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Localized states of acoustic waves in three-dimensional periodic composites with point defects

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Abstract. Acoustic point defect states in the three-dimensional simple-cubic arrays of water spheres embedded in a mercury host are studied. Two kinds of defects are introduced, one is a sphere defect created by changing its radius, and another is a cubic defect obtained by replacing one of the spheres with a cube. The results show that a defect band appears in the band gap of the perfect crystals. The calculations show that the defect modes are localized around the defect. The influence of the filling fraction and the geometry of the defect on the defect modes are investigated in detail.

PACS. 43.20.+g General linear acoustics – 62.60.+v Acoustical properties of liquids – 61.72.Ji Point defects (vacancies, interstitials, color centers, etc.) and defect clusters

In recent years, the propagation of acoustic or elastic waves in periodic and random elastic composite materials, known as "phononic band gap materials" or "phononic crystals", has received a great deal of attention [1–24]. Much effort has been focused on the search for large band gaps in the acoustic or elastic band structure, in which sound and vibration are all prohibited. The motivation for these studies is to better understand the Anderson localization of sound and vibrations in inhomogeneous media [3], as well as their numerous engineering applications such as frequency filters, vibrationless environments for high-precision mechanical systems or the design of new transducers.

In the two dimensional (2D) and three dimensional (3D) periodic composite media with solid host, the longitudinal and transverse vibrations are always coupled, which makes the nature of the eigenmodes and corresponding computation much more complicated. The situation can be simplified if the host media is gas and/or liquid, in which only longitudinal waves can propagate, no matter whether the system is 2D or 3D. Large acoustic (sonic) band gaps have been found in the 2D and 3D binary liquid and gas systems, such as liquid-liquid systems [4–7], liquid-gas systems [8,9], and solid inclusions inside air [10–15]. Although there have been many works trying to determine the optimal conditions for the appearance of acoustic wave band gaps, only few works have been related to the defects and disorder-induced phenomena in 2D and 3D phononic crystals. Sigalas [16,17] has treated point and linear defect states in 2D phononic crystals composed of solid cylinders in air or in a solid host by means of the plane-wave expansion (PWE) method. The results show that the defect in those structures creates localized states inside the band gap. Kafesaki *et al.* [18,19] and Khelif *et al.* [20] have studied linear wave-guides in 2D elastic wave band gap materials made up of either fluid or solid constituents. The calculations of band structure and transmission coefficient were performed by using PWE method and the finite difference time domain (FDTD) method, respectively. They studied the guiding of elastic waves through linear defect modes created by a line of defects in a 2D elastic wave band gap material, and found that these defects could act as waveguides in the frequency regime of the gap. Miyashita *et al.* [21] also reported the numerical investigations of transmission and waveguide properties of 2D sonic crystals by the FDTD method. The localization phenomena in linear and point defects were also observed experimentally [22]. However, within all the above works [16–22], only circular cross-section of cylinders were considered, and the point defects were created by changing the radius of a cylinder or simply removing the whole cylinder. Recently, we have studied the 2D defect problem by using different geometry of cross section from the regular cylinders to introduce the

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point defect. The results show that the defect states not only relate to the filling fraction of defect, but also to its geometry [23].

For the defect states of 3D phononic crystals, to the best of our knowledge, only one theoretical paper has appeared [24]. A possible reason is that for the 3D cases the mathematical treatment and corresponding computation are much more complicated than that of 2D phononic crystals. In their work, Psarobas *et al.* [24] investigated the planar defects in 3D solid phononic crystals composed of nonoverlapping lead spheres centered on the sites of an FCC lattice. The defects were introduced by changing the radius of spheres in one of the planes, *i.e.*, what they studied was a defect layer in a 3D periodic system. The result shows that the plane of impurity spheres introduces modes of vibration localized on this plane at frequencies within a frequency gap of a pure phononic crystal.

In the present article, we study the point defects in 3D phononic crystals. For the sake of simplicity, we consider the system of water (with longitudinal velocities $c_l = 1.48$ km/s and density $\rho = 1.0 \times 10^3$ kg/m^3) spheres with a simple-cubic (SC) array embedded in a mercury ($c_l = 1.45$ km/s, $\rho = 13.5 \times 10^3$ kg/m^3) host. The acoustic wave equation for a homogeneous isotropic medium of fluid or gas can be written as [4–6]

$$\frac{1}{\lambda}\frac{\partial^2 p}{\partial t^2} = \nabla\left(\frac{\nabla p}{\rho}\right), \tag{1}$$

where $\lambda(\vec{r})$, $\rho(\vec{r})$ and $p(\vec{r})$ are the bulk modulus, the mass density and pressure of the fluid or gas, respectively.

