Influence of defect states on band gaps in the two-dimensional phononic crystal of 4340 steel in an epoxy*

Kong Xiao-Yan(孔肖燕), Yue Lei-Lei(岳蕾蕾), Chen Yu(陈 雨), and Liu Ying-Kai(刘应开)†

Institute of Physics and Electronic Information, Yunnan Normal University, Kunming 650092*, China*

(Received 28 December 2011; revised manuscript received 24 April 2012)

The band structures of a new two-dimensional triangle-shaped array geometry of 4340 steel cylinders of square cross section into epoxy resin were studied by the plane-wave expansion and supercell calculation method. The band gaps of this type of phononic crystals with different defects were calculated such as defect-free, 60° crystal linear defect states, 120° crystal linear defect states, and 180° crystal linear defect states. It was found that the band gap will emerge in different linear defects of the phononic crystals and the bandwidth of linear defect states is larger than that of the free-defect crystal by about 2.14 times within the filling fraction $F = 0.1$–0.85. In addition, the influence of filling fraction on the relative width of the minimum band gap is discussed.

Keywords: defect state, band width, number of band gap

PACS: 61.50.Lt, 61.72.–y, 62.65.+k **DOI:** 10.1088/1674-1056/21/9/096101

1. Introduction

In recent years there has been growing interest in the propagation of elastic waves in periodic elastic composite materials known as phononic crystals.[1−4] Of particular interest is the existence of band gaps in which sound with a certain frequency range are forbidden. Further study also indicates that defect states exist inside the band gaps.[2−6] Moreover, because of the ability of phononic crystals to effectively block sound waves with a range of frequencies, they can be used as acoustic filters, suppressing noise in places where a vibrationless or noise-free environment is desired.[2,7−13] Consequently, it is of great importance to determine and optimize the factors that influence the width of the band gap. The motivation for these studies is to better understand the Anderson localization of sound in composite media[14] and use its properties.

For the two-dimensional (2D) phononic band gap materials, various structures have been investigated. Large acoustic band gaps in square, triangular, boron nitride, and rectangular lattices have been found. However, the constituent materials are either solid, or both fluid (gas) and solid–fluid.[15−22] Plane-wave method have been used to calculate the band gap of 2D triangle-shaped array and square-shaped array solid–solid phononic crystal with square cross section. The results indicated that triangle-shaped array is more likely to get wider band gap than square-shaped array.[23] In this paper, we study 2D triangular lattices of 4340 steel cylinders of square cross section inserted into epoxy resin (2D-SCER) by the plane-wave expansion method and supercell calculations.[24−26] Forbidden gap appeared in small filling fraction (e.g., $F = 0.1$) in solid-solid state. Its bandwidth increases to a maximum, and then decreases as the filling fraction increases.[27,28] The band gaps of 2D-SCER with different defects, such as defect-free 60° crystal linear defect states, 120° crystal linear defect states, and 180° crystal linear defect states are calculated. The band gap number and relative width of the minimum band gap with the filling fraction are also obtained.

2. Model

We consider elastic waves propagating in a perfect phononic crystal with cylindrical of 4340 steel (denoted by A) periodically embedded in the epoxy resin (denoted by B), as shown in Fig. 1(a).

*Project supported by the National Natural Science Foundation of China (Grant Nos. 10764005 and 11164034) and the New Century Training Program Foundation for Talents from the Ministry of Education of China (Grant No. NCET-08-0926).

†Corresponding author. E-mail: liuyingkai99@163.com

© 2012 Chinese Physical Society and IOP Publishing Ltd

For the 4340 steel, the density is $\rho_{\rm A} = 7.8$ g/cm^3, the shear wave speed $c_{\rm tA} = 3200$ m/s, and the vertical wave velocity $c_{\rm lA} = 5830$ m/s. For epoxy resin, the density $\rho_{\rm B} = 1.4$ g/cm^3, the shear wave speed $c_{\rm tB} = 1300$ m/s, and the vertical wave velocity $c_{lB} = 2700$ m/s. The filling fraction for component A is $F = 4l^2/(\sqrt{3}a^2/2)$ $(0 \leq F \leq 0.86)$, where $2l$ is the edge length of square rods, and a is the lattice constant. The edge length of defect square is $2l_1 \leq \sqrt{3}a/2$, and thus the filling ratio is $F \leq 0.86$. The x and y directions are periodic, but the z direction is homogeneous. In reciprocal lattice vector space with triangle-shaped array, the first Brillouin zone is hexagonal, and the Bloch wave vector $\boldsymbol{k}$ is along the triangle ΓXM, as shown in Fig. 1(b).

