Formation of absolute frequency gaps in three-dimensional solid phononic crystals

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We report on the occurrence of absolute elastic band gaps in three-dimensional binary systems made up of steel spheres in polyester, and examine how the width of such gaps depends on the geometry of the structure.

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Phononic crystals are composite materials with elastic coefficients which vary periodically in space. A most interesting aspect of these materials arises from the possibility of frequency regions, known as absolute phononic band gaps, over which there can be no propagation of elastic waves in the crystal, whatever the direction of propagation; an interesting phenomenon which promises applications as well (see, e.g., Ref. 1 and references therein). Absolute spectral gaps do not occur easily in three-dimensional (3D) solid phononic crystals. Elastic waves in a 3D solid phononic crystal have longitudinal and transverse components, and corresponding gaps must overlap, for any direction of propagation, if an absolute gap is to appear. One may think that this is not likely in view of the different propagation velocities of longitudinal and transverse waves. However, under specific conditions, absolute gaps do occur in 3D solid phononic crystals. It has been established that periodic binary composites consisting of nonoverlapping high-density spheres in a low-density host material,[2] as well as three-component phononic crystals consisting of coated spheres inside an embedding medium,[3,4] exhibit absolute phononic gaps. In this paper we further investigate the physics of the formation of absolute gaps in phononic crystals, and show in particular that the crystal structure plays an important role in the formation of these gaps.

We consider (this is a good example of a phononic crystal consisting of high-density spheres in a low-density host) an infinite 3D array of nonoverlapping steel spheres ($\rho_s = 7800$ kg/m^3, $c_{sl} = 5940$ m/sec, and $c_{st} = 3200$ m/sec), of radius S, arranged periodically in a polyester matrix ($\rho = 1220$ kg/m^3, $c_l = 2490$ m/sec, and $c_t = 1180$ m/sec), neglecting losses in both constituent materials. The infinite crystal is viewed as a sequence of planes of spheres perpendicular to the z axis. The spheres of a plane (xy plane) are arranged on a 2D lattice defined by the primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$. The $(n+1)$th plane along the z axis is obtained from the nth plane by a primitive translation $\mathbf{a}_3 = (a_{3x}, a_{3y}, a_{3z})$, so that $d = a_{3z}$ is the distance between successive planes. For example, a square lattice, obtained with $\mathbf{a}_1 = a_0(1,0,0)$, $\mathbf{a}_2 = a_0(0,1,0)$, generates a variety of 3D lattices depending on the choice of $\mathbf{a}_3$. Putting $\mathbf{a}_3 = a_0(0,0,1)$ gives a simple cubic (sc) crystal, $\mathbf{a}_3 = a_0(1/2,1/2,1/2)$ gives a base-centered-cubic (bcc) crystal, $\mathbf{a}_3 = a_0(1/2,1/2,\sqrt{2}/2)$ gives a face-centered-cubic (fcc) crystal, $\mathbf{a}_3 = (0,0,d)$ with $d \neq a_0$ gives a simple tetragonal (st) crystal, etc. By comparing the phononic band structures corresponding to a variety of crystal structures we learn how the geometry of the structure influences the formation of frequency gaps. The calculations are carried out using the on-shell layer-multiple-scattering formalism we have developed for this purpose.[5] This formalism applies to phononic crystals consisting of nonoverlapping spheres (fluid or solid) in a homogeneous host medium (fluid or solid). The convergence of numerical calculations by this method is determined by the cutoff values actually used in the spherical-wave and plane-wave expansions involved. In the present work we required a relative accuracy better than 0.01 in the determination of the edges of the frequency gaps. This was achieved in the most demanding cases (large fractional volume occupied by the spheres) by considering an angular momentum cutoff $l_{\max} = 8$ and by including 149 2D reciprocal vectors.

To begin with, we consider a fcc crystal of steel spheres in polyester with a fractional volume occupied by the spheres $f = 18.4\%$. Figure 1(a) shows the frequency band structure of the elastic field in this crystal, normal to its (001) surface, i.e., when the component $\mathbf{k}_\parallel = (k_x, k_y)$ of the reduced wave vector, within the corresponding surface Brillouin zone (SBZ), is equal to zero. The thin solid lines in Fig. 1(a) are longitudinal bands and the thick solid lines are transverse bands; these couple, respectively, with longitudinal and transverse elastic waves incident normally on a (001) slab of