For the 3D fluid-fluid periodic systems, Bloch's theorem asserts that the pressure $p(\vec{r})$ can be written as $p(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} p_{\vec{K}}(\vec{r})$, where $\vec{k}$ is restricted within the first Brillouin zone (BZ) and $p_{\vec{K}}(\vec{r})$ is a periodic function with the same periodic structure as $\lambda^{-1}(\vec{r})$, $\rho^{-1}(\vec{r})$. They can be expanded in Fourier series with corresponding coefficients $p_{\vec{K}+\vec{G}}$, $\lambda^{-1}_{\vec{G}}$, and $\rho^{-1}_{\vec{G}}$, respectively. In term of these coefficients, equation (1) becomes

$$\sum_{\vec{G}'}\left[\omega^2\lambda^{-1}_{\vec{G}-\vec{G}'} - \rho^{-1}_{\vec{G}-\vec{G}'}\left(\vec{k}+\vec{G}\right)\cdot\left(\vec{k}+\vec{G}'\right)\right] p_{\vec{G}'} = 0. \tag{2}$$

Equation (2) is an infinite set of linear equations. In practice, only a finite number of reciprocal vectors $\vec{G}$ are taken into account for the numerical calculation. If the infinite series is approximated by a sum of N reciprocal vectors, equation (2) is reduced to $N \times N \times N$ matrix eigenvalue equations. In the present paper, we use 1331 reciprocal vectors per supercell to perform the numerical calculations. The results have shown a good convergence. The eigenvalues do not exceed 2% by using more reciprocal vectors in the low-frequency regime where the complete band gaps were found.

We introduce the point defects in two ways: one is by radius-modification, *i.e.*, changing the radius of one of the spheres in 3D phononic crystal, another is by replacing one of the spheres with a cube. The theoretical analysis of the defect modes can be carried out by the supercell method that has been performed for the defects in 2D phononic crystals [16,17] and photonic crystals [25–27]. We consider now such a system, in which the supercell consists of $5 \times 5 \times 5$ spheres. The locations of the spheres with one sphere of radius r (corresponding to the filling fraction $F_0 = \frac{4}{3}\pi\left(\frac{r}{a}\right)^3$) are at $[(2n_x+1)/2,\ (2n_y+1)/2,\ (2n_z+1)/2]$, where n_x, n_y, n_z = 0, 1, 2, 3, 4 and a is the lattice constant. A defect located at (2.5, 2.5, 2.5) is introduced by changing the spherical radius r_d, or width L_d of the cube in the center of the supercell (corresponding to the defect filling fraction $F_d = \frac{4}{3}\pi\left(\frac{r_d}{a}\right)^3$ for the sphere defect, and $F_d = \left(\frac{L_d}{a}\right)^3$ for the cubic defect). It means that the supercell lattice has a period $a' = 5a$, each supercell is composed of 5^3 original cells.

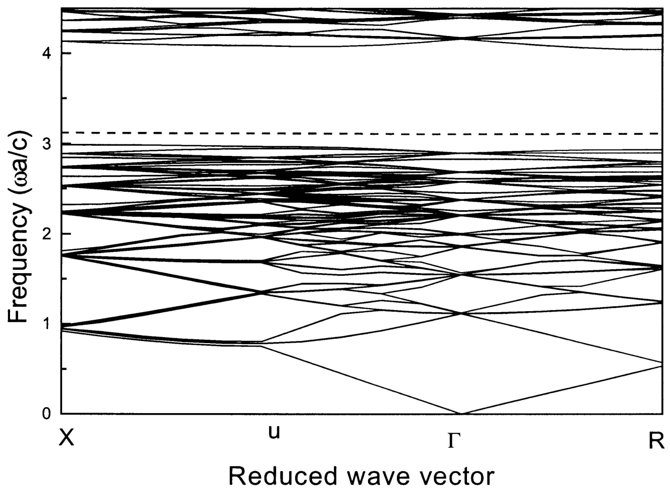

Fig. 1. Acoustic band structure with a point defect. The filling fraction is $F_0 = 0.27$, and defect filling fraction is $F_d = 0.25F_0$. A defect band with bandwidth $\Delta\omega = 0.013c/a$ is shown by the dashed line. The band gap ranges from $\omega = 2.99c/a$ to $4.05c/a$. ω is the frequency, a is the lattice constant, and c is the sound velocity in mercury.

We first study the defect states of the systems consisting of water spheres inside a mercury host. The point defect is introduced by changing the radius of one water sphere located in the center of the supercell. We begin with a perfect crystal, when the filling fraction of the regular water sphere is $F_0 = 0.27$ the corresponding ratio of radius r to the lattice constant a is $r/a = 0.40$. The numerical result shows the existence of a band gap with the lower edge at $\omega = 3.00c/a$ and the upper edge at $\omega = 4.05c/a$, where c is the sound velocity in mercury. Then we reduce gradually the radius of the defect sphere. Figure 1 shows the band structure when the defect water sphere has a different radius $F_d = 0.25F_0$. One defect band with a narrow width $\Delta\omega = 0.013c/a$ can be seen within the frequency range of the original band gap. Figure 2 shows the pressure distribution of the defect state at point Γ of Figure 1 in the XY plane ($z = 2.5$) of the supercell. A peak of pressure is found to occur at the location of the defect sphere, and there was a very low pressure distribution along the

