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LOW-FREQUENCY ABSOLUTE GAPS IN THE PHONON SPECTRUM OF MACROSTRUCTURED ELASTIC MEDIA

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Abstract. The propagation of elastic waves in macroscopically periodic composites consisting of core-shell spherical scatterers in a homogeneous host medium is studied by means of numerical calculations using the layer-multiple-scattering method. By an appropriate choice of the constituent materials, these crystals exhibit wide absolute frequency gaps, over which no elastic wave can propagate in the composite medium, whatever the direction of its propagation. We analyze the detailed structure of transmission spectra of finite slabs of such crystals in conjunction with the corresponding complex-band-structure and density-of-states diagrams, and emphasize aspects of the underlying physics which have not been discussed previously.

1. INTRODUCTION

The low-frequency phonon spectra of materials can be efficiently manipulated by periodic structuring on a length scale comparable to the corresponding wavelength. A typical example would be a composite system consisting of a periodic array of inclusions in a homogeneous host medium. The elastic characteristics of the host medium, i.e. its mass density ρ and the sound velocities c_l and c_t (the subscripts l and t refer to longitudinal and transverse waves, respectively), are different from those of the inclusions. The dimensions of the inclusions must be large enough in order for a macroscopic description of their elastic properties to be valid but, otherwise, their size and the lattice constant a of the crystal is a matter of choice. The most interesting property of such materials, so-called phononic crystals, appears to be the existence of absolute gaps in their frequency band structure, i.e. regions of frequency over which no elastic wave can propagate in the composite material, whatever the direction of propagation. A wave incident on a sufficiently thick slab of such material will be reflected (practically completely) if its frequency lies within the gap.

Phononic crystals operating at sonic, ultrasonic, and hypersonic frequencies are realizable in the laboratory and attract a continuously growing interest [1] because of technological applications ranging from acoustics to control systems, remote sensing, medical imaging, and military industry. Phononic

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crystals are interesting also in relation to basic physics in a number of ways. For example, they can be the starting point in a process of gradual introduction of disorder and a study of consequent phenomena, including Anderson localization.

There are mainly two mechanisms that can lead to a frequency gap in a phononic crystal. One is Bragg scattering which is responsible for the opening of gaps at the Brillouin zone boundaries. These gaps appear at about an angular frequency ω of the order of $c_{l(t)}/a$ and at higher frequencies, which tells us how to choose a if we want a gap in a certain frequency region. The other mechanism originates from localized resonances. For instance, it has been established that a scatterer made of a relatively hard elastic core and a soft shell, embedded in an elastically hard host medium, exhibits localized resonant modes which lead to hybridization gaps in phononic crystals realized from such building components [2,3]. These gaps are quite robust against structural changes, and their position in frequency can be tuned by a proper choice of the constituent materials. In this manner, we can create absolute phononic gaps in a desired frequency region without the need to change the dimensions of the unit cell of the crystal. In this paper we analyze the formation of such hybridization gaps in a phononic crystal of core-shell spherical inclusions in a silicon matrix, an example that has been also considered by Liu *et al.* [3], and we clarify aspects of the underlying physics to a degree that has not been done before.

2. METHOD OF CALCULATION

Our calculations are carried out by the layer-multiple-scattering method we have developed in relation to phononic crystals [4,5]. The method employs multiple-scattering techniques, analogous to those applied in the first instance to the treatment of electron scattering in solids. These techniques are very efficient for systems of nonoverlapping scatterers in a homogeneous host medium. The shape of the scatterers can be, in principle, arbitrary, but the calculations are simpler if one assumes that they are spherical, as it will be the case in the present work. The basic principle of the method is that the wave incident on a given scatterer is the sum of the waves outgoing from all the other scatterers and the externally incident wave. The scattering matrix **T**, which relates the amplitudes (expansion coefficients in a given representation) of the scattered wave with those of the incident wave, is obtained, for the composite system, from the corresponding matrices of the individual scatterers and proper propagator functions in the host medium. In a multiple-scattering calculation, whether one is interested in the transmittance/reflectance of a slab of the material or the complex frequency band structure of an (infinite) phononic crystal, the angular frequency ω of the elastic field is a given conserved quantity. This 'on-shell' character of the method makes its application to phononic crystals made of materials with complex and/or frequency-dependent elastic coefficients straightforward.