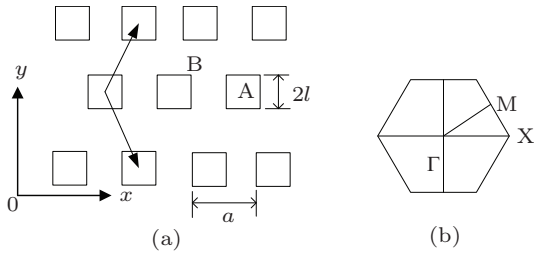


Fig. 1. Structure of phononic crystal. (a) Triangular-square lattice. (b) The first Brillouin zone for a 2D triangle lattice.

Figure 2 shows the cross sections of the supercells having typical bending linear defects, which are created by removing cylinders along the bend path in phononic crystals. All models are periodic in the x and y directions but homogeneous in the z direction.

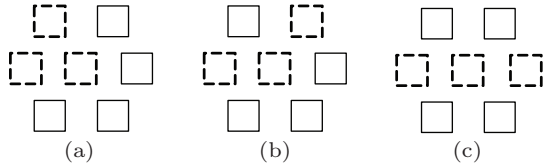


Fig. 2. (a) Supercell structure with 60° linear defect; (b) supercell structure with 120° linear defect; (c) supercell structure with 180° linear defect. Square: 4340 steel; blank area and dotted line box: epoxy resin.

3. Theory

Defect states appearing inside the band gaps were studied by the plane-wave expansion and supercell calculation method. $2N\times2N$ matrix eigenvalue equations were obtained for the x–y mode in 81 reciprocal vectors $\boldsymbol{G}$ (i.e., the integers n_x and n_y in G take the values from -4 to 4), where N is the number of reciprocal lattice vectors. For a given Bloch wave vector $\boldsymbol{k}$ in the first Brillouin zone, an infinite number of eigen solutions is obtained, which is characterized by a natural number n (rather than k). The results indicate a good convergence.[3–9]

4. Results and discussion

Figure 3 displays the band structure along the paths M–Γ and Γ–X in the first irreducible Brillouin zone with filling fraction $F = 0.4$ and $a = 0.04$ m, as shown in Fig. 1(b). The frequency is normalized by $a/2\pi c_{\rm t}$, where $c_{\rm t}$ is the transverse wave velocity. For the free defect structure in Fig. 1(a), the largest width of the band gap is $L = 0.1709$ with $L = \omega a/2\pi c_{\rm t}$ ranging from 4.7720 to 4.9429, where ω is the eigen frequency (see Fig. 3(a)). For 60° linear defect in Fig. 2(a), the largest width of the band gap is $L = 0.3661$ with L ranging from 8.6682 to 9.0343, as displayed in Fig. 3(b). For 120° linear defect in Fig. 2(b), the largest width of the band gap is $L = 0.1661$ with L ranging from 7.2912 to 7.4573, as shown in Fig. 3(c). For 180° linear defect in Fig. 2(c), the largest width of the band gap is $L = 0.0390$ with L ranging from 3.8575 to 3.8865, as illustrated in Fig. 3(d). It is found that the band gap widths of the above-mentioned structures decrease in the sequence of 60° linear defect, free defect, 120° linear defect, and 180° linear defect. The band gap width of 60° linear defect is about 2.14 times larger than that of the free defect. The band gap width of 120° linear defect is about 0.97 times as large as that of free defect. The band gap width of 180° linear defect is about 0.23 times as large as that of free defect. However, the band gap width of the linear defects does not increase with the angle of linear defect.

