Splitting and tuning characteristics of the point defect modes in two-dimensional phononic crystals

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Point defect modes of acoustic wave in two-dimensional square arrays of square water rods in a mercury host were studied. The defects are created by three kinds of geometry, namely, square defect, circular defect, and rectangular defect, respectively. The results show that for both square defect and circular defect, the defect modes are only related to the defect filling fraction F_d , but not with the geometry of defects (square or circular), as well as the orientations of the square defect. For the rectangular defect, the defect modes could be tuned by changing the ratio of edge width of the defect, moreover, the double degenerate one will split into two nondegenerate modes when the ratio of edge widths $L_x/L_y > 9.0$. Meanwhile the corresponding pressure distributions also will be changed.

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I. INTRODUCTION

In past few years, the phononic crystals, periodic elastic composite materials, have attracted much attention (Refs. [1–13]). Such artificial crystals can exhibit phononic band gaps in which sound and vibration are all forbidden in any direction. The existence of the acoustic/elastic wave band gaps is significant for us to better understand the Anderson localization of sound and vibrations in composite media, as well as their numerous applications. One particularly interesting aspect of these crystals is the possibility of creating crystal defects that confine the elastic/acoustic waves in the localized modes. Because of the locally breaking the periodicity of the structures, the defect modes can be created within the acoustic (elastic) wave band gaps, which are strongly localized around the local defects. So a point defect can act as a microcavity and a line defect can be used as a waveguide. These controllable defect modes have played key roles in their possible applications (such as acoustical filters and transducers).

Although there have been many works in searching the optimal conditions of the appearance of acoustic wave (elastic wave) band gaps (Refs. [1–6]), only a few works have been devoted to the defects and disorder-induced phenomena in two-dimensional (2D) and 3D phononic crystals. Sigalas [7] had treated the point and linear defect states in 2D phononic crystals composed of solid cylinders in an air or in a solid host by means of the plane-wave expansion (PWE) method. The results show that the defects in those structures create the localized states inside the band gaps. Kafesaki *et al.* [8] and Khelif *et al.* [9] have studied the linear waveguides in 2D elastic wave band gap materials consti-

tuted by either the fluid or solid constituents. The calculations of the band structures and the transmission coefficients were performed by using the PWE method and the finite difference time domain (FDTD) method, respectively. They have studied the guiding of the elastic waves through the 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.* [10] also reported the numerical investigations of transmission and waveguide properties of the 2D acoustic crystals by FDTD method. The localization phenomena in the linear and point defects were also observed experimentally [11].

However, all the above works [7–11], only the circular cross section of the cylinders was considered, and the point defects are created by changing the radius of a cylinder or simply removing the whole cylinder. Recently the present authors have studied the 2D defect problem by using different geometry of cross section from the rest cylinders to introduce the point defects. The results show that the defect states not only depend on the filling fraction of the defect, and also on its geometry [12]. On the other hand, we had studied the acoustic band gaps in the 2D liquid phononic crystals composed of water (mercury) square rods inside mercury (water) host [13]. It is found that acoustic band gaps could be tuned effectively by rotating the square rods. The lowest gap width increases monotonously as the rotation angle increases for the systems of mercury square rods in a water host. But for the systems of water square rods in a mercury host, the opposite result is found, the lowest gap width will decrease monotonously as the rotation angle increases.



FIG. 1. The cross section of XY plane in a 5×5 supercell. The square defect locates at (2.5,2.5). The two constituents are denoted by the black and white sectors, respectively. The mesh stands for defect.

In the present article, we study the point defects in the 2D phononic crystals composed of water (with longitudinal velocities $c_1 = 1.48 \text{ km/s}$ and density $\rho = 1.0 \times 10^3 \text{ kg/m}^3$) square rods with a square array embedded in a mercury (c_1) =1.45 km/s, ρ =13.5×10³ kg/m³) host, we try to examine if the rotation effect could be also used to tune the acoustic defect modes, and how to split the double degenerate modes. We introduce the point defects by three ways, the first is by the edge width modification (square defect), i.e., changing the edge width of the defect square rods and/or rotating them with the angle θ , the second is by replacing one of the square rods with a circular one (circular defect), the last one is by replacing one of the rods with a rectangular one (rectangular defect). The theoretical analyses of the defect modes can be carried out by the supercell method that has been performed successfully for the studies of defects in 2D phononic crystals [7,12] and photonic crystals [14,15].

As suggested by several groups [2,3,9,12,13,16–18], to be practical, some latex material would be used for the inner layer of the cylinders containing the liquid (air). The mass density and speed of rubber are comparable to those of water, so the effect of this thin film can be neglected.



FIG. 2. Acoustic band structure with a square defect. The defect filling fraction. F_d =0.03. Its rotation angle θ =0°. The filling fraction F=0.30. Symbol lines represent two defect bands. *C* is the sound velocity in mercury.



FIG. 3. The pressure distributions of the two defect modes at point Γ Fig. 2. (a) and (b) correspond to the double degenerate modes, dipoles. (c) the nondegenerate mode, monopole.