Usually, when one deals with a slab of a phononic crystal parallel to a given crystallographic plane, $\mathbf{k}_{\|}$, the component of the wave vector parallel to this plane (this is taken to be the *xy* plane), reduced within the surface Brillouin zone (SBZ), is also a given conserved quantity. The layer-multiple-scattering method proceeds by evaluating the scattering properties of a slab from those of the constituent layers, for given ω and $\mathbf{k}_{\|}$. The layers can be either planes of scatterers with the same two-dimensional (2D) periodicity, or homogeneous plates (this includes also the case of planar interfaces between two homogeneous media). For each plane of scatterers, the method calculates the full multipole expansion of the total multiply scattered wave field and deduces the corresponding transmission and reflection matrices in the plane-wave basis. For homogeneous plates, the transmission and reflection matrices are directly obtained in the plane-wave basis.

In relation to the frequency band structure, the question we ask is: for the given $\omega; \mathbf{k}_{\|}$, are there propagating Bloch waves in the infinite crystal? These represent of course the eigenmodes of the elastic field in the crystal. The method provides us with these propagating Bloch waves and at the same time with a number of evanescent waves which play an indirect role in the phenomena we are considering. By repeating the calculation for different values of ω, we obtain the frequency bands $k_z(\omega)$ for the given $\mathbf{k}_{\|}$ over a selected region of frequency. If $k_z(\omega)$ is real, the corresponding mode is a propagating Bloch wave. If it is complex, we have a wave which decays exponentially along the positive or negative *z* direction. A region of frequency where propagating waves do not exist, for given $\mathbf{k}_{\|}$, constitutes a frequency gap of the elastic field for the given $\mathbf{k}_{\|}$. If over a frequency region no propagating wave exists whatever the value of $\mathbf{k}_{\|}$, then this region constitutes an absolute frequency gap.

3. RESULTS AND DISCUSSION

We consider, to begin with, a single spherical scatterer consisting of a gold core (ρ_1 = 19500 kg/m^3, c_{1l} = 3360 m/sec, c_{1t} = 1240 m/sec), of radius S_1, coated with a lead spherical shell (ρ_2 = 11400 kg/m^3, c_{2l} = 2160 m/sec, c_{2t} = 860 m/sec) of external radius $S = 18S_1/13$. The scatterer is embedded in a silicon matrix (ρ= 2330 kg/m^3, c_l = 8950 m/sec, c_t = 5359 m/sec). Fig. 1 shows the change $\Delta N(\omega)$ in the number of states and the change $\Delta n(\omega) = d\Delta N(\omega)/d\omega$ in the density of states of the elastic field induced by the above core-shell sphere in the silicon host. These quantities have been calculated from the general formula [6]: $\Delta N(\omega)=(1/\pi)\mathrm{ImTr}\ \ln[\mathbf{I}+\mathbf{T}]$ using the appropriate **T** matrix [5]. It can be seen that, in the frequency region under consideration, there are two peaks at frequencies $\omega S/\pi c_t$ = 0.174, 0.201. These peaks originate from dipole resonant modes of the scatterer, of coupled longitudinal-transverse (*L*-*N*) and of purely transverse (*M*) type, respectively. The first peak has the form of a relatively broad Lorentzian and is associated with a resonant state of short lifetime. The second peak is a very sharp Lorentzian, corresponding to a virtual bound state with a long lifetime. Because of the ($2l$+1) degeneracy of the eigenmodes of a spherical scatterer, both dipole resonances exhibit a corresponding change in the number of states of nearly 3.

