes are normalized in terms of w instead of u since the considerations of Appendix A make it clear that it is convenient to use w = ypu; the displacement operator U(r) is then given by

The quantum number n labels modes with the same m and q in the set wmn,q (r), where q represents the z-component

of the wavevector qz. In determining the normalization constants for the normal modes wmn q (r), it is convenient to write

Wmn,q (r) = Wmn,q (r) eimv+iqz/a = u(r) eimv+iqz/a, (7.202)

Vn a2N

where u(r) is the classical displacement given by the elastic continuum model and the normalization constant N is then determined by the normalization condition

d r p(r)wn>m>q (r) • wn',m',q'(r) — $n,m,q\n',m',q', (7.2°3)

and q = aqz.

Let the density and Lame constants of the cylindrical waveguide be p1, A1 and ^1 respectively, and those of the surrounding material be p2, X2 and fi2. The general solution of the classical elastic continuum equations for such a cylindrical structure may be written (Beltzer, 1988; Stroscio et ai., 1996) in terms of three scalar potentials 0, f, and x as

u = Vtp + V ez f + aV ~xV~x <izx, (7.204)

where ez is a unit vector along the z-direction. The second and third terms in this last result correspond to the usual irrotational contribution to u, expressed as a sum of two mutually normal vectors. The potentials 0 ’ f, and x satisfy scalar wave equations with longitudinal and transverse sound speeds given by

ci$ = V (k$ + 2M$)/P$ and ct $ = j n$/P$; (7.205)

the subscript $ takes on the value 1 to designate the material parameters of the

cylinder and the subscript 2 to designate those of the surrounding material. Solutions of the classical elastic continuum equations are sought with vibration frequency m, wavevector qz = q/a, and azimuthal quantum number m. Seeking acoustic modes confined near the cylindrical waveguide, the scalar potentials for r < a are taken to be

and the bl1 etc. are normalization constants, to be determined. In the expressions for 0 , f, and x, it is assumed that k21 > 0 and Kft > 0, since confined acoustic modes are desired. Substituting these potentials into the general expression for u it follows that

for r > a. By applying the boundary conditions of continuity of displacement and continuity of the normal components of the stress tensor at r = a, it follows that

where the normalization condition gives

Again, at such a symmetry point only the irrotational - that is, the longitudinal - components of u(r) contribute to Hdf Accordingly, only the the potential 0, (7.204), contributes to Hdf. Indeed, from the normalized components wmn _ q (r) (7.202) , U(r) is obtained readily and by using the relation V20 = — (rn/cl)20 it follows that

Let us consider the case of a thin cylindrical shell. For a cylindrical shell, the boundary conditions on the inner and outer surfaces are

where P represents an external pressure that would be present, for example, in the case where the cylindrical shell is in contact with a liquid, TMV is the stress

tensor, and nv is the normal to the surface of the shell. In particular, P = ±P in er

n = ^er where er is the unit vector in the r-direction. The subscripts ‘in’ and ‘out’ are alternatives. For a cylindrical shell of infinite length in the z-direction and of thickness h and radius R such that h ^ R, the boundary conditions are

|r^/2 = Trzl R^h/2 = 0 ’ Trr 1 R^h/2 = P in . (7.225)