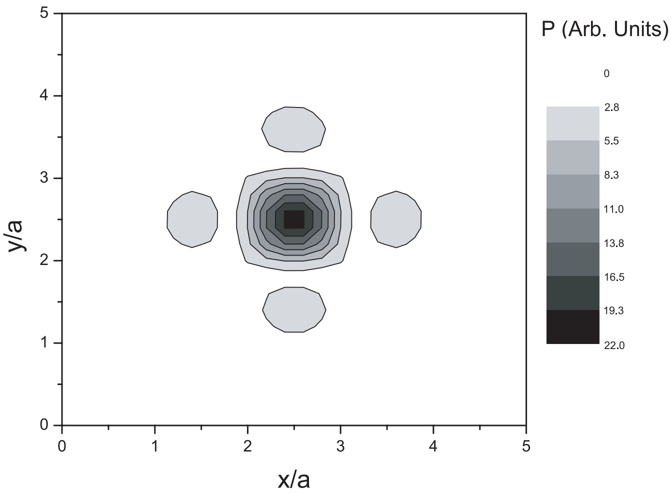

Fig. 2. In the XY plane with $Z = 2.5$ of the supercell, the spatial distribution of pressure P for the defect state at the Γ point in Figure 1.

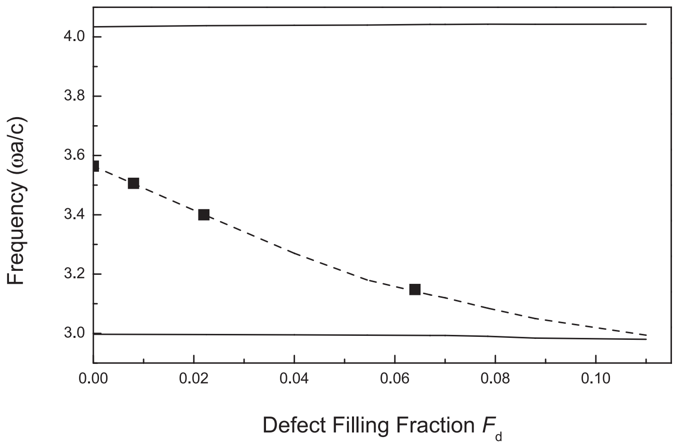

Fig. 3. The frequencies of the defect midband as a function of the defect filling fraction. The filling fraction is $F_0 = 0.27$. The solid lines indicate upper and lower edge of the band gap. The dashed line stands for the midband of the defect mode. The square symbols denote the defect midband of the cubic defect.

edges of the supercell. This result shows a well-isolated spatial distribution without overlapping with other supercells. Almost the same pressure distribution behavior can be obtained for other defect states.

Figure 3 shows the results of the defect midband as a function of the defect filling fraction F_d for a given filling fraction $F_0 = 0.27$. When $F_d = 0$, the frequency of the defect midband reaches $\omega = 3.56c/a$. The defect band moves towards the lower edge of the gap as the defect filling fraction F_d increases. Eventually, the defect band disappears when the defect filling fraction $F_d > 0.12$. It infers that the defect band can appear for a small defect filling fraction F_d, but when the defect filling fraction is larger than a certain value ($F_d = 0.12$), the perturbation is too small to create a defect mode in the band gap of the perfect system.

In 2D phononic crystals with water rods in a mercury host [23], we have found that the acoustic point defect modes are sensitive to the geometry of defect rods as well as the rest rods. For the system of water rods with a circular cross section in mercury, the two defect bands only appear in a certain range of defect filling fractions in the case of circular defects, while the defect midband almost does not change for a wider range of defect filling fraction in case of the square defect. For the system of water rods with square cross section, the defect modes depend only on the defect filling fraction regardless of the geometry of defect (circular or square). So it is very interesting to see what happens when the geometry of the defect or the regular inclusions are changed in the 3D phononic crystals. We first examine the effect of the geometry of the defect on defect band in the system of water spheres in mercury (SWM) when a water cube replaces the spherical defect. The four square symbols (■) in Figure 3 show the midbands of the defect modes for ratios between edge width (L_d) of the cubic defect and the lattice constant (a) of $L_d/a = 0.00$, 0.20, 0.28, and 0.40, respectively. It can be clearly seen that if the cubic defect has the same filling fraction as the spherical defect, there will be almost the same defect states. This result is different from the case of 2D phononic crystals [23]. Similar results can be obtained in the system of water cube in mercury host (CWM) with the sphere defects as well as the cubic defects.

In conclusion, using the PWE method and supercell calculations, we have studied the point defect states of the 3D simple cubic arrays of water spheres in a mercury host. The defects are created by two kinds of geometry: one is a sphere, which has a different radius from the other spheres, and another is a cube. The results show that the defect band only appears in a certain range of defect filling fractions, and will move down with increasing defect filling fraction. For these two kinds of defects, the defect band is only related to the defect filling fraction F_d, not the geometry of defect (sphere or cube). Similar results can be found in the CWM systems. The numerical results also show that the pressure distribution of such defect states is well localized in the vicinity of the defect.

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