When such core-shell spheres are assembled into a phononic crystal, the resonant states of the individual spheres interact with each other and form frequency bands about the corresponding eigenfrequency of the single sphere. The width of these bands depends on the overlap of the corresponding modes of the elastic field: the more localized a resonant state, the narrower the corresponding band. We consider the specific case of an fcc crystal with a fractional volume occupied by the spheres f = 10%. We view the crystal as a sequence of (001) planes: on any of these planes the spheres are arranged on a square lattice defined by the primitive vectors $\mathbf{a}_1 = a_0(1,0,0)$ and $\mathbf{a}_2 = a_0(0,1,0)$. Each plane is obtained from the one preceding it by a primitive translation $\mathbf{a}_3 = a_0(1/2,1/2,\sqrt{2}/2)$. Obviously, $d = a_0\sqrt{2}/2$ is the distance between successive planes.

Along the fcc [001] direction, the first resonant mode of the spheres (a dipole *L*-*N* mode) gives, according to group theory [7,8], a band of Δ_1 symmetry which is nondegenerate and a band of Δ_5 symmetry which is doubly degenerate. These two bands converge at the center of the Brillouin zone to a three-fold degenerate point, of Γ_{15} symmetry.

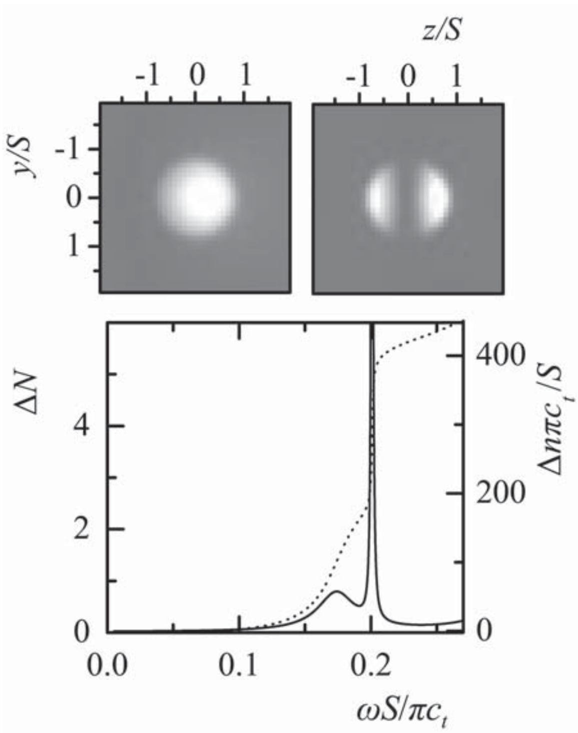

Fig. 1. Change in the number of states ΔN (dotted line) and in the density of states Δn (solid line) induced by a gold sphere of radius S_1 coated with a lead spherical shell of external radius $S = 18S_1/13$, in silicon. The field intensity distribution corresponding to the resonant modes is shown at the top (we assume a *x*-polarized transverse wave incident on the sphere along the *z* axis).

Correspondingly, the second virtual bound state of the spheres (a dipole *M* mode) gives a (nondegenerate) $\Delta_{1'}$ band and a Δ_5 band, which at the center of the Brillouin zone converge to a three-fold degenerate point of $\Gamma_{15'}$ symmetry. In addition to the above bands, there are, of course, bands corresponding to propagation of elastic waves in a homogeneous effective medium, which are described by linear dispersion curves in the long-wavelength limit. These bands have the Δ_1 and the Δ_5 symmetry for longitudinal and transverse waves, respectively, along the fcc [001] direction. When bands of the same symmetry cross each other, their hybridization leads to band diagrams such as those shown in the middle panel of Fig. 2. According to this analysis, the physical origin of the bands shown in Fig. 2 is obvious.