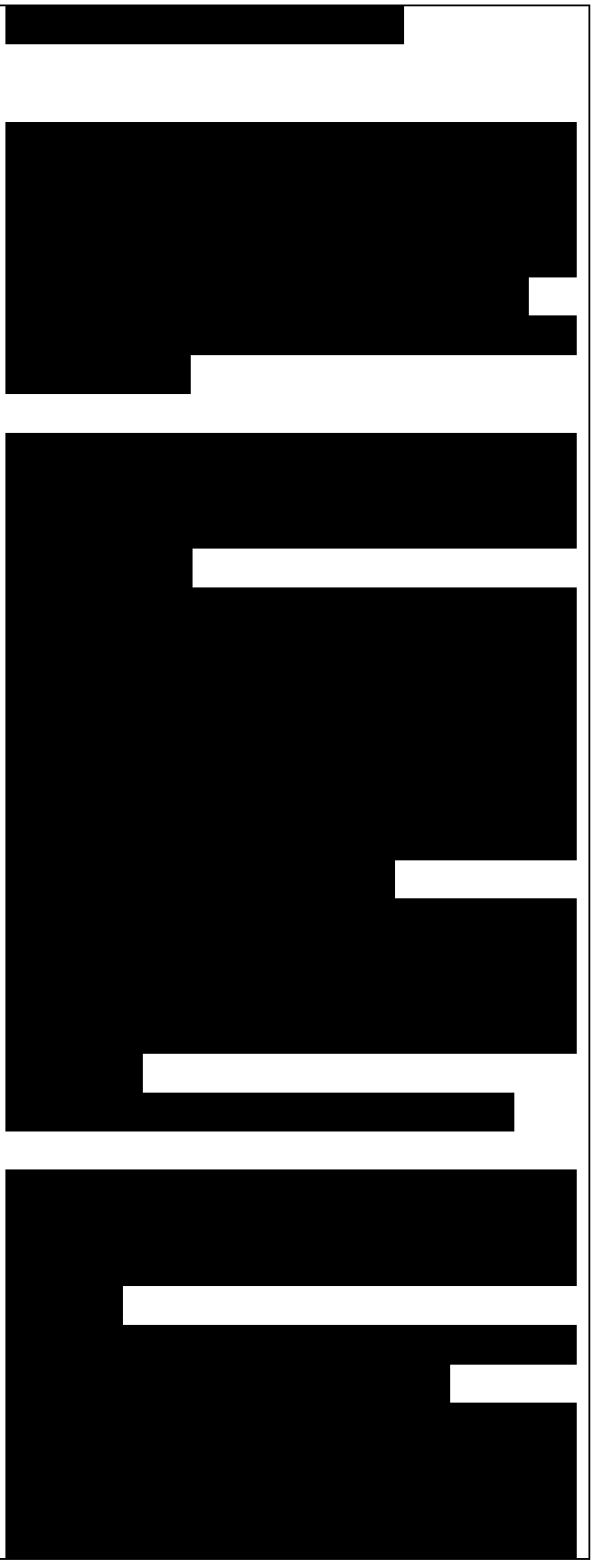
Assuming that all quantities except Trr are nearly constant with respect to r over the interval from R — h/2 to R + h/2, it is possible to show that

These results follow straightforwardly by integrating the right- and left-hand sides of each force equation over the interval from R — h/2 to R + h/2, invoking the boundary conditions in the radial force equation, and cancelling factors of h. From the stress-strain relation (7.198), it follows that

Using these stress-strain relations and eliminating the Lame constants in favor of Young’s modulus and the Poisson ratio, the force equations may be written as

it follows that the longitudinal mode has frequency Qlongitudinal = Qim = ~JV-m. Since Q^ ~ 0 was obtained in the lowest order in q it is necessary to find the first non-vanishing term. For m = 0, by making the assumption that = aq2 and collecting terms up to order q4 in the dispersion equation, it follows that

One of the roots of this equation, a = V-, corresponds to the mode Q^^=0, and another root, a = 1 - v2, implies that Q^^ ^ V1 - v2q. For the case where m =



0, by making the assumption (Q^)2 = aq4 and collecting terms up to q4 in the dispersion relation, it follows that

so that a1 = 1, a2 = V-, and a3 = 0. The result a3 = 0 is inconsistent with the initial guess, so solutions are of the form Q2 ^ constant. Then from the last two terms of the dispersion relation, with leading fourth power of q, it follows that v-q4Q2 - V- (1 - V2)q4 ~ 0, and Q2 ^ 1 - v2. Convenient interpolation formulae between the small-q and large-q solutions are given by

In the axisymmetric case with m = 0 the I, II, and III modes correspond to pure radial, torsional, and longitudinal modes respectively. When m = 0, the radial and torsional modes are coupled. In the limit where q » m + 1 the asymptotic expressions do not depend on m; indeed, in this limit Qm (q) - q, Q% (q) - ~JV-q, and Qlm(q) - V1 - v2 . Analysis of the coefficients cr, cf, and cz (Sirenko et ai., 1996a, b) reveals that in the limit of large q the I, II, and III modes correspond to pure longitudinal, torsional, and radial vibrations, respectively.

speed and density of water are taken to be 1.50 km s-1 and 1 g cm-3. The calculated dispersion relations, Qlm(q), for m = 1, 2, and 3 are shown in Figures 7.21, 7.22, and 7.23, respectively.

From Figures 7.21-7.23, it is apparent that for qz » m/R the mode frequencies of the immersed MTs tend to those of the free-standing MTs and do not depend on m. These modes are seen to

have maximum frequencies of the order of tens of GHz. Moreover, the sound speeds of the axisymmetric acoustic modes are in the range 200-600 ms-1.

