Resonant-mode conversion and transmission of phonons in superlattices

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We study the transmission and reflection of phonons incident on a superlattice at an oblique angle. For frequencies in the vicinity of an anticrossing frequency in the superlattice phonon-dispersion relation we find that the wave energy oscillates back and forth between the different polarizations as the wave propagates through the superlattice. These oscillations are analogous to the Pendellösung effect for electrons and x rays.

I. INTRODUCTION

Since the first demonstration of phonon filtering by periodic semiconductor superlattices (SL's),[1] there have been extensive studies of the propagation of high-frequency acoustic phonons in multilayered structures composed of crystalline or amorphous thin films of nanometer thickness.[2–4] The basic transmission and reflection characteristics of phonons in periodic SL's can be understood in terms of the dispersion relations for phonons propagating within the structure. Figure 1(a) illustrates the dispersion curves for phonons propagating normal to the layers in a (001) GaAs/AlAs superlattice. These calculations are based on an isotropic continuum model in which the sound velocities are taken to be 5.03×10^5 and 5.98×10^5 cm s^{-1} (L mode) and 3.03×10^5 and 3.60×10^5 cm s^{-1} (T mode) for GaAs and AlAs, respectively. The mass densities are 5.32 and 3.76 g cm^{-3}, respectively, and the thickness of each layer is 40 Å. The phonon modes have either purely longitudinal (L) or purely transverse (T) polarization. The artificially imposed periodicity of a SL induces the folding of the dispersion curves into a mini-Brillouin zone whose size is determined by the length of the SL period. The branches of the dispersion relation corresponding to different polarizations cross at a number of points. For each polarization there are gaps at the zone center and zone boundary arising from the intramode phonon Bragg reflections characteristic of a periodic structure.[1,5–7] For the GaAs/AlAs system the difference between the elastic properties of the two materials is fairly small, and so the gaps are not large. These gaps mean that there are ranges of frequency over which there are no propagating modes in the superlattice. These frequency ranges act as phonon stop bands, i.e., if a phonon with a frequency in these ranges is incident on a superlattice made up of a large number of periods, the phonon will be reflected and there will be no transmission.

For phonon propagation at oblique incidence the dispersion relation exhibits some different features, as shown in Fig. 1(b). These results are based on the same model as Fig. 1(a). The calculations are for a phonon wave vector with a component parallel to the superlattice layers such that the L and T phonons propagate at 45° and 25.2° to the normal in the GaAs layers, and at 56.9° and 30.4° in the AlAs layers, respectively. As a first approximation one can still consider that the L and T phonons propagate independently. Within this approximation, however, the dispersion curves for the L and T phonons intersect at various points within the minizone due to their different sound velocities. The inclusion of coupling between waves of different polarizations leads to level repulsion, and ''anticrossing'' behavior at these points. These anticrossings occur in two different manners. (i) The first type of anticrossing occurs in a region where one of the dispersion curves comes up from the zone center and the other from the zone edge, i.e., at places where the dispersion curves make a ''head-on'' collision. (ii) The second type occurs where the L branch of the dispersion curves attempts to ''overtake'' the T branch because of the larger velocity of longitudinal sound.

The first type of anticrossing is associated with the intermode Bragg reflection of phonons in a SL. Let the repeat distance of the structure be D_{AB}. An incident L phonon will generate a T-polarized reflection in each unit cell. These reflections will add up constructively and lead to anticrossing if

$$q_L + q_T = mG_0, \tag{1}$$

where q_L and q_T are the z components of the wave vectors of the envelope functions of the L and T phonons in the extended zone scheme, m is an integer, and $G_0 = 2\pi/D_{AB}$ is the magnitude of the smallest reciprocal SL vector.[3,4,8] Naturally, one could obtain the same condition by considering an incident T phonon.

The second type of anticrossing comes from transmission with mode conversion. An incident L wave generates a T wave propagating in the forward direction at each unit cell in the structure. These secondary T waves will add up constructively if

$$q_T - q_L = mG_0, \tag{2}$$

where again m is an integer.

