Elastic band gaps in a fcc lattice of mercury spheres in aluminum

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Elastic waves propagating in a periodic system consisting of mercury spheres arranged in a fcc lattice and surrounded by aluminum have been studied using the layer-multiple-scattering method. The band structure shows wide elastic band gaps along certain high-symmetry directions. For filling ratios of mercury spheres around 8.2%, there is a narrow full band gap with maximum width of the gap over mid-gap frequency of 2.5%. The full band gap can be further enhanced by using a heterostructure containing seven slabs of different sizes of mercury spheres and can be as wide as 14.4%.

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Phononic crystals are composite materials whose density and/or the Lame coefficients vary periodically in space.[1,2] Under certain conditions,[1–12] phononic crystals can exhibit frequency regions where elastic waves are not allowed to propagate, the so-called elastic band gaps. Phononic crystals with full band gaps may be used in filters, transducers, and for creation of vibration-free environments. It is also interesting to compare their properties with their electromagnetic counterparts, the photonic crystals.[13,14]

Most of the experimental work has been focused on the fabrication and measurement of two-dimensional (2D) phononic crystals. Acoustic measurements in a minimalistic sculpture consisting of steel rods surrounded by air showed that there was a band gap.[3] A system consisting of air holes in a marble was studied and the motivation for this work was the possibility of applying the concept of phononic crystals to attenuate surface seismic waves.[4] In another experiment, cylinders of mercury, air, or oil in aluminum and forming a square lattice were studied and band gaps were found.[5] Absolute band gaps were also found in a system consisting of steel cylinders in epoxy forming a triangular lattice.[6] There are several theoretical studies of 3D phononic crystals,[1,7–12] but there is only one experimental work.[7] In this study, lead balls coated with silicon rubber form a simple cubic lattice with epoxy matrix. These phononic crystals exhibit spectral gaps with a lattice constant two orders of magnitude smaller than the relevant wavelength.

Here, we study three-dimensional phononic crystals consisting of mercury (Hg) spheres arranged in a face-centered-cubic (fcc) lattice and surrounded by aluminum (Al). The layer-multiple-scattering method[9,10] has been used to calculate the band structure and the transmission coefficient of elastic waves. The Hg/Al system was one of the first systems suggested as having a full elastic band gap.[1] This stems from the high relative difference between the densities of Hg and Al. The plane-wave-expansion (PWE) method has been used in Ref. 1 to calculate the band structure. It is well known that the PWE method does not converge for liquid-solid periodic composites. So, it is still not known if the Hg/Al system has indeed a full band gap. In addition, the 2D system of Hg rods in Al has already been studied[5] and wide band gaps have been found. In this respect, it would be interesting to know what is the behavior of a 3D system.

The projection of the phononic band structure on the surface Brillouin zone (SBZ) of the (001) plane of a fcc crystal of mercury spheres in aluminum and of lattice constant a is shown in Fig. 1. One should bear in mind that the crystal under consideration is viewed as a succession of (001) fcc planes of spheres. The filling ratio of the mercury spheres is $f=8.2\%$. The mass density and the sound velocities for aluminum are $\rho_{Al}=2.71$ g/cm^3, $c_{l(Al)}=6150$ m/s, $c_{t(Al)}=3090$ m/s, and the corresponding values for mercury are $\rho_{Hg}=13.5$ g/cm^3, $c_{Hg}=1450$ m/s. The calculations were performed with an angular momentum cutoff $\ell_{max}=4$ and 13 2D reciprocal-lattice vectors **g** (for more details consult Ref. 9) and the estimated relative accuracy of the eigenfrequencies is better than 10^{-4}. The width of the absolute gap over the midgap frequency is 2.5% and it is defined solely by considering the lower and upper gap edges at the $\bar{X}$ point. It should be noted that for higher volume filling fractions, we have larger partial gaps but no full gap exists.

The phononic band structure normal to the (001) surface (point $\bar{\Gamma}$) and the corresponding transmission spectrum of

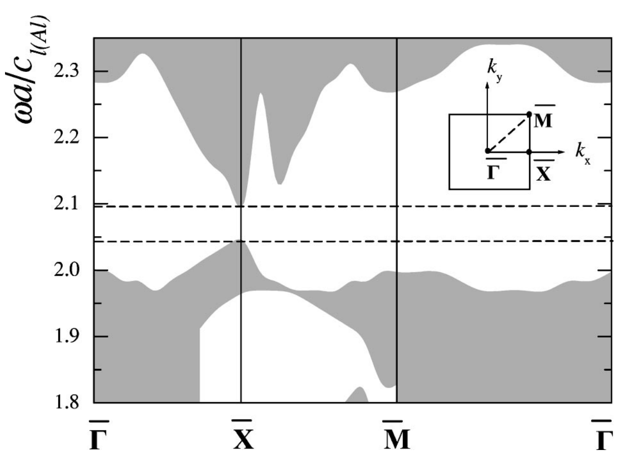

FIG. 1. Projection of the phononic band structure of a fcc crystal of mercury spheres in aluminum, with $f=8.2\%$, on the SBZ of the (001) surface along the high-symmetry lines shown in the inset.

