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Acoustic properties of a layered medium with randomly distributed layer thicknesses

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Abstract. We study here the acoustic properties of a layered medium with randomly distributed layer thicknesses. The propagation of transverse elastic waves with polarization in the direction parallel to the laminations is investigated. The bulk modes and the transmission coefficients in a finite sample are calculated by the use of the transfer-matrix method. It is found that the density of states of these modes is drastically affected by the extent of disorder of such a system. Owing to the randomness, most of the waves are localized in the direction perpendicular to the laminations, but there still exist some waves with special frequencies which are completely extended. In some special cases we can analytically determine the frequencies of these extended waves. On the basis of this calculation a possible application of such structures is suggested.

1. Introduction

There has been a great deal of interest in recent years in the study of various vibrational modes supported by heterostructures and multilayered structures or superlattices. From theoretical investigations [1-5], it is believed that the periodic alternation of layers of materials with different acoustic properties in a superlattice has essential effects on the propagation of acoustic phonons in the direction perpendicular to the layers $(x_1 \text{ direction})$. Owing to the artificial periodicity, the dispersion relation of acoustic waves propagating along x_1 is folded into mini Brillouin zones of the superlattice, and frequency gaps open up at their centres or boundaries. Experimental investigations of the spectra of possible acoustic modes in various superlattices made of metals, semiconductors or amorphous materials have shown fairly good agreement with the theory [6–10]. In recent years, the artificially constructed aperiodic layered structures have also attracted much attention in investigations. These include the quasi-periodic systems and the systems with randomly distributed layer thicknesses. In such systems, crystalline periodicity remains in directions parallel to the laminations, but one-dimensional (1D) quasi-periodicity or randomness appears in the growth direction. For a given wavevector component parallel to the layers, the propagation of waves along the perpendicular direction is just like the motion in a 1D aperiodic system. It is found that the electronic states in a 1D quasi-periodic system have exotic Cantor-set-like features [11]. At the same time, in a 1D disordered system, most of the states are localized, as indicated by the scaling theory [12], but for special disorder types there still exist a small number of extended states [13, 14].

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The random-thickness layered structure provides another possibility for producing new devices. The acoustic properties can be artificially tailored by controlling the randomness of the thicknesses or doping profiles. The presence of randomness in such systems necessarily results in lattice vibrations totally different from those in bulk crystals or in periodic superlattices. At the same time, one may expect that some particular extended modes of acoustic phonons can also be found in special 1D disordered systems; meanwhile the other modes are drastically damped out owing to the randomness. So it is possible to develop high-quality acoustic filters by use of a layered structure with a specially designed thickness randomness.

In the present paper, we study the acoustic properties of the system which is formed by alternative stacking of layers of two materials with different acoustic parameters, and the layer thicknesses are randomly distributed. The phononic spectra of bulk modes and the transmission coefficients of the transverse waves are calculated for finite samples with different extents of randomness by use of the transfer-matrix method. It is found that the density of states is drastically affected by the disorder. Owing to the randomness, most of the waves are localized in the growth direction, but, for special forms of disorder, there still exist some waves with particular frequencies which are completely extended. We shall analytically determine the frequencies of these extended waves and qualitatively discuss the possible applications.

The paper is organized as follows. In section 2 we describe the structural features of the system and illustrate the expression of the transfer-matrix method in the continuum approximation which is used in the calculation. In section 3 we give the result of the phononic spectrum for different degrees of disorder. In section 4, we calculate the transmission of the transverse waves through such a layered structure, prove that for special forms of disorder there exist completely extended waves and analytically determine their frequencies. Our conclusions are summarized and discussed in section 5.