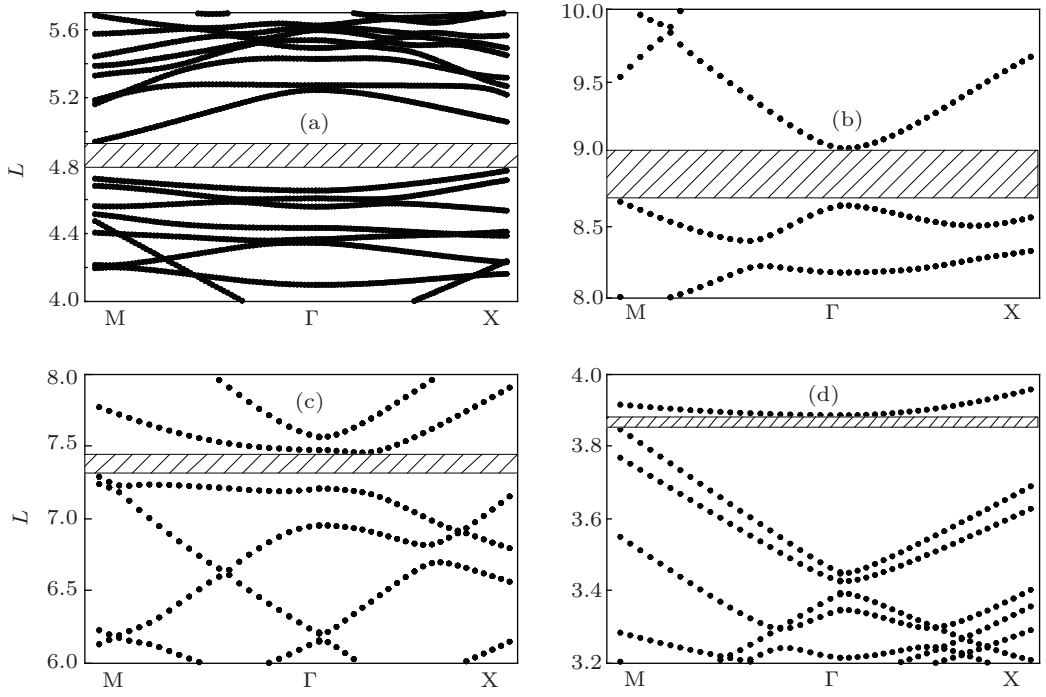


Fig. 3. Acoustic band structure of (a) free defect, (b) 60° linear defect, (c) 120° linear defect, and (d) 180° linear defect for F=0.4.

Variation of the band gap number with the filling fraction is shown in Fig. 4 and that for the relative width of the minimum band gap is shown in Fig. 5. The cases of the free defect, 60° linear defect, 120° linear defect, and 180° linear defect are considered. It is noticed that the band gap exists for filling fractions varying from 0.1 to 0.85 for the free defect in Figs. 4(a) and 5(a). As the filling fraction increases, the band gap number increases and reach a maximum value of 22 when the filling fraction is 0.2, and then decreases. The maximum relative width of the minimum band gap is 0.1144 as the filling fraction equals 0.25. For 60° linear defect, there exists the band gap for the filling fractions in the range from 0.1 to 0.85. As the filling fraction increases, the band gap number changes smoothly. When the filling fraction is 0.15, the maximum number of band gap is 12. When the filling fraction is 0.8, the maximum relative width of the minimum band gap is 0.1959, as shown in Figs. 4(b) and 5(b). For the 120° linear defect, there is the band gap for filling fractions varying from 0.1 to 0.85 except 0.55. With the increase in the filling fraction, the band gap number decreases to zero, and then increases. When the filling fraction is equal to 0.85, the maximum number of band gap is 6. However the filling fraction is 0.8, the maximum relative width of the minimum band gap is 0.2809, as displayed in Figs. 4(c) and 5(c). For 180° linear defect, as shown in Figs. 4(d) and 5(d), it is seen that the band gap exists for the filling fraction varying from 0.25 to 0.85. As the filling fraction increases, the band gap number increases to a maximum and then decreases. The maximum number of band gap is 4 when the filling fraction is 0.75. The maximum relative width of the minimum band gap is 0.0706 when the filing fraction is equal to 0.45.

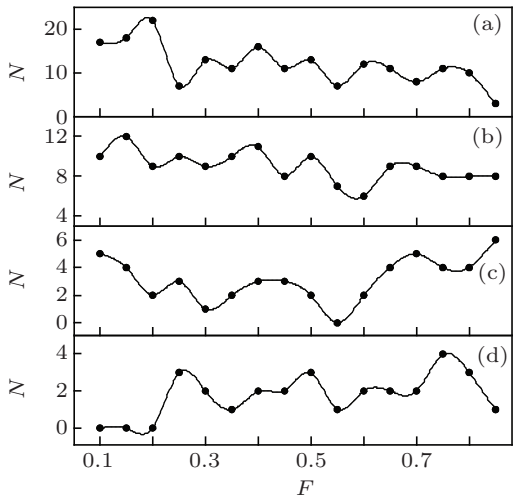


Fig. 4. Band gap number of (a) the free defect, (b) 60° linear defect, (c) 120° linear defect, and (d) 180° linear defect as a function of the filling fraction.

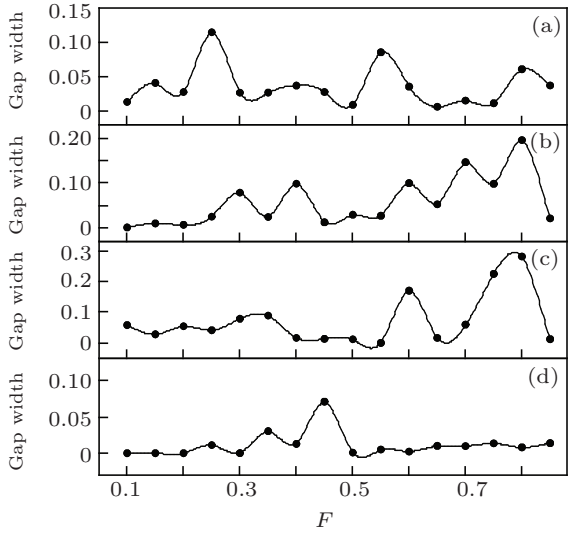


Fig. 5. Relative widths of the minimum band gap of (a) the free defect, (b) 60° linear defect, (c) 120° linear defect, and (d) 180° linear defect as a function of the filling fraction.