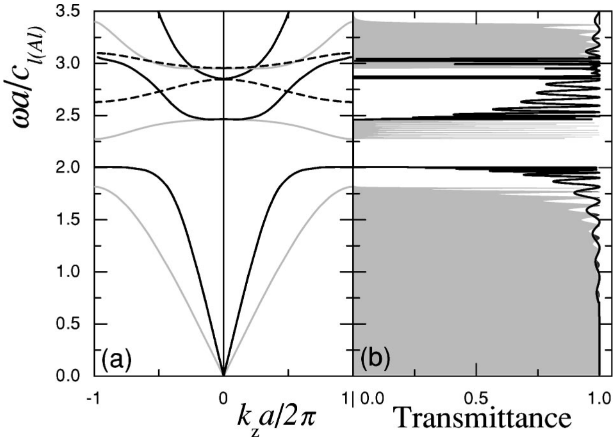

FIG. 2. Phononic band structure at the center of the SBZ ($\bar{\Gamma}$ point) of a (001) surface of a fcc crystal of Hg spheres in Al (a); and the corresponding transmittance curve of slab of 16 planes of spheres parallel to the same surface at normal incidence (b). As in Fig. 1 the fractional volume occupied by the spheres is $f=8.2\%$. In (a) the solid black (gray) lines represent compressional (shear) modes and the dotted lines are deaf bands. Correspondingly in (b) the shaded area (black solid line) shows the transmittance of incident shear (compressional) acoustic waves.

compressional and shear acoustic waves incident normally on a slab of the crystal, consisting of 16 (001) fcc planes of spheres, are shown in Fig. 2. The bands shown in Fig. 2(a) by black (gray) lines correspond to compressional (shear) modes of the vibration of the elastic field inside a sufficiently thick slab of the material. These modes are excited only by compressional (shear) waves incident normally on the surface of the slab. This is demonstrated quite clearly in Fig. 2(b) that shows the transmission coefficient of a plane wave incident normally on a slab of the material consisting of 16 planes of spheres parallel to the (001) surface. The shaded curve (black line) shows the transmission coefficient for a shear incident wave (compressional incident wave). Off the normal direction the frequency bands are clearly hybridized and they are excited by either compressional or shear incident plane waves. The bands shown in dotted lines are deaf bands, meaning that they cannot be excited by an incident plane wave, leading to total reflection of the latter. Finally, we point out the oscillations in the transmission coefficient, over the allowed regions of frequency, which are due to interference effects resulting from multiple reflection between the surfaces of the slab (Fabry-Perot-type oscillations). As can be seen from Fig. 2(a), in the long-wavelength limit ($\omega \to 0$) we obtain linear dispersion curves, the slopes of which give the effective velocity of compressional and shear sound waves in a homogeneous effective medium. The first Bragg gap for shear modes opens up from $\omega a/c_{l(Al)}=1.82$ to $\omega a/c_{l(Al)}=2.28$, while the corresponding gap for compressional modes is expected at much higher frequencies. However, a hybridization gap for compressional modes exists from $\omega a/c_{l(Al)}=2.01$ to $\omega a/c_{l(Al)}=2.47$, which overlaps with the first Bragg gap of shear modes. This gap originates from a hybridization between a flat band resulting from interacting resonant compressional modes of neighboring fcc (001) planes of spheres and the band that describes free propagation of compressional waves in a corresponding homogeneous effective medium.

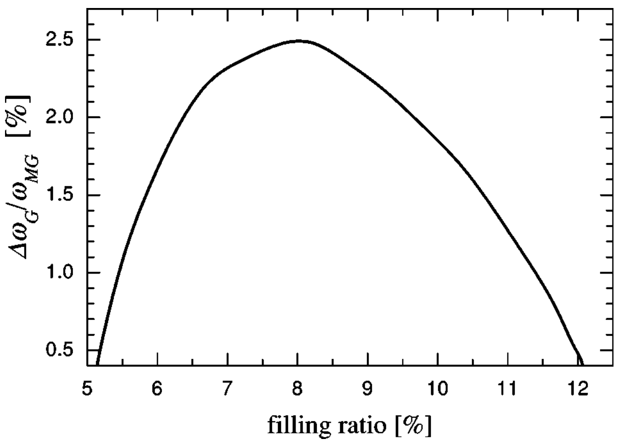

FIG. 3. The width of the gap over midgap frequency for the fcc crystal of Hg spheres in Al as a function of the filling ratio.