The coupling between L and T arises because at oblique incidence a phonon of one polarization will generate a small reflected or transmitted wave of the other polarization at each interface. In previous work, the intermode Bragg reflection (the first type of anticrossing) in SL's has been studied extensively by several groups both theoretically and

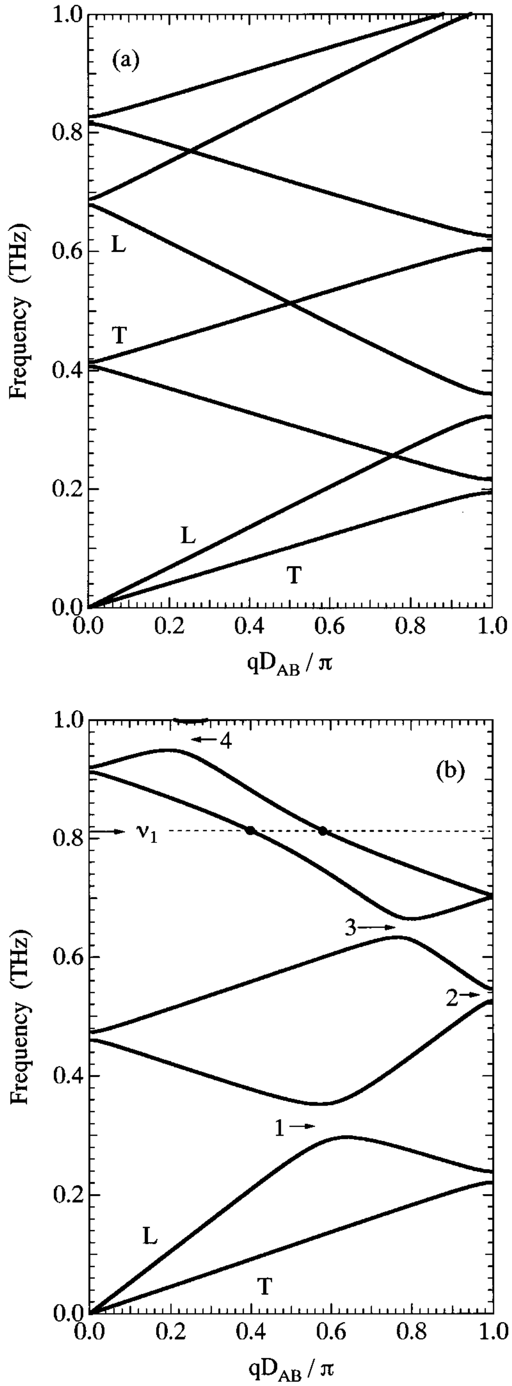

FIG. 1. Phonon-dispersion relations in a GaAs/AlAs superlattice in the isotropic, continuum approximation. The thicknesses D_A of the AlAs (A) and D_B of GaAs (B) layers are both 40 Å, and the sound velocities and densities of the materials are listed in the text. (a) Propagation at normal incidence. (b) Propagation at oblique incidence. The propagation direction is such that the direction of the L (T) mode is 45° (25.2°) in the GaAs layers, and 56.9° (30.4°) in the AlAs layers, respectively. The numbered frequency gaps are those related to L phonons. Note that the intrazone gaps (numbered 1, 3, and 4) are due to intermode phonon Bragg reflections. For the definition of ν_1, see the text.

experimentally.[3,4,8–10] However, the second type of anticrossing has not been studied, and is the subject of the present paper. We find the interesting result that within certain ranges of frequency this process can lead to a large amplitude of the mode-converted wave. In addition, the transmitted acoustic energy of a given polarization is an oscillatory function of the number of periods in a given SL. These oscillations are to some extent analogous to the Pendellösung effect that occurs when electrons or x rays are diffracted in a highly perfect crystal.[11–13]