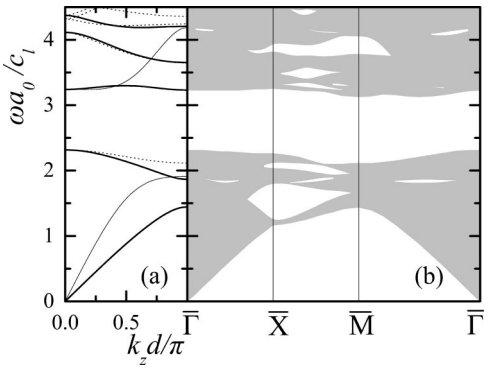

FIG. 1. The phononic frequency band structure of a fcc crystal of steel spheres in polyester, with $f = 18.4\%$. (a) Frequency bands normal to the (001) surface. The thin (thick) solid lines refer to longitudinal (transverse) bands and the dotted lines refer to deaf bands. (b) Projection of the frequency band structure on the symmetry lines of the SBZ of the (001) surface.

the material. The dotted lines are deaf bands which do not couple with waves incident normally on the slab (for a clarification of what is meant by longitudinal, transverse, and deaf bands in phononic crystals, see Sec. VII of Ref. 5). It is seen that, in the frequency range from $\omega a_0/c_l = 2.32$ to $\omega a_0/c_l = 3.23$, there are no propagating modes of the elastic field in the crystal along the [001] direction. This relatively wide frequency gap exists throughout the SBZ, and its edges vary little with $\mathbf{k}_\parallel$; this is seen in Fig. 1(b), which shows the projection of the frequency band structure of the elastic field in the given crystal on the symmetry lines of the SBZ of its (001) surface. The shaded regions define the frequency bands of the elastic field: at any one frequency within a shaded region, for a given $\mathbf{k}_\parallel$, 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 corresponding to $\mathbf{k} = (\mathbf{k}_\parallel, k_z)$ with $\mathbf{k}_\parallel$ within the irreducible part of the SBZ—a triangle with vertices at $\bar{\Gamma}$ [$\mathbf{k}_\parallel = (0,0)$], $\bar{X}$ [$\mathbf{k}_\parallel = (\pi/a_0, 0)$], and $\bar{M}$ [$\mathbf{k}_\parallel = (\pi/a_0, \pi/a_0)$]— and k_z in the region: $0 \leqslant k_z \leqslant \pi/d$ is sufficient for a complete description of all the modes in the infinite crystal. The modes corresponding to the remaining of the reduced $\mathbf{k}$ space are obtained through symmetry. As can be seen from Fig. 1(b), for the phononic crystal under consideration one obtains an absolute frequency gap extending from $\omega a_0/c_l = 2.32$ to $\omega a_0/c_l = 3.13$. We verified that this is indeed so by calculating the projection of the band structure at a sufficient number of $\mathbf{k}_\parallel$ points in the SBZ. The bottom of the absolute gap is determined by the frequency band structure at the $\bar{\Gamma}$ point, and its top by the frequency band structure at the $\bar{M}$ point.

As shown in Fig. 1(a), the long-wavelength limit ($\omega \to 0$) is represented by the linear segments of the dispersion curves, which correspond to the longitudinal (nondegenerate) and transverse (doubly degenerate) modes of propagation of the elastic field in an effective homogeneous medium. It is worth noting that the slopes of these curves give effective propagation velocities in the composite medium, $\bar{c}_l = 2045$ m/sec and $\bar{c}_t = 1019$ m/sec, which are in very good agreement with the results, $\bar{c}_l = 2064$ m/sec and $\bar{c}_t = 1030$ m/sec, of the effective-medium approximation.[6] In an effective-medium picture of the phononic crystal, one would have only these continuum bands, extending over all frequencies. A periodic distribution of *weak* scattering centers would alter this picture only by folding the bands onto the first Brillouin zone and by opening up small gaps, the so-called Bragg gaps, at the Brillouin-zone boundaries. Evidently the absolute frequency gap in Fig. 1 is not a Bragg gap. In reality, apart from the above-mentioned continuum bands, there are also bands originating from resonant elastic modes of the individual spheres: resonant states on neighbor spheres couple weakly with each other, resulting in corresponding relatively narrow bands. We know, in fact, that the elastic field about a single steel sphere in polyester exhibits a sharp dipole resonance, the so-called rigid body resonance,[7] near the frequency region of the gap shown in Fig. 1. This points to the physical origin of this gap: it opens up as a result of hybridization between the narrow bands originating

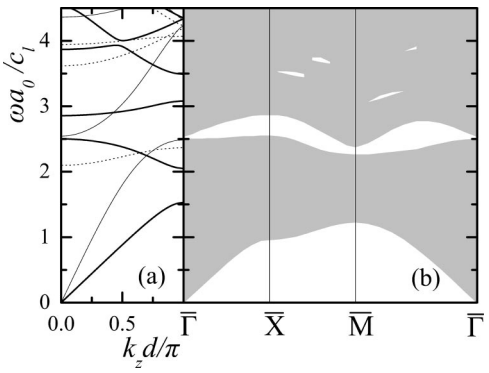

FIG. 2. The same as in Fig. 1, but for a st crystal of steel spheres in polyester with $d = a_0\sqrt{2}/2$ and $f = 18.4\%$.