2. Propagation of acoustic waves in a superlattice with randomly distributed layer thicknesses

The system considered here is a superlattice made from alternating deposition of layers of two different materials A and B. The thicknesses of the layers are randomly distributed. This means that the thickness of a particular layer is a random variable. We denote $P_A(l_A)$ and $P_B(l_B)$ as the stochastic functions describing the distributions of thicknesses of layers of species A and layers of species B, respectively. The form and extent of the disorder are completely controlled by these functions. In the present paper we consider a uniform continuous distribution

$$P_{\mathbf{A}(\mathbf{B})}(l_{\mathbf{A}(\mathbf{B})}) = \begin{cases} 1/\delta_{\mathbf{A}(\mathbf{B})} & \text{if } \bar{l}_{\mathbf{A}(\mathbf{B})} - \frac{1}{2}\delta_{\mathbf{A}(\mathbf{B})} \leqslant l_{\mathbf{A}(\mathbf{B})} \leqslant \bar{l}_{\mathbf{A}(\mathbf{B})} + \frac{1}{2}\delta_{\mathbf{A}(\mathbf{B})} \\ 0 & \text{otherwise} \end{cases}$$
(1)

where $\bar{l}_{A(B)}$ is the average layer thickness of species A(B) and $\delta_{A(B)}$ is the width of the random distribution. Here the subscript A or B indicates the species of the layer. The thicknesses of the layers of the system that we consider are sequentially generated from a random-number generator in a computer according to this distribution. As soon as the sample is generated, the calculation is carried out upon this structure.

For the propagation of transverse acoustic waves, the elastic properties of a layer A (B) are described by two parameters: the density $\rho_{A(B)}$ and the transverse sound velocity $c_{A(B)}^{t}$.

We assume that the layers are perpendicular to the x_1 direction, and the displacement of the transverse elastic waves is in the x_2 direction, parallel to the plane of the layers; so the propagation of the transverse waves is in the x_1-x_3 plane. The elastic equation of motion within a layer may be written as

$$\ddot{u}(x_1, x_3, t) = (c_{A(B)}^t)^2 (\partial^2 / \partial x_1^2 + \partial^2 / \partial x_3^2) u(x_1, x_3, t)$$
(2)

where $u(x_1, x_3, t)$ is the displacement at position (x_1, x_3) and time t, and $c_{A(B)}^t$ is the velocity of transverse acoustic waves in material A (B). Thus the general solution of the equation can be written as

$$u(x_1, x_3, t) = \exp[i(k_3 x_3 - \omega t)] u(x_1)$$
(3)

with

$$u(x_1) = A_i \sin[\alpha_i (x_1 - x_{1i})] + B_i \cos[\alpha_i (x_1 - x_{1i})]$$

where the position x_1 is in the *i*th layer, x_{1i} is the coordinate of the interface between the *i*th layer and the (i - 1)th layer, k_3 is the component of wavevector in the x_3 direction, and

$$\alpha_i = [(\omega/c_i^{\rm t})^2 - k_3^2]^{1/2}.$$

Here c_i^t equals c_A^t when the species in the *i*th layer is A and equals c_B^t when the species in the *i*th layer is B; ω is the frequency of the acoustic mode.

The continuities of the displacement and the stress at interface $x_{1,i+1}$ yield

$$A_i \sin(\alpha_i l_i) + B_i \cos(\alpha_i l_i) = B_{i+1} \tag{4}$$

and

$$F[A_i \cos(\alpha_i l_i) - B_i \sin(\alpha_i l_i)] = A_{i+1}$$
(5)

with

$$F = \alpha_i \rho_i (c_i^t)^2 / \alpha_{i+1} \rho_{i+1} (c_{i+1}^t)^2$$
(6)

where ρ_i and l_i are the density and thickness, respectively, of the *i*th layer. At the same time, at interface $x_{1,i+2}$, the requirement of the continuities gives

$$B_{i+2} = A_{i+1}\sin(\alpha_{i+1}l_{i+1}) + B_{i+1}\cos(\alpha_{i+1}l_{i+1})$$
(7)

and

$$FA_{i+2} = A_{i+1}\cos(\alpha_{i+1}l_{i+1}) - B_{i+1}\sin(\alpha_{i+1}l_{i+1}).$$
(8)

