

Wave propagation and acoustic band gaps of two-dimensional liquid crystal/solid phononic crystals

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Abstract The vast majority of acoustic wave propagation in phononic band studies has been usually carried out by scattering inclusions embedded in a viscoelastic medium, such as air or water. In this study, we present calculated band structure results for the two-dimensional square array geometry of a solid cylindrical scatterer surrounded by a liquid crystal (LC) matrix. Liquid crystals provide a unique combination of liquid-like and crystal-like properties as well as anisotropic properties. The purpose of using LC material is to take advantage of longitudinal acoustic waves propagating parallel (\parallel) and perpendicular (\perp) to the nematic liquid crystal (NLC) director n . The compound used in this study was a room temperature NLC, called 5CB (4-pentyl-4'-cyanobiphenyl). The acoustic band structure of a two-dimensional phononic crystal containing a 5CB NLC and lithium tantalate was investigated by the plane wave expansion method. The theoretical results show that the solid/LC system can be tuned in a favorable configuration for adjusting or shifting acoustic band gaps.

1 Introduction

Phononic crystals (PnCs) [1, 2], also known as phononic band gap materials, are artificial structures designed for controlling and manipulating the propagation of

mechanical waves. They have received a great deal of interdisciplinary research attention across condensed matter physics and materials science for both fundamental and applied researches, and are expected to find commercial applications soon. The periodicity of the elastic moduli and mass densities of the constituents in space generates the phononic crystal effects [3]. They show interesting physical characteristics due to their ability to block the propagation of acoustic waves by forming energy band structures, called phononic bands. Phononic band gaps (PnBGs) can be adjusted to allow desired frequency to pass through as well as tune the PBG [4, 5]. This can be done through the careful design of the geometry of the structure as well as adjusting the crystal lattice parameters, and selecting appropriate materials to find partial or complete band gaps. Therefore, phononic crystals are engineered acoustic band gap materials that belong to the group of metamaterials with designed properties that are usually unknown in nature. The periodic spatial modulation of elasticity and mass density with an appropriate choice of the geometrical and physical parameters have found several potential applications, such as acoustic shielding, acoustic mirrors, demultiplexers [6], and also in the field of wave guiding and filtering [7] (including the modes due to the linear and point defects) as well as in the field of sound isolation [8]. In addition, acoustic negative refraction and an imaging effect of acoustic waves were achieved in the phononic crystals [9]. In general, most of the investigations for solid–fluid periodic structures, known as mixed phononic crystals, focused on placing rigid or liquid materials in air background, water, glycerin, chloroform, or mercury by creating relative density difference between the component materials [10, 11]. However, these are all fixed parameters and cannot be changed easily unless one of the materials is physically replaced by placing another

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material. On the other hand, the effect of other material parameter values such as the speed of sound in a fluid medium (gas or liquid) also has an effect on the band structure. The sound waves travel through each of these mediums as longitudinal waves, and their propagation depends on the elasticity or bulk modulus and the mass density. Therefore, it appears that the sound velocity cannot be changed without changing the density or the bulk modulus. That leaves us with not many parameters to make adjustments for the structure under study. Therefore, we suggest a phononic structure that may allow us to change the acoustic velocity nonlinearly to observe the effects on the phononic band gaps.

Liquid crystals (LCs) are remarkable materials with strange properties [12, 13]. They are more like liquids than they are like solids, but their molecules are aligned like those in crystals. That leaves them with symmetries that are intermediate between those of isotropic liquids and crystalline solids. 4-n-pentyl-4-cyanobiphenyl (5CB) is one of the most interesting and well-known liquid crystals and also the most widely studied one. 5CB is a thermotropic nematic compound which manifests polymorphism upon variation of temperature. The compound has a nematic phase, known as the most simple liquid crystal phase, temperature between 297 and 308.3 K [14]. It is evident that the liquid–crystal phase exists within a limited temperature range. In fact, temperature always plays an important role in affecting liquid crystalline properties; birefringence [15], viscosity [16], elastic constant [17, 18], and dielectric anisotropy [19] all decrease with increasing temperature. Beyond the nematic phase transition range, some other mesophases may exist. There are many different types of LC mesophases discovered in the last decades such as nematic, smectic A (SmA), smectic C (SmC), columnar, and blue phases, respectively [20]. Based upon material selection, like LC polymers, different phases can exist in one material at different temperatures.