from the rigid-body-resonance modes of the individual spheres and the continuum bands corresponding to propagation in an effective homogeneous medium. For a fcc crystal, the large coordination number and the highly symmetric arrangement of neighbors around a given sphere imply a relatively isotropic and homogeneous distribution of the elastic field associated with the above-mentioned resonance bands. This, in turn, facilitates their interaction and their hybridization with modes of the elastic field corresponding to propagation in a homogeneous effective medium. For the same reason, strong hybridization and, consequently, large gaps are expected in the case of other compact structures: hexagonal close-packed (hcp), bcc or sc structures.[2] As a measure of compactness we adopt the maximum value of f, to be denoted by $f_{\max}$, that is possible in the given structure (of nonoverlapping spheres). To clarify the above, in Fig. 2 we present band-structure results for a st crystal of steel spheres in polyester, with $f = 18.4\%$ and $d = a_0\sqrt{2}/2$. This crystal, obtained from the previously studied fcc crystal by a simple shift of every second (001) plane by $a_0(1/2,1/2,0)$, is less compact (it has $f_{\max} = 26.2\%$ compared to $f_{\max} = 74\%$ for the fcc). We see that the hybridization-induced gap for $\mathbf{k}_\parallel = 0$ is very narrow [Fig. 2(a)] and that, as result of its variation with $\mathbf{k}_\parallel$, no absolute gap exists in this case [Fig. 2(b)].

In order to further clarify the physical origin of a hybridization gap we refer to Fig. 3. There we show schematically, by dotted lines, two unhybridized bands, along the direction $\mathbf{k} = (0,0,k_z)$: a flat longitudinal band, originating from weakly interacting rigid-body-resonance modes of the inclusions, and the band corresponding to the longitudinal displacement field in the homogeneous effective medium that one would obtain in the absence of interaction with the resonance modes. Because an interaction between them does exist, one obtains the hybridized bands represented by the solid lines in Fig. 3. The bands denoted by 1 are the longitudinal bands shown in Fig. 1(a); in their case the hybridization is strong and a wide gap opens up. The bands denoted by 2 are the longitudinal bands shown in Fig. 2(a); in their case the hybridization is weaker and the corresponding gap is much smaller. We note that the hybridization we have described is analogous to the well known *s-d* hybridization in the energy-band structure of transition metals;[8] it also occurs in metall-odielectric photonic crystals.[9] Of course hybridization occurs

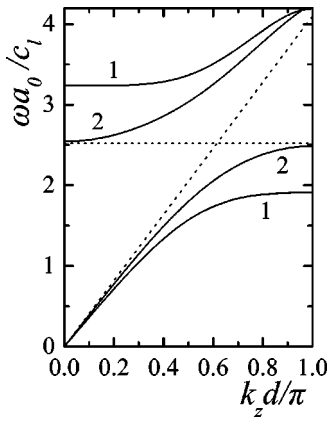

FIG. 3. Schematic representation of a hybridization-induced gap. The dotted lines show the (hypothetical) unhybridized bands. The solid lines 1 and 2 show the (actual) hybridized longitudinal bands shown in Figs. 1(a) and 2(a), respectively.

between transverse bands [see Figs. 1(a) and 2(a)]; there the shape of the hybridized bands is indeed more complicated because of the greater number of unhybridized bands involved in their generation.

In Fig. 4 we show the ratio of the gap width to its respective midgap frequency, $\Delta\omega_G/\overline{\omega}_G$, against the volume fraction f occupied by the spheres, for a variety of lattices having the same interplane distance $d=a_0\sqrt{2}/2$. They are defined by the primitive vectors $\mathbf{a}_1=a_0(1,0,0)$, $\mathbf{a}_2=a_0(0,1,0)$, and $\mathbf{a}_3=a_0(\alpha,\beta,\sqrt{2}/2)$; we also put $(\alpha,\beta)=(0.5,0.5)$ (fcc lattice), $(\alpha,\beta)=(0.5,0.25)$, $(\alpha,\beta)=(0.5,0)$, $(\alpha,\beta)=(0.25,0.25)$, $(\alpha,\beta)=(0.25,0)$, and $(\alpha,\beta)=(0,0)$ (st lattice). It is seen that the widest absolute gaps are obtained for the most compact structure of the family (the fcc structure), with progressively narrower gaps as we go to less compact structures (corresponding to smaller values of $f_{\max}$). It is worth noting that the maximum value of $\Delta\omega_G/\overline{\omega}_G$ for a given structure does not occur at $f=f_{\max}$. This can be understood as follows. The opening of the hybridization gap is favored by an increased f, but at the same time it is compromised by the widening of the resonance bands which is also favored by an increased value of f.