Equations (4), (5), (7) and (8) can be rewritten in the transfer-matrix form

$$\begin{bmatrix} A_{i+2} \\ B_{i+2} \end{bmatrix} = \mathbf{T}_i \begin{bmatrix} A_i \\ B_i \end{bmatrix}$$
(9)

where \mathbf{T}_i is a 2 × 2 matrix:

$$\mathbf{T}_{i} = \begin{bmatrix} \cos(\alpha_{i+1}l_{i+1})/F & -\sin(\alpha_{i+1}l_{i+1})/F \\ \sin(\alpha_{i+1}l_{i+1}) & \cos(\alpha_{i+1}l_{i+1}) \end{bmatrix} \begin{bmatrix} F\cos(\alpha_{i}l_{i}) & -F\sin(\alpha_{i}l_{i}) \\ \sin(\alpha_{i}l_{i}) & \cos(\alpha_{i}l_{i}) \end{bmatrix}.$$
 (10)

As the layers of species A and B are alternatively deposited, the *i*th layer and the (i + 2)th layer are of the same species; so matrix T_i is a unimodular matrix. We consider a finite system with 2N layers, and its (2N)th layer is connected to a medium of the same species as the first layer. The amplitudes of the wave at the first layer and at this medium ((2N + 1)th layer) are related by

$$\begin{pmatrix} A_{2N+1} \\ B_{2N+1} \end{pmatrix} = \mathsf{T}_{\text{total}} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$$
(11)

where

$$\mathbf{T}_{\text{total}} = \bigg(\prod_{i=1}^{N} \mathbf{T}_{2i-1}\bigg).$$

From this equation we can obtain the phonon spectrum by use of the boundary conditions at the ends and calculate the acoustic wave at a special eigenfrequency and the transmission through the whole system.

3. Spectrum of bulk modes of acoustic phonons for finite samples with different degrees of disorder

The randomness of the layer thicknesses breaks the periodicity in the growth direction; so the Bloch theorem cannot be employed in the calculation of the spectrum of the phonons. Owing to this difficulty we have to restrict ourselves to a system containing only a finite number 2N of layers. Some modes in an infinite system are lost owing to this truncation because of the disappearance of the long-range structures which are longer than the length of the finite system. On the other hand, some new modes are created by the truncation; these are the modes associated with the two surfaces of the finite system and depending on how we deal with the boundary conditions. In fact, we are not interested in these surface modes; so we look for frequencies where corresponding solutions do not grow exponentially and can be regarded as the 'bulk modes' of the finite system. This leads to a condition that the ratio between the amplitudes at the two surfaces is finite. Alternatively, in a more restricted version, similar to the standard procedure employed in the investigations of the quasi-periodic systems [15, 16], we impose a Bloch ansatz on the amplitudes at the two surfaces:

$$\begin{bmatrix} A_{2N+1} \\ B_{2N+1} \end{bmatrix} = \exp(ikL) \begin{bmatrix} A_1 \\ B_1 \end{bmatrix}$$
(12)

where k is the Bloch index reflecting this periodic boundary condition, and

$$L = \sum_{i=1}^{2N} l_i$$

is the total length of the finite system. From equation (11) we have

$$\mathbf{T}_{\text{total}}\begin{bmatrix} A_1\\ B_1 \end{bmatrix} = \exp(\mathbf{i}kL)\begin{bmatrix} A_1\\ B_1 \end{bmatrix}.$$