Phases with a wider temperature range are usually desired for scientific applications. It is well known that the pure substances of type nCB cannot be directly used in real-time applications since the temperature range of the nematic phase is either too narrow or too high. Hence, extending the temperature range of the nematic phase without reducing the nematic–isotropic transition temperature is required. In order to significantly increase the useful nematic temperature range, eutectic mixtures of some single-substance LCs (e.g., E7, E8, and E9 by Merck) are used. Eutectic mixtures have wider nematic range, and hence, they provide relatively wider operating temperature range. The simplest method consists of mixing the different products in proportions corresponding to the eutectic point. The proportions of eutectic mixtures are easy to determine. For instance, a eutectic mixture of roughly 35% 5CB with

65% 8OCB has a nematic range from 5 to 50 °C [21]. The nematic range can therefore be further extended to a wide range of temperature through the use of making not only binary mixtures, but also ternary, quaternary, etc., mixtures by taking some proper components. For example, in a mixture of 36% 7CB, 18% 3CB, 15% 5OCB, 12% 7OCB, and 19% 8OCB, the nematic phase exists between 0 °C and 61 °C [22]. Fortunately, it is also interesting to mention that nematic temperature ranges from −30 to +100 °C from some LCs are commercially available for state-of-the-art results [23]. It must be noted that here we specifically focus on 5CB LC despite the fact that it has a limited temperature range since speed of sound and acoustical properties of the many alkylcyanobiphenyls (e.g., 6-CB) or alkyloxycyanobiphenyls (e.g., 8OCB), or eutectic mixtures (e.g., E7) have not been fully studied in the nematic range. The LC material 5CB has the advantage of being an excellent candidate for making eutectic mixtures to widen the nematic range. In a nematic phase, 5CB molecules have directional order rather than positional order by self-aligning themselves with their long axes almost parallel. This direction is referred to as the director of the liquid crystal, and its orientation is responsible for determining the unique optical properties of the material. The anisotropic nature and uniaxial symmetry of liquid crystals must give rise to acoustic anisotropy related to sound velocity, elastic properties, and the attenuation coefficient. The acoustics of liquid crystals are based on scientific progress in various fields, such as crystal physics, optics, and acoustical physics [24–26]. Hence, their acoustic properties, like acoustic attenuation, acoustic impedance, and absorption coefficients, have not yet been completely reported. Therefore, it is also an open field to explore the acoustic properties of LCs and they can be promising materials for constructing tunable phononic crystals.

2 Model and the calculation method

Liquid crystals (LCs) are highly structured organic fluids that consist of rod-shaped molecules. The most commonly studied thermotropic liquid crystal 4-pentyl-4'-cyanobiphenyl (5CB) was used in this study since it is a relatively stable room temperature nematic liquid crystal (NLC). At temperatures above the nematic–isotropic phase transition temperature T_{NI} , the long axes of the liquid crystal molecules are randomly oriented, resulting in isotropic properties. At lower temperatures, below the nematic–isotropic transition temperature T_{NI} , the elongated molecules, on average, align themselves approximately parallel to one another along an arbitrarily chosen preferred direction in space (x, y, z). This long-range orientational order is called the nematic phase. The nematic phase exhibits a unique

property that comes from the geometry and dynamics of that particular direction. The mean value of the direction of the molecular long axes is described by a vector as a function of space. This is known as the director vector $n(r)$. The magnitude of the director has no significance since it is taken as a unit vector.