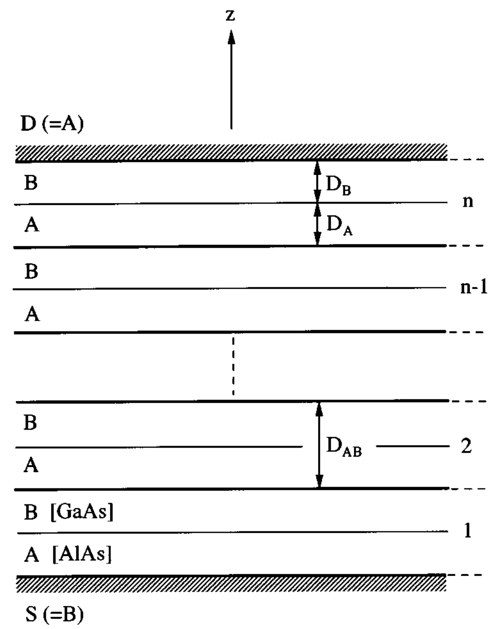

FIG. 2. The geometry of the superlattice structure considered. The A layers are AlAs, and the B layers GaAs. The substrate (S) and detector (D) are assumed to have the elastic properties of GaAs and AlAs, respectively.

As a specific model, we discuss all these features by considering a multilayered structure (Fig. 2) in which an alternating sequence of elastic layers of different materials A and B, is sandwiched between a substrate (S) where the waves are excited and a layer D where the waves are detected. The substrate is taken to have the same elastic properties as layer B. Layer D is assumed to have the properties of layer A, and all waves entering D are absorbed so that they do not return into the superlattice. We take the z axis to be perpendicular to the interfaces between layers, and choose the x-z plane as the saggital plane. For simplicity, elastic anisitropy is not considered, and only the two phonon branches polarized in the saggital plane are treated.

II. PERTURBATION RESULTS

In this section we consider the reflected and transmitted mode-converted waves based on a perturbation treatment. To calculate the reflection the approach is to restrict attention to waves that have been reflected at no more than one interface. Moreover, the depletion of the incident wave is ignored. We call the sum of phonon amplitudes the SL-structure factor. For an incident L wave the reflected T wave is given by the reflection structure factor S_R given by

$$S_R = r_{BA} + (r_{BA} + r_{AB} e^{-i\theta^{(B)}}) e^{i\Theta} \frac{1-e^{in\Theta}}{1-e^{i\Theta}}, \qquad (3)$$

where

$$\theta^{(i)} \equiv (k_L^{(i)} + k_T^{(i)}) D_i \quad (i = A, B), \tag{4}$$

$$\Theta = \theta^{(A)} + \theta^{(B)}. \tag{5}$$

r_{ij} is the coefficient giving the amplitude of the T wave reflected when an L wave is incident on the interface between a layer of type i and type j, n is the number of double layers, $k_j^{(i)}$ is the z component of the phonon wave vector of mode J in the layer i, and D_i is the thickness of the sublayer of type i. For definiteness, we will suppose that r_{ij} are reflection coefficients for displacements.

It is clear from Eq. (3) that the reflected amplitude will be very large when

$$\Theta = 2m\pi \quad (m = 1,2, \ldots) \tag{6}$$

or

$$(k_L^{(A)} + k_T^{(A)}) D_A + (k_L^{(B)} + k_T^{(B)}) D_B = 2m\pi. \tag{7}$$

If we identify $k_j^{(A)} D_A + k_J^{(B)} D_B$ with $q_J D_{AB}$, Eq. (7) is an alternative expression for the first condition $q_L + q_T = mG_0$ given in Sec. I.