II. RESULTS AND DISCUSSION

Now we consider such a system, in which the supercell consists of 5×5 rods. The locations of the square rods of edge width *L* (corresponding the filling fraction F_0) are at $[(2m_x+1)/2, (2m_y+1)/2]$, where $m_x, m_y=0, 1, 2, 3, 4$. A defect located at (2.5,2.5) is introduced by changing its edge width L_d and/or its rotation angle θ for the square defect, or the radius r_d for the circular defect, or the width L_x, L_y along x, y directions for the rectangular defect, respectively. Figure

TABLE I. The frequency of the edge of the band gap and the defect midbands in the 2D phononic crystal with a square defect or a circular defect. (F=0.30, $F_d=0.03$).

Defect of shape	θ	$\omega_1 (c/a)^a$	$\omega_2(c/a)^{\mathrm{b}}$	$\omega_3 (c/a)^{\rm c}$	$\omega_4(c/a)^d$
Square	0°	1.825	2.416	4.736	4.901
	9°	1.825	2.416	4.736	4.901
	18°	1.825	2.415	4.736	4.901
	27°	1.825	2.414	4.736	4.901
	36°	1.825	2.414	4.736	4.901
	45°	1.825	2.413	4.736	4.901
Circular		1.825	2.412	4.734	4.897

^a ω_1 —the frequency of the lower edge of the band gap.

 ${}^{b}\omega_{2}$ —the midband frequency of the lower defect band (no degenerate).

 $^{c}\omega_{3}$ —the midband frequency of the upper defect band (double degenerate).

 ${}^{d}\omega_{4}$ —the frequency of the upper edge of the band gap.

1 shows the cross section of XY plane of the supercell with a square defect. In the present paper, we use 729 reciprocal vectors per supercell to perform the numerical calculations. The results show a good convergence.

First, we study the defect modes of the systems consisting of square water rods inside mercury host. The point defect is introduced by changing the edge width of one square water rod located in the center of the supercell. Figure 2 shows the band structure when there exist a defect water rod, which has different filling fraction F_d from the rests F_0 . Two flat defect bands can be found within the frequency range of the band gap of the perfect array. The upper one is a double degenerate one; the lower one is a nondegenerate. Figure 3 shows the pressure distributions of the defect modes at point Γ in Fig. 2. The results show their peculiar symmetry, for the double degenerate mode, there are two distributions shown in Figs. 3(a) and 3(b), which are labeled dipoles since they have two nodes in the plane, and moreover, one is an almost replica of the other given by a 90° rotation. For the lower one, only one peak appears in the center of the defect, and the pressure decays rapidly away from the defect. Since there is not a node in the supercell [see Fig. 3(c)], it is labeled a monopole.

Next we study the effect of the orientation of the square defect on the defect modes. Five sets of date corresponding to five rotation angles $\theta = 9^{\circ}, 18^{\circ}, 27^{\circ}, 36^{\circ}, 45^{\circ}$ are given in Table I for a fixed defect filling fraction $F_d = 0.03$. One could immediately find that there are almost the same results for the five cases. More detailed numerical calculations also show that the defect modes are independent of the orientation of the defect rod. In Table I we also present the results for the circular defect, which have the same defect filling fraction as the above square defect. The same results as the square defect case can be found. Although the symmetry of the system is reduced by rotating the square defect, this mechanism is not sufficient to tune the modes as well as split the double defect modes.

In order to split the double mode, we should break further the symmetry of the system. Now we examine the effect of



FIG. 4. Acoustic band structure with a rectangular defect. The defect filling fraction F_d =0.03. The filling fraction F=0.30. The ratio between edge widths L_x/L_y =25. Three defect bands appear and are represented by symbol lines.

the rectangular defect on the defect states. Figure 4 shows the band structure when the ratio between the edge width L_x and L_y along x, y directions is $L_x/L_y=25$. It can be clearly seen that the upper double degenerate defect band in the case of the square defect is split into two no degenerate ones. Moreover, both split defect modes have different pressure



FIG. 5. The pressure distributions of the two split defect modes at point Γ in Fig. 4. (a) The higher split mode, quadrupole. (b) The lower split defect mode, dipole.



FIG. 6. The frequencies of the defect midband as a function of the ratio of edge widths for rectangular defect. The filling fraction F=0.30. The defect filling fraction $F_d=0.03$. The symbol lines stand for the midbands of defect modes.

patterns shown in Fig. 5 from the case of the square defects. The high one is a quadrupole and the lower is also a dipole [see Figs. 5(a) and 5(b)]. But the distribution of the lowest one remains a monopole.

Figure 6 shows the frequencies of the defect midbands as a function of the ratio of the edge widths in the case of rectangular defect for a given defect filling fraction F_d =0.03. We can find that the midband frequency of the lower defect band increases slowly as the ratio L_x/L_y increases, at the same time the upper defect band also slowly increases following the increase of the ratio, L_x/L_y , but when, $L_x/L_y > 9.0$, the double degenerate one splits to two defect bands.

III. CONCLUSION

In a conclusion, using the PWE method and the supercell calculations, we have studied the point defect modes of the 2D square arrays of the square water rods in a mercury host. The defects are created by three kinds of geometry, i.e., square defect, circular defect, and rectangular defect, respectively. The numerical results show that for both the square defect and the circular defect, the defect modes are uniquely related to the defect filling fraction F_d , but not with the geometry of the square defect. But for the rectangular defect, the defect modes could be tuned by changing the ratio of the edge width. Moreover, in this case the double degenerate band will split into two defect bands when the ratio $L_x/L_y > 9.0$.

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