Figure 3 shows the width of the gap over the midgap frequency. Absolute gaps appear for filling ratios between 5.2% and 12.1% and the maximum absolute gap is 2.52% at $f=8.2\%$. The full-band-gap feature of the system under study can be enhanced by using a heterostructure containing slabs corresponding to different f (spheres of different size). This tandem structure concept has been also investigated in the past by Kushwaha *et al.*,[15] with a PWE approach. In Fig. 4 we show how, by stacking together seven slabs with overlapping full gaps we obtain a resulting $\Delta\omega_G/\omega_{MG}=14.4\%$. In particular, the filling ratios used were 5.9%, 6.3%, 6.8%, 7.5%, 8.23%, 8.93%, and 9.6%. It should be noted that slabs of at least eight planes of spheres are needed in order to preserve with accuracy the full-band-gap feature of the crystal. Therefore a minimum width of $4a$ per slab should be appropriate for stacking and a width of $28a$ for the above heterostructure is recommended at least. The stacking properties of two consecutive (001) fcc slabs are given in Fig. 5 and they correspond to the above minimum width configuration.

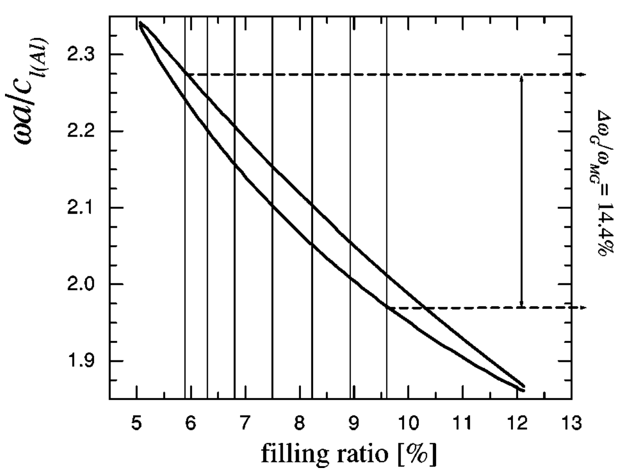

FIG. 4. The edges of the full gap for the fcc crystal of Hg spheres in Al as a function of the filling ratio.

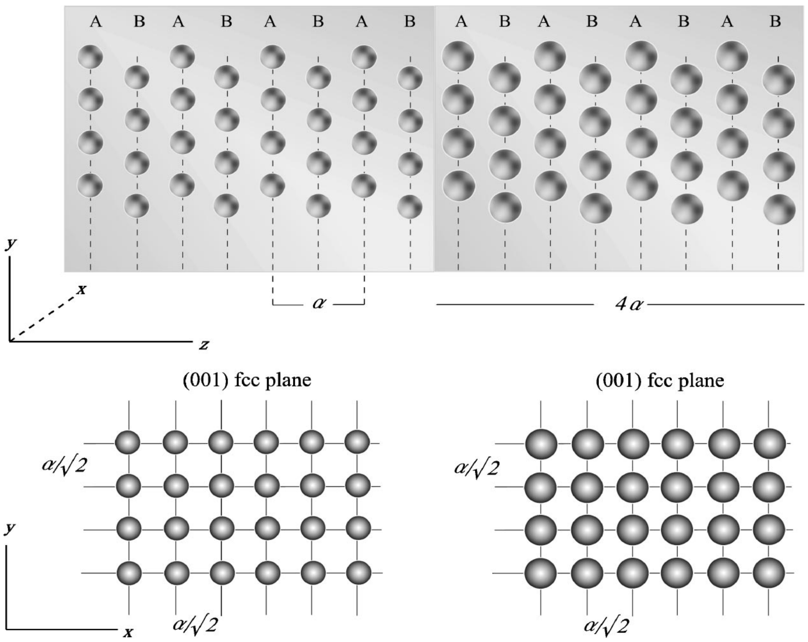

FIG. 5. Consecutive slabs of different *f* along the (001) fcc stacking. At the bottom, the 2D structure of the individual (001) fcc planes is given.

In conclusion, a three-dimensional elastic periodic composite of mercury spheres in aluminum matrix forming a fcc lattice was studied. The layer-multiple-scattering method has been used for the calculation of the band structure and the transmission of elastic waves. Although, wide frequency partial gaps were found along certain directions within the lattice, the absolute band gaps were much narrower. The maximum width of the absolute elastic band gap over the midgap frequency was 2.52% at a filling ratio of mercury spheres of 8.2%. Using an assembly of seven composites of different filling ratios, a heterostructure was created having a width of the absolute band gap over the midgap frequency of 14.4%. This concept applied to assemblies of phononic or photonic band-gap materials may enhance greatly full gaps.

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