A longitudinal or a transverse elastic wave, incident normally on a finite (001) slab of the crystal under consideration, excites bands of Δ_1 or Δ_5 symmetry, respectively, and through them is transmitted to the other side of the slab. Bands of any other symmetry cannot be excited in this case; they are inactive and correspond to bound states of the slab. In the regions of frequency gaps there are no propagating Bloch modes, and there the transmission coefficient is determined from the complex band of the proper symmetry which has the smallest imaginary part: the wave decreases exponentially within the slab with an attenuation coefficient equal to Im$k_z(\omega)$ of this band, as shown in the left panel of Fig. 2. It is worthnoting that in the transmission spectrum of longitudinal waves in the gap region (upper left diagram in Fig. 2) there are eight sharp resonances (as many as the number of planes of spheres in the slab) at frequencies ω_κ, which are superimposed on an otherwise smooth background. These resonances correspond to eigenmodes of the slab for $\mathbf{k}_{||} = \mathbf{0}$. If we associate with ω_κ the discrete values of the wave number $k_{z;\kappa} = \kappa\pi/9d$; κ=1,2, …,8, implied from the finite thickness of the slab, the points ($k_{z;\kappa}d/\pi=\kappa/9$, ω_κ), κ= 1,2, …,8 (shown by open circles in the upper middle diagram of Fig. 2) reproduce the real part of the Δ_1 band which originates from the corresponding resonant states of the spheres. This band lies in a frequency gap: it has been pushed into the complex k_z plane as a result of the hybridization with the Δ_1 effective-medium band. In the present case this resonance complex band has the smallest imaginary part from all the (complex) bands in the given gap region. Therefore this band determines the transmission coefficient of a longitudinal elastic wave incident normally on a (001) slab of the crystal, in this frequency region.

The above results can be also analyzed in conjunction with relevant density-of-states diagrams [6]. As shown in the right panel of Fig. 2, the change of the density of states induced in the silicon host by a single (001) plane of the crystal under consideration for $\mathbf{k}_{||} = \mathbf{0}$ exhibits two resonant states with a relatively short lifetime, one of Δ_1 and one of Δ_5 symmetry that originate from the first resonant state of the individual spheres. We also have one bound $\Delta_{1'}$ state and one virtual bound Δ_5 state with long lifetime, which originate from the second resonant state of the individual spheres. In the given slab, the interaction between states of neighboring planes leads to eight resonant states Δ_1 for $\mathbf{k}_{||} = \mathbf{0}$ which manifest themselves in the transmission of longitudinal waves as mentioned above. In the same manner, the Δ_5 resonant states with the short lifetime form a relatively broad band which hybridizes with the Δ_5 effective-medium band, but in this case no sharp resonances appear in the corresponding transmission spectrum of transverse waves because at no frequency the imaginary part of this band is the smallest one. Similarly, we obtain in the slab bound $\Delta_{1'}$ states which reproduce the corresponding inactive band and resonant Δ_5 states with long lifetimes which reproduce the flat Δ_5 band. The latter manifest themselves as resonance structures in the corresponding transmission spectrum (lower left diagram of Fig. 2), however they cannot be discerned in the figure because they appear in a very narrow frequency range.

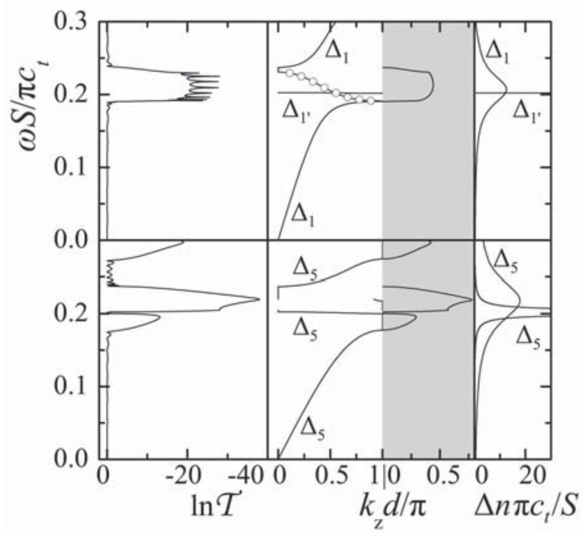

Fig. 2. Left: Transmission coefficient of a longitudinal (upper diagram) and a transverse (lower diagram) elastic wave incident normally on a slab of eight (001) planes of the phononic crystal under consideration. Middle: The corresponding complex band structure for nondegenerate (upper diagram) and doubly degenerate (lower diagram) bands. In the gap regions we show the eigenvalues k_z with the smallest imaginary part (plotted in the shaded area) which may belong to different bands over different regions of frequency. Right: Change of the density of states, with respect to the silicon background, for a single (001) plane of the above crystal for $\mathbf{k}_{||} = \mathbf{0}$.