For transmission with mode conversion from an L mode to a T polarization, the relevant structure factor is S_T given by

$$S_T = t_{BA} + (t_{BA} + t_{AB} e^{i(\phi_T^{(B)} - \phi_L^{(B)})}) e^{i(\Phi_L - \Phi_T)} \frac{1 - e^{in(\Phi_L - \Phi_T)}}{1 - e^{i(\Phi_L - \Phi_T)}}, \tag{8}$$

where

$$\phi_J^{(i)} \equiv k_J^{(i)} D_i, \tag{9}$$

$$\Phi_J = \phi_J^{(A)} + \phi_J^{(B)}, \tag{10}$$

and t_{ij} is the coefficient giving the amplitude of the T wave transmitted when an L wave is incident on the interface between a layer of type i and type j. The condition for a large transmitted T wave is then

$$\Phi_T - \Phi_L = 2m\pi \quad (m = 1,2, \ldots) \tag{11}$$

or

$$(k_T^{(A)} - k_L^{(A)}) D_A + (k_T^{(B)} - k_L^{(B)}) D_B = 2m\pi. \tag{12}$$

Again, this is essentially equivalent to the equation $q_T - q_L = mG_0$ given in Sec. I.

Of course, results similar to Eqs. (3) and (8) hold for an incident T wave. In particular, one notes that the condition for a large transmitted L wave given an incident T wave is the same condition that gives a large transmitted T wave for an incident L wave. The terms in parentheses in Eqs. (3) and (8) can be viewed as the structure factor for a *single* unit cell of the superlattice.

This perturbation approach can be valid only for a superlattice with a small number of periods. At resonance the transmitted or reflected mode-converted wave has an amplitude which is proportional to the number of layers n. Clearly, the theory must break down when the energy in the mode-converged wave becomes comparable to the incident energy.

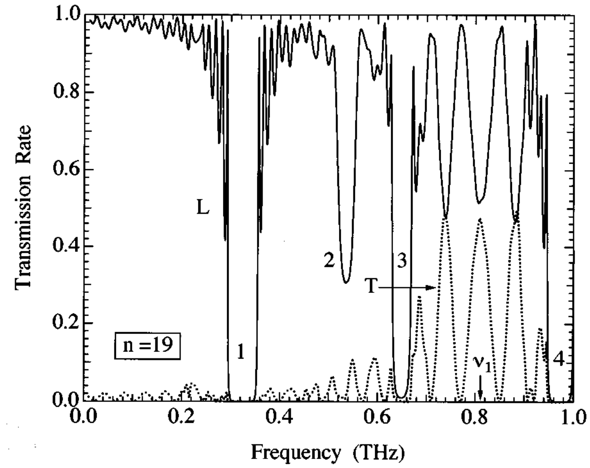

FIG. 3. Frequency dependence of the transmission rate in a GaAs/AlAs SL or L phonons incident from substrate side. The solid line is the fraction of energy transmitted with L polarization, and the dashed line is that transmitted with T polarization. The number of periods of the SL is 19 and $D_A = D_B = 40$ Å. The propagation directions chosen are the same as in Fig. 1(b). The dips in transmission labeled correspond to the frequency gaps in the dispersion curves shown in Fig. 1(b).

In this regard, one can consider the approach to be analogous to the so-called kinematic theory of x-ray scattering from crystals. For x rays, the reflection occurring at a single atomic layer is very small, and so the kinematic theory can hold for crystals composed of a very large number of atomic planes. The range of validity of the perturbation approach for acoustic waves in a superlattice is strongly dependent on the angle of incidence, since at normal incidence mode conversion does not occur.

III. NUMERICAL CALCULATIONS OF THE TRANSMISSION RATE

To go beyond the perturbation approach we first present some numerical results for particular cases. To do this we use the transfer matrix method[4] to calculate the transmission and reflection.