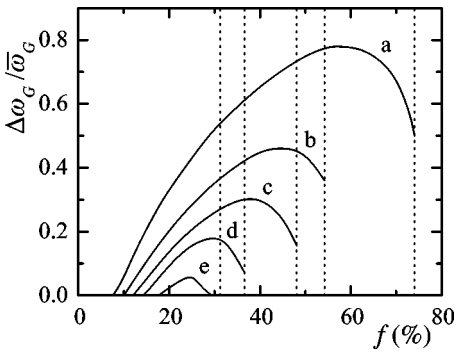

FIG. 4. Absolute frequency gaps in phononic crystals of steel spheres, centered at the sites of various Bravais lattices specified by the primitive vectors $\mathbf{a}_1=a_0(1,0,0)$, $\mathbf{a}_2=a_0(0,1,0)$, and $\mathbf{a}_3=a_0(\alpha,\beta,\sqrt{2}/2)$, in a polyester matrix. (a) $\alpha=0.5$, $\beta=0.5$ (fcc lattice). (b) $\alpha=0.5$, $\beta=0.25$. (c) $\alpha=0.5$, $\beta=0$. (d) $\alpha=0.25$, $\beta=0.25$ (e) $\alpha=0.25$, $\beta=0$. The dotted lines (normal on the abscissa) indicate the values of $f_{\max}$ corresponding to these structures. For $\alpha=\beta=0$ (st lattice, $f_{\max}=26.2\%$) no absolute gap appears.

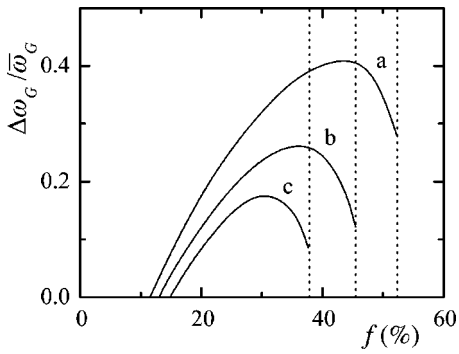

FIG. 5. Absolute frequency gaps in phononic crystals of steel spheres, centered at the sites of various tetragonal lattices specified by the primitive vectors $\mathbf{a}_1=a_0(1,0,0)$, $\mathbf{a}_2=a_0(0,1,0)$, and $\mathbf{a}_3=d(0,0,1)$, in a polyester matrix. (a) $d=a_0$ (sc lattice). (b) $d=1.15a_0$. (c) $d=0.85a_0$. The dotted lines (normal on the abscissa) indicate the values of $f_{\max}$ corresponding to these structures.

We have also looked at the variation of the width of the absolute gap with d, in the case of tetragonal symmetry. Our results (see Fig. 5) again show that the widest gaps are obtained for the sc structure ($d=a_0$), which is the most compact of all tetragonal structures, and become narrower as we go to less compact structures for both $d>a_0$ and $d<a_0$.

The above arguments do not imply that structures with the same $f_{\max}$ will have identical $\Delta\omega_G/\overline{\omega}_G$ versus f curves. These curves depend on the specific geometry of the structure to some degree, but on the whole we expect structures of the same compactness to have more or less the same $\Delta\omega_G/\overline{\omega}_G$ versus f curves.

In all the structures considered so far we have one sphere per primitive cell. We have also looked at two structures with two (identical) spheres per primitive cell: the hcp and diamond structures. The hcp is a compact structure with $f_{\max}=74\%$, equal to that of the fcc. Not surprisingly, we find that $\Delta\omega_G/\overline{\omega}_G$ as a function of f is the same in this case (within 1%) with that of the fcc case [Fig. 4(a)]. By the same token, in the diamond structure, not a compact structure ($f_{\max}=34\%$), we find small absolute gaps for $f>15\%$. $\Delta\omega_G/\overline{\omega}_G$ as a function of f lies in this case between Fig. 4(d) ($f_{\max}=36.6\%$) and curve Fig. 4(e) ($f_{\max}=31.2\%$), and has a maximum value, equal to 0.09, at $f=27\%$.

Finally, in our calculations the scatterers were spheres of a single material. Coating the spheres may shift a hybridization gap toward a desired frequency region,[3,4] but the width of the gap should depend on the geometry of the structure in much the same way as in the examples considered here. It is also likely that the arguments we have presented here relating the width of hybridization gaps to the compactness of 3D structures will apply to 2D systems as well.[10,11]

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