In Fig. 3 we present the projection of the frequency band structure of the phononic crystal under consideration on the symmetry lines of the SBZ of the fcc (001) surface. The shaded regions extend over the frequency bands of the elastic field: at any one frequency within a shaded region, for given $\mathbf{k}_{||}$, there exists at least one propagating elastic mode in the infinite crystal. The blank areas correspond to frequency gaps. We note that knowing the modes

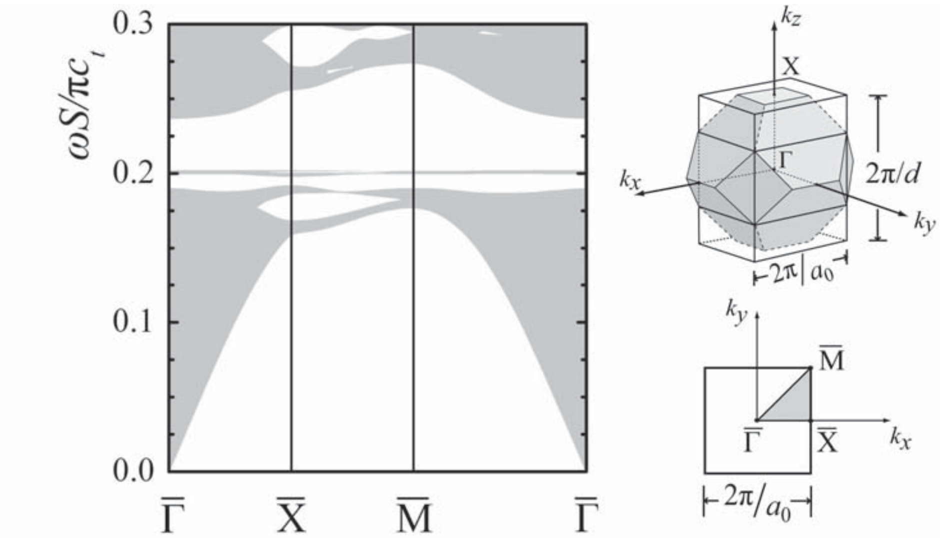

Fig. 3. Left: Projection of the phononic band structure of the crystal under consideration on the high symmetry lines of the SBZ of its (001) surface. Right: The reduced **k**-zone associated with the fcc (001) surface (top) and the corresponding SBZ (bottom). The (bulk) fcc Brillouin zone (shaded decatetrahedron) is also shown for comparison.

with $\mathbf{k}_{\|}$ in the shaded area $\overline{\Gamma \mathrm{XM}}$ of the SBZ shown in the right panel of Fig. 3 and k_z in the interval $[0, \pi/d]$ is sufficient for a complete description of all the modes in this crystal. The modes in the remaining of the reduced **k** space are obtained through symmetry. Finally we note the existence of a narrow, almost dispersionless band about $\omega S/\pi c_t = 0.201$ within an otherwise absolute frequency gap extending from 0.193 to 0.237 in units $\pi c_t/S$. We verified that this is indeed so by calculating the band structure at a sufficient number of $\mathbf{k}_{\|}$ points in the SBZ.

4. CONCLUSION

In summary, we presented a theoretical study of the elastic properties of a three-dimensional phononic crystal consisting of gold core-lead shell spherical inclusions in a silicon host using the layer-multiple-scattering method, clarifying the underlying physics. We analyzed transmission spectra of finite slabs of this crystal by reference to relevant complex-band-structure and density-of-states diagrams, demonstrating the physical origin of the field eigenmodes as well as the mechanism which leads to the formation of absolute frequency gaps in this system.

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