Figure 3 shows the frequency dependence of the transmission rate, i.e., the fraction of energy transmitted, calculated numerically for a GaAs/AlAs superlattice. An L wave incident from the substrate is assumed and the rates of energy flux transmitted as L and T modes are both plotted. The repeat distance of the superlattice is chosen to be 80 Å, and the number of bilayers is 19. The direction of propagation is 45°, i.e., the same as in Fig. 1(b). The transmission rate of L phonons drops sharply in the frequency ranges corresponding to the gaps 1–4 indicated in Fig. 1. Over most of the frequency range away from these gaps the transmitted energy is carried predominantly by the L mode. However, at frequencies around 800 GHz, a strong transmission of acoustic energy of T polarization can be seen. The frequency predicted by Eq. (2) for strong mode-converted transmission (for $m = 1$) is $\nu_1 = 816$ GHz, and this coincides well with the location of the peak ($\nu_1^* = 812$ GHz) of the T-wave transmission. It should be noted that the energy transmission via T phonons is also prohibited at frequencies inside the gaps due

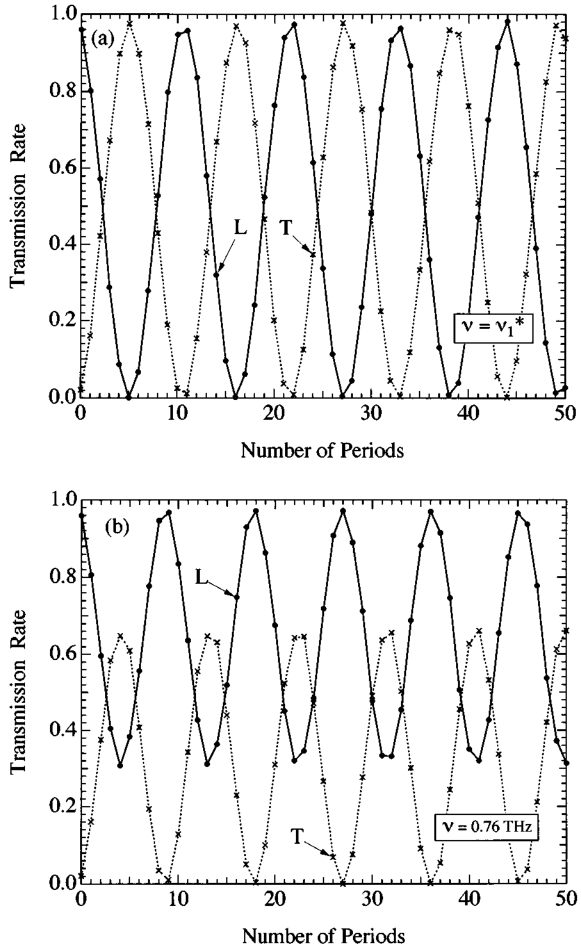

FIG. 4. Transmission rate vs number of periods for a longitudinal phonon incident obliquely on a GaAs/AlAs superlattice. The direction of propagation and the properties of the superlattice are the same as in Figs. 1(b) and 3. (a) Transmission at the frequency $\nu_1^* = 812$ GHz, for which the strongest mode mixing occurs; and (b) at 760 GHz, for which the mode mixing is incomplete. Dots with solid lines and crosses with dashed lines are the rates of the transmitted L and T phonons, respectively.

to the intermode Bragg reflections (the dips labeled 1, 3, and 4).

The transmission rates plotted in Fig. 3 are obtained for 19 bilayers. Interesting results are obtained by plotting the transmission rate at a fixed frequency near ν_1 against the number of unit periods of the SL. In Fig. 4(a) we plot the transmission rate for frequency ν_1 versus the number of periods for the same system as in Fig. 3. We see that the conversion of the transmitted energy into the T mode for an incident L polarization increases as the number of periods increases when the number of periods is small. For $n = 5$ the transmitted energy is nearly 100%, and appears almost entirely as transverse polarization. As the number of layers is increased, the transmission rates for L and T each oscillate with a period of about 11 bilayers, while their sum remains nearly constant at a value close to unity. In Fig. 4(b) a similar plot is presented for a frequency slightly different from ν_1. At this frequency the behavior is similar, but the maximum fraction of the energy being transmitted as T phonons is approximately 66%.