The existence of non-trivial solutions of these linear equations for A_1 and B_1 , together with the fact that T_{total} is a unimodular 2×2 matrix, leads to

$$x = \frac{1}{2} \operatorname{Tr}(\mathsf{T}_{\text{total}}) = \cos(kL) \tag{13}$$

or

 $|x| \leqslant 1. \tag{14}$

As x depends on a frequency, from this equation we can obtain the spectrum of the acoustic modes of the system. The result is a set of minibands of frequencies which meet condition (14). Such a miniband structure comes from the imposed Bloch ansatz, and their widths are reduced to zero at the limit $N \to \infty$. In the calculation of the spectrum, we employ a finite sample with N large enough that the widths of the minibands are of the same order as the frequency resolution in the figures and take a miniband as a phononic state with frequency at its centre; thus the number of states in a given frequency interval can be accumulated to obtain a density of states as a function of frequency. The calculated results for a sample with a small degree of randomness, for a sample with a large degree of randomness and for a sample without randomness are shown in figures 1(a), 1(b) and 1(c), respectively. All the samples have the same average layer thickness (1000 Å) and the same total number of layers (N = 200). As a comparison, the density of states for the ordered sample (figure 1(c)) is calculated by the above-mentioned method, without applying the periodic symmetry. The values of the density and sound velocity for species A and B used in the calculation are given in table 1. These parameters are appropriate for a Nb/Cu layered structure. From the figures we can see that the band structure of the ordered sample shown in figure 1(c) is broken by the introduction of the randomness; some modes in the bands disappear and some new modes emerge in the gaps. Such an effect is more apparent in the high-frequency range. There are some remnants of band structure at low frequencies in figures 1(a) and 1(b). When the degree of randomness increases, the spectrum is resolved into a more discrete structure.

Table 1. Values of ρ and c^{t} for A and B.

_	ρ (g cm ⁻³)	$c^{t} (10^{5} \ cm \ s^{-1})$
A	8.57	1.83
В	8.92	2.905

Other boundary conditions can be used for the two surfaces of the finite system. For example, we can assume that the surfaces are free of the stress. Then,

$$A_1 = A_{2N} \cos(\alpha_{2N} l_{2N}) - B_{2N} \sin(\alpha_{2N} l_{2N}) = 0.$$
⁽¹⁵⁾

This means that

$$\begin{bmatrix} A_{2N+1} \\ B_{2N+1} \end{bmatrix} = \begin{bmatrix} 0 \\ B_{2N+1} \end{bmatrix} \begin{bmatrix} A_1 \\ B_1 \end{bmatrix} = \begin{pmatrix} 0 \\ B_1 \end{pmatrix}.$$
 (16)





$$[T_{\text{total}}]_{12} = 0.$$

The frequencies of the allowed modes can be solved by this equation. These include the surface modes which have not been considered above, and the bulk modes which lead to a finite ratio of B_1 to B_{2N+1} . If we restrict the module of this ratio to unity, the bulk modes obtained are just levels within the respective minibands obtained from the Bloch *ansatz*. At the limit $N \rightarrow \infty$, the influence of the surfaces is eliminated, and there is no difference between the results obtained from different boundary conditions.

(17)

4. Transmissions

In the propagation of the acoustic waves in such a random superlattice, the amplitudes of the waves are spatially varying in the growth direction. It is interesting to investigate the spatial distribution of the amplitudes. In particular, the information about the transmission of the waves through a system with a finite number of layers may be useful for possible application. We consider the above-mentioned system inserted into a bulk material of species C and assume that the wavevector of the incident wave is in the x_1-x_3 plane and the polarization of the wave is still in the x_2 direction. We write the function $u(x_1)$ in the left- and right-hand parts of the bulk material as

$$u(x_{1}) = \begin{cases} \exp[ik_{10}(x_{1} - x_{10})] + r \exp[-ik_{10}(x_{1} - x_{10})] \\ r \exp[ik_{10}(x_{1} - x_{1,2N})] \end{cases} \quad \text{for} \begin{cases} x_{1} \leq x_{10} \\ x_{1} \geq x_{1,2N} \end{cases}$$
(18)