5. Conclusions

In summary, the band gaps, the number of the band gap trends, and the maximum relative width of the minimum band of 2D-SCER with different defects were obtained. The main results are as follows: 1) the largest widths of the band gaps are 0.1709, 0.3661, 0.1661, and 0.0390 for free defect, 60° linear defect, 120° linear defect, and 180° linear defect, respectively; 2) the band-gap width of 60° linear defect crystal is about 2.14 times larger than that of the free-defect one, the band-gap width of 120° linear defect is about 0.97 times as large as that of the free-defect one, and the band-gap width of 180° linear defect is about 0.23 times as large as that of the free-defect crystal. In other words, for phononic crystal with different linear defects, the propagation of sound waves will have different locations. Therefore, we can change the defect structure and the filling fraction, and then adjust the width and the number of the conduction band, to control the propagation of sound waves with different frequencies.

References

[1] Martinez-Sala R, Sancho J, Sánchez J V, Gómez V, Llinares J and Meseguer F 1995 *Nature* **378** 241

[2] Sigalas M M 1998 *J. Appl. Phys.* **84** 3026

[3] Chen S B, Wen J H, Yu D L, Wang G and Wen X S 2011 *Chin. Phys.* B **20** 014301

[4] Qi G G, Yang S L, Bai S X and Zhao X 1993 *Acta Phys. Sin.* **52** 668 (in Chinese)

[5] Wu F G and Liu Y Y 2002 *Acta Phys. Sin.* **51** 1434 (in Chinese)

[6] Gao G Q, Ma S L, Jin F and Jin D F 2010 *Acta Phys. Sin.* **59** 393 (in Chinese)

[7] Belzons M, Devillard P, Dunlop F, Guazzelli E, Parody O and Suillard B 1987 *Europhys. Lett.* **4** 909

[8] Weaver R L 1990 *Wave Motion* **12** 129

[9] Weaver R L 1993 *Phys. Rev.* B **47** 1077

[10] Parmley S, Zobrist T, Clough T, Perez-Moller A, Makela M and Yu R 1995 *Appl. Phys. Lett.* **67** 777

[11] Vasseur J O, Deymier P A, Khelif A, Lambin Ph, Djafari-Rouhani B, Akjouj A, Dobrzynski L, Fettouhi N and Zemmouri J 2002 *Phys. Rev.* E **65** 056608

[12] Garcia-Pablo D, Sigalas M, Montero de Espinosa F R, Torrs M, Kafesaki M and García N 2000 *Phys. Rev. Lett.* **84** 4349

[13] Li X C and Liu Z G 2005 *Phys. Lett.* A **338** 413

[14] Xu C, Hu L F and Liu Y K 2010 *Piezoelectrics & Acoustooptics* **32** 859 (in Chinese)

[15] Wu F G, Liu Z Y and Liu Y Y 2002 *J. Phys.* D **35** 162

[16] Zhang X, Liu Z Y, Liu Y Y and Wu F G 2004 *Solid State Commun.* **130** 67

[17] Kushwaha M S and Halevi P 1996 *Appl. Phys. Lett.* **69** 31

[18] Kushwaha M S and Halevi P 1994 *Appl. Phys. Lett.* **64** 1085

[19] Kushwaha M S and Halevi P 1997 *Appl. Phys. Lett.* **70** 3218

[20] Kushwaha M S and Djafari-Rouhani B 1998 *J. Appl. Phys.* **84** 4677

[21] Kafesaki M, Sigalas M M and Garcia N 2001 *Physica* B **296** 190

[22] Li X L, Wu F G, Hu H F, Zhong S and Liu Y Y 2003 *J. Phys.* D **36** L15

[23] Xu H 2009 *Special Topic of Condensed Matter Physics* (Changsha: Central South University) pp. 168–171 (in Chinese)

[24] Yue L L, Chen Y, Fan G H, He J, Zhao D X and Liu Y K 2011 *Acta Phys. Sin.* **60** 106103 (in Chinese)

[25] Wen X S 2009 *Phononic Crystals* (Beijing: National Defense Industry Press) p. 61 (in Chinese)

[26] Xu C, Dong X C, Yue L L and Liu Y K 2010 *Journal of Yunnan Normal University* **30** 49

[27] Wen X S 2009 *Phononic Crystals* (Beijing: National Defense Industry Press) p. 136 (in Chinese)

[28] Wen X S 2005 *Photons/Phnoonic Crystal Theory and Technology* (Beijing: Science Press) p. 46 (in Chinese)