IV. PHYSICAL ORIGIN OF THE OSCILLATIONS

One can understand the physical origin of the oscillations in the energy of the mode converted wave in a number of different ways. At the qualitative level one can simply consider that when an L wave is introduced into the superlattice at oblique incidence a small amount of T polarization is generated at each interface. If the interference condition [Eqs. (2) or (12)] is satisfied, the energy in the T wave will steadily grow. However, at some point all of the energy will be in the T wave, and then energy begins to be transferred back to the L wave. It is clear that the number of periods n_0 required for the energy to completely return to the L wave will be larger the smaller the value of the mode-conversion transmission coefficient at each interface.

An alternative view is to consider the process in terms of the normal modes of the superlattice as shown in Fig. 1(b), for example. An incident wave of frequency ν will couple to superlattice modes of this frequency. We can therefore consider the following three cases:

(1) When ν lies within the range that corresponds to one of the frequency gaps, there will be no propagating modes to which the incident wave can couple. Then the transmission of energy through the structure is exponentially small.

(2) For most values of the frequency ν, there will be two propagating superlattice modes whose frequency matches that of the incident wave. Let us denote the wave numbers of these modes by q_1 and q_2. Provided that these two wave numbers are far removed from points at which anticrossing occurs, one of these modes will have essentially the character of an L wave and the other a T wave. Then the incident wave will excite the L wave with a large amplitude and the T wave with a much smaller amplitude. Because of the difference in the wave numbers of the two superlattice modes that are excited, there will be beating between these two waves as they propagate through the structure. However, because the amplitude of the L-like wave is much larger than the amplitude of the T wave, the amplitude of the beating will be very small.

(3) For an incident frequency in the vicinity of an anticrossing the difference between the wave numbers q_1 and q_2 is small. Because both of these modes lie near to an anticrossing each is a mixture of longitudinal and transverse. The two modes have different wave numbers and consequently an orthogonality relation does not hold between their two polarization vectors. Thus an incident longitudinal wave will excite both of the modes with comparable amplitudes. When the waves propagate through the structure, beats will occur. Initially, the two waves will interfere in a way such that the L components of their displacements add and the T components cancel. (This is, of course, necessary in order for the sum of the two waves to match with the incident L wave.) After the waves have propagated a number of layers n such that

$$|q_1 - q_2| n D_{AB} = \pi, \tag{13}$$

the waves will combine so the L components cancel and the T components add. This corresponds to the distance for complete transfer to T polarization. Therefore the energy returns to the L wave after n_0 bilayers, where

$$n_0 = \frac{2\pi}{|q_1 - q_2| D_{AB}}. \tag{14}$$

It follows from these considerations that the energy of the T component of the wave varies as

$$\sin^2(\pi n/n_0), \tag{15}$$

where n is the number of layers travelled into the superlattice. The energy in the L component varies as $\cos^2(\pi n/n_0)$.

One can also express these results directly in terms of the transmission coefficients introduced in Sec. II. Consider the predictions of the perturbation theory approximation [Eq. (8)], when the interference condition (11) is satisfied. Then the energy in the transverse wave builds up as

$$|S_T|^2 \approx n^2 |t_{BA} + t_{AB} e^{i(\phi_T^{(B)} - \phi_L^{(B)})}|^2. \tag{16}$$

We assume that $n \gg 1$ so that the first term (t_{BA}) on the right-hand side of Eq. (8) can be neglected. The perturbation theory holds provided that the fraction of energy converted is much less than 1. Now let us compare Eqs. (15) and (16). It follows that

$$n_0 = \frac{\pi}{|t_{BA} + t_{AB} e^{i(\phi_T^{(B)} - \phi_L^{(B)})}|}. \tag{17}$$

We checked both results for the period [Eqs. (14) and (17)] against the numerical results, and found agreement. It should, of course, be emphasized that these results rely on the assumption that the amount of mode conversion occurring in each layer of the superlattice is very small. This will certainly be true when the incident wave is propagating at close to normal incidence.