where x_{10} and $x_{1,2N}$ are the coordinates of left- and right-hand ends, respectively, of the random superlattice and k_{10} is the component of the wavevector in the direction perpendicular to the laminations. The function $u(x_1)$ within the sample is still expressed by equation (3). Since the frequency ω and the component of wavevector k_3 are the same for the vibrations within and outside the sample, we have

$$k_{10} = [(\omega/c_{\rm C}^{\rm t})^2 - k_3^2]^{1/2}$$
⁽¹⁹⁾

where c_{C}^{t} is the sound velocity in medium C. From the continuities of the displacement and the stress at the ends, we have

$$A_1 = i(1-r)F_1$$
(20)

$$B_1 = 1 + r \tag{21}$$

$$[A_{2N}\cos(\alpha_{2N}l_{2N}) - B_{2N}\sin(\alpha_{2N}l_{2N})]F_2 = it$$
(22)

$$A_{2N}\sin(\alpha_{2N}l_{2N}) + B_{2N}\cos(\alpha_{2N}l_{2N}) = t$$
(23)

where

$$F_{1} = \alpha_{\rm C} \rho_{\rm C} (c_{\rm C}^{\rm t})^{2} / \alpha_{\rm A} \rho_{\rm A} (c_{\rm A}^{\rm t})^{2} \qquad F_{2} = \alpha_{\rm B} \rho_{\rm B} (c_{\rm B}^{\rm t})^{2} / \alpha_{\rm C} \rho_{\rm C} (c_{\rm C}^{\rm t})^{2}.$$
(24)

From equations (7)–(11), we have

$$\begin{bmatrix} A_{2N}\cos(\alpha_{2N}l_{2N}) - B_{2N}\sin(\alpha_{2N}l_{2N}) \\ A_{2N}\sin(\alpha_{2N}l_{2N}) + B_{2N}\cos(\alpha_{2N}l_{2N}) \end{bmatrix} = \begin{bmatrix} F & 0 \\ 0 & 1 \end{bmatrix} \mathbf{T}_{\text{total}} \begin{bmatrix} A_1 \\ B_1 \end{bmatrix}.$$
 (25)

By the use of equations (20)–(25), we obtain

$$r = [T_{12} + T_{21}F_1^2 + iF_1(T_{11} - T_{22})]/[T_{21}F_1^2 - T_{12} + iF_1(T_{11} + T_{22})]$$
(26)
and

$$t = \{F_1 T_{21}(F_1 - 1)(T_{11} + T_{22}) + i[2F_1 + T_{12}T_{21}(F_1 - 1)]\} / [T_{21}F_1^2 - T_{12} + iF_1(T_{11} + T_{22})]$$
(27)

where $T_{ij}(i, j = 1, 2)$ is the element of the matrix \mathbf{T}_{total} . So the transmission coefficient of the wave through the random superlattice is

$$|t|^{2} = \{ [F_{1}T_{21}(F_{1}-1)(T_{11}+T_{22})]^{2} + [2F_{1}+T_{12}T_{21}(F_{1}-1)]^{2} \} / \{ [T_{21}F_{1}^{2}-T_{12}]^{2} + [F_{1}(T_{11}+T_{22})]^{2} \}.$$
(28)

It depends on the frequency and the component of wavevector k_3 . For simplicity, hereafter we assume that medium C is of species A. So $F_1 = 1$, and

$$|t|^{2} = 4/[(T_{11} + T_{22})^{2} + (T_{21} - T_{12})^{2}].$$
(29)

Owing to the randomness in the superlattice, the transmissions for most of the waves vanish provided that the number of the layers is sufficiently large. However, it can be proved that for some special types of disorder there still exist waves which have a transmission of unity. An example is superlattices with randomly distributed thicknesses of species A but regular thickness of species B, i.e.