Sirenko et al. (1996b) also considered the dynamical behavior of cytoskeletal filaments, by using the elastic continuum model to determine the mode structure for the vibrations of a solid cylinder. Particular attention was given to (a) the axisymmetric torsional mode, (b) the axisymmetric radial-longitudinal mode, and (c) the flexural mode, as depicted in Figure 7.24.

7.6.5 Acoustic phonons in quantum dots

In quantum dots, phonons and carriers alike are modified as a result of abrupt changes in the material properties at the interface between the quantum dot and the surrounding material. Indeed, carrier wavefunctions are modified as a result of the variations in the electron and hole band energies near the boundaries of the quantum dot. In the case of acoustic phonons, the changes in elastic properties near the quantum-dot boundaries lead to modifications in the displacement amplitudes. The acoustic phonon modes for spherical quantum dots and for quantum dots with rectangular-face confinement have been considered previously (Stroscio et al., 1994). For the case of a free-standing spherical quantum dot, the quantization of the acoustic phonons may be performed by taking

Here, a is the radius of the quantum dot, N is the number of unit cells in the normalization volume V, dq is the

phonon annihilation operator, q is the phonon wavevector, mq is the angular frequency of the phonon mode, M is the mass of the ions in the unit cell, and r,0,$ are the usual spherical coordinates. For a quantum dot with rectangular faces the normalization condition for the acoustic phonon mode amplitude is given by (7.258)

The classical acoustic modes in an isotropic elastic medium have been analyzed previously, and many of the most useful known results summarized, by Auld (1973). The lowest-order pure-compressional mode is referred to frequently as the breathing mode. The displacement field associated with this lowest order compressional mode of a sphere of radius a is given by

where y is the normalization constant, r is the unit vector in the radial direction, j is the spherical Bessel function of order unity, j1 (x) = sin x /x2 — cos x/x, —q is the mode frequency, and the longitudinal sound speed cl is equal to V (k + 2fi)/p. The frequency for a free-standing sphere is determined by the condition that the normal component of the traction force at the surface of the sphere vanishes; that is, Trr = 0 at r a:

where j0(x) = sin x/x is the spherical Bessel function of order zero. This last result implies that

The normalization condition for this lowest-order breathing mode is

with a>i representing the quantity rnqa/ci. This integral may be performed analytically and it follows that

(7.263)

where the second-order spherical Bessel

function, j2(x), is defined by j2(x) = [(3/x3) — (1/x)] sin x — (3/x2) cos x. The lowest-order breathing and torsional modes for a spherical quantum dot are shown in Figure 7.25.

The lowest-order torsional mode - a pure shear mode - of an free-standing isotropic spherical quantum dot may be determined from the known elastic-continuum solution for the lowest-order classical pure shear mode of an isotropic elastic medium (Auld, 1973):

Figure 7.25. Lowest-order (a) breathing mode and (b) torsional mode in a spherical quantum dot. From Stroscio et ai. (1994), American Institute of Physics, with permission.

where p is the unit vector in the p-direction, T is the normalization constant to be determined from the phonon normalization condition, and the transverse sound speed of the shear wave is given by ct = Vi/p. This mode is depicted in Figure 7.25(b). The normalization condition for this mode is with at = rnqa/ct. Thus, the normalization constant T may be evaluated in terms of the same integral used to calculate Y ; indeed,

Following the same procedure as for the breathing mode, it follows that the dispersion relation for the lowest-order torsional mode is

Krauss and Wise (1997) have recently observed the coherent acoustic phonons in spherical quantum dots. The damping of the lowest-order acoustic phonon modes observed by Krauss and Wise has been described in terms of the

elastic continuum model by Stroscio and Dutta (1999).

McSkimin (1944) gave approximate classical flexural thickness modes for a structure with rectangular faces. The structure considered in this section has faces joining each other at right angles, and the faces in the xy-, yz-, and xz-planes are rectangles such that the width of the structure - in the x-direction - is a, the height of the structure - in the y-direction - is b, and the length of the structure - in the z-direction - is c. The approximate flexural thickness modes given by McSkimin are

u(x, y, z) = A sinmx (sin/1 y + a sinl2y + fi sinl3y) cosnz, v(x, y, z) = A cos mx

where a and i are determined by applying desired boundary conditions on two sets of rectangular faces. The discrete mode indices for the x- and z-dimensions are labeled by m and n respectively. For the y-dimension, the mode index for the

The deformation potential for these flexural thickness modes has an especially simple form at a non-degenerate V -point, namely,

In fact, the spatially dependent terms in Hdef do not depend on a and i.