Finally, we mention the analogy between the effect we have studied and two other wave phenomena which are more familiar. It is clear that the oscillations between the two polarizations are, to some extent, analogous to the Pendellösung effect that occurs when x rays or electrons scatter at the Bragg angle from very perfect crystals, i.e., under conditions such that the dynamical theory of scattering must be used, rather than the kinematical theory.[11–13] This analogy to the Pendellösung effect raises some interesting questions. Under conditions such that the Pendellösung effect is observed, it is necessary to consider very carefully the nature of the wave packet (x ray or electron) that is incident on the crystal. The same concern clearly must arise for an elastic wave packet incident on a superlattice. Such a wave packet could contain a spread of frequencies either larger or smaller than the characteristic frequency range over which the level repulsion occurs. We have not investigated this in detail, but it appears likely that the spatial directions in which the energy flows in these two cases are quite different.

The second analogy is to the oscillations predicted to occur between different neutrino flavors if neutrinos have mass. When only two flavors are considered, a fraction of the probability oscillates back and forth between the flavors over a length scale determined by the difference in mass of the flavors. An additional effect can occur when neutrinos propagate through matter, rather than through free space. The interaction of the neutrinos with the electron density via the charged current interaction (W-boson exchange) leads to an interesting modification of the propagation, referred to as the Mikheyev-Smirnov-Wolfenstein (MSW) effect.[14,15] When there is a gradient in the electron density as occurs within the sun, for example, the effective masses of the different neutrino flavors vary in space. If the neutrino oscillations take place sufficiently rapidly on the length scale over which the electron density varies, it is possible to have an almost complete conversion of one neutrino flavor into the other. It appears that there should be an analogous effect for waves propagating in a superlattice in which the period slowly increases (or decreases) with distance. Suppose, for example, that L waves are incident on a superlattice that has a repeat distance D_{AB} such that conditions (2) or (11) for buildup of a T wave are *not* satisfied at the front of the structure. If the repeat distance slowly increases with distance into the superlattice, a region will eventually be reached in which the conversion condition is satisfied. In this region the energy in the wave will oscillate back and forth between the L and T polarizations. If the period of the superlattice continues to increase, the wave will eventually reach a region where the conditions (2) and (11) are no longer satisfied. At this point the energy will have been almost completely converted to T polarization, and the energy will then remain as transverse until another region of the superlattice is reached in which resonant conversion can occur. Of course, these effects will all be more complicated in real anisotropic SL's when the propagation is in an arbitrary crystallographic direction (i.e., not lying in a symmetry plane), so that coupling to both transverse modes is also possible.

V. SUMMARY

We have studied the transmission of elastic waves (phonons) through a superlattice in a direction oblique to the interfaces. We find that for certain frequencies an incident longitudinal (transverse) wave will be strongly converted into a transverse (longitudinal) wave. When this happens the fraction converted to the other polarization oscillates as the distance of propagation increases. We note that a wave packet propagating in a superlattice may exhibit a number of interesting effects which depend on the range of wave vectors contained in the packet. Finally, propagation in a superlattice with a slowly varying repeat distance is considered.

Experimentally, the predicted enhancement in the mode-converted transmissions of phonons in SL's should be observable by phonon spectroscopy experiments utilizing the phonon-imaging technique,[16] which is particularly useful for anisotropic media exhibiting the phonon-focusing effect.[17] Multilayered heterostructures grown by molecular-beam epitaxy (MBE) techniques can be used as phonon optics devices for high-frequency phonons.[18] The resonant mode-conversion effect that we have discussed in this paper could be used as the basis for a frequency or mode-selective reflector or transmitter of phonons. The characteristics of such a device could be modified over a wide range through the choice of the superlattice repeat distance, the mismatch of the layers, the number of layers, and the angle of incidence of the phonons.

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