$$\delta_{\rm A} \neq 0 \qquad \delta_{\rm B} = 0. \tag{30}$$

If the frequency of a mode satisfies

$$\alpha_{\rm B} \bar{l}_{\rm B} = m\pi \tag{31}$$

with *m* being an integer, the transfer matrices T_i in equation (10) become

$$\mathbf{T}_{i} = (-1)^{m} \begin{bmatrix} \cos(\alpha_{A}l_{i}) & -\sin(\alpha_{A}l_{i}) \\ \sin(\alpha_{A}l_{i}) & \cos(\alpha_{A}l_{i}) \end{bmatrix} \quad \text{for all } i.$$
(32)

This means that the matrix string \mathbf{T}_{total} is the same as the transfer matrix of a uniform medium A with thickness

$$L = \sum_{i=1}^{N} l_{2i-1} \tag{33}$$

except for a possible negative sign. Since the system is embedded in an infinite medium of species A, the transmission for these waves is unity. At the same time, the other waves are heavily scattered by the randomness and have a nearly vanishing transmission. In figure 2 we plotted the transmissions as functions of frequencies for samples with different layer numbers. The peaks with a magnitude of unity correspond to these unscattered waves. It can be seen that the peaks rapidly become sharper when the layer number increases. Such a property can be used in an acoustic filter.

Now we consider another structure which has sharper peaks. It is a random superlattice with the following thickness distribution:

$$P_{A(B)}(l_{A(B)}) = \begin{cases} 1/M_{A(B)} & \text{if } l_{A(B)} = l_{A(B)}^{(0)} + m l_{A(B)}^{(1)}, m = 1, 2, \dots, M_{A(B)} \\ 0 & \text{otherwise.} \end{cases}$$
(34)

If the frequency ω of a wave satisfies

$$\alpha_{\rm A} l_{\rm A}^{(1)} = m_1 \pi \tag{35}$$

$$\alpha_{\rm B} l_{\rm B}^{(1)} = m_2 \pi \tag{36}$$

where m_1 and m_2 are integers, and ω is in the range of spectrum of a periodic superlattice with regular layer thicknesses $l_A^{(0)}$ and $l_B^{(0)}$, in a similar way we can prove that this wave is completely unscattered. In this case, the frequency should satisfy three conditions simultaneously; so we can choose appropriate values of $l_{A(B)}^{(0)}$ and $l_{A(B)}^{(1)}$ to select the necessary frequency. In figure 3 we plot the transmission as a function of frequency for such a system. It can be seen that the peaks in this curve are much sharper than those in figure 2(a), although the systems have the same layer number.



Figure 2. The transmission as a function of the frequency for acoustic waves with $k_3 = 0$ through a sample with fixed layer thicknesse d_1 of Nb equal to 500 Å and random layer thicknesses d_2 of Cu, uniformly distributed between 1000 Å and 10^5 Å. The sample is embedded in an infinite uniform medium of Nb. The total numbers of layers in the sample are as follows: (a) 200; (b) 50.



Figure 3. The transmission as a function of the frequency for acoustic waves with $k_3 = 0$ through a sample with Nb layer thicknesses $d_1 = 850$ Å +m1260 Å and Cu layer thicknesses $d_2 = (n + 1)1000$ Å, where m and n are both random integers, uniformly distributed between 0 and 100. The sample is embedded in an infinite uniform medium of Nb. The total number of layers in the sample is 200.

5. Discussion

We have calculated the phononic spectrum and the transmission of superlattices with randomly distributed layer thicknesses. It is found that the structure of phonons with comparatively high frequencies is very sensitive to the extent of the randomness. In these systems, there are abundant parameters which can be used to tailor the properties of the material. The calculation of the transmission reveals the existence of a small number of waves which are completely unscattered by such a random structure. This provides the possibility of using these structures in a high-quality filter. The frequencies and sharpness of the filter can be easily designed by selecting the type and extent of the randomness. The result obtained here may be useful for further studies, e.g. study of the electron-photon interaction, and study of Raman scattering and other optical properties.

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