Here, we focus on the acoustic wave propagation through a periodic array of cylindrical scatterers. We model the matrix as a fluid medium in order to make use of solid/fluid approximation. Such approximation is reasonable if we only consider that the waves propagate as longitudinal waves by means of adiabatic compression and decompression. Fortunately, the longitudinal waves propagating along the director n of 5CB will provide that opportunity. In order to do that, we will consider two possible orientations of the director vector. For simplicity, an axial alignment will be assumed, in which the liquid crystal director is firstly parallel to the long axis of the cylindrical scatterers, and secondly perpendicular to that of the cylinders. The direction of the directors with respect to cylinder is shown in Fig. 1. According to Fig. 1a, the sound velocity $c_{||}$ is in direction parallel to the direction vector n while c_{\perp} is in direction perpendicular to the director n .

For an arbitrary orientation, the wave velocity can be expressed as

$$V(\phi) = \frac{1}{\sqrt{2\rho}} \left[\frac{(C_{11}\sin^2\phi + C_{33}\cos^2\phi)}{+ \sqrt{(C_{33}\cos^2\phi - C_{11}\sin^2\phi)^2 + C_{13}^2\sin^22\phi}} \right]^{1/2}, \tag{1}$$

where ρ is the LC density, ϕ shows the angular direction of the director [26, 27]. It is noteworthy that the shear mode of the nematic phase is in general considered to be negligible. Therefore, the elastic components related to this mode are neglected and assumed to be zero, $C_{44} = C_{55} = C_{66} = 0$ [26].

Lithium tantalate (LiTaO₃ or LTA) is our material of choice, since it possesses unique properties, which as a material finds uses in electro-optical and acousto-optical applications. Some of the technological applications of this well-suited material include: bulk acoustic wave devices, acoustic transducers, piezoelectric transducers and piezoelectric sensors [28]. Its good mechanical stability and

chemical stability make LTA already widely used as a substrate in surface acoustic wave (SAW) devices [29]. LiTaO₃ has twelve independent acoustic physical constants. They are six elastic constants, four piezoelectric stress constants, and two dielectric constants. For the sake of simplicity, we will only consider the elastic constant component related to longitudinal velocity. All the piezoelectric, electro-optical effects and medium viscosity will be neglected since piezoelectric phase mostly influences the z -mode [30].

Assuming a homogeneous and isotropic medium, we can separate the wave modes and use methods based on acoustic wave theory. To calculate the band gaps for phononic crystals, a plane wave expansion (PWE) method in frequency domain [31] is used due to its simplicity. The considered system is a 2D phononic crystal composed of LiTaO₃ inclusions in a 5CB LC host in a square lattice. A square lattice formed of cylindrical rods has a lattice constant of $a = 0.1$ m and the scatterers' radius, $r_0 = 0.05$ m. The calculation model of the studied system and its unit cell is shown in Fig. 2.

The material properties are $\rho_1 = 1022$ kg/m³ at 297 K [32] and $c_{\perp} = c_{L1} = 1784$ m/s and $c_{||} = c_{L1}' = 1620$ m/s for the 5CB LC, and $\rho_2 = 7450$ kg/m³ and $c_{L2} = 5592$ m/s for LiTaO₃. The equation that describes the wave motion is given by the acoustic wave equation as

$$(C_{11})^{-1} \frac{\partial^2 p}{\partial t^2} = \vec{\nabla} \cdot (\rho^{-1} \nabla p), \tag{2}$$

where p is the pressure wave, $C_{11} = \rho c_L^2$ is the longitudinal velocity and ρ is the mass density, and $\nabla = (\partial/\partial x, \partial/\partial y)$ is the two-dimensional nabla. This equation is a scalar wave equation. The periodicity of the phononic system may be utilized to expand $C_{11}^{-1}(r)$ and $\rho^{-1}(r)$ in two-dimensional Fourier series. Hence, the Fourier coefficients for C_{11} and ρ can be expressed as

$$F(\vec{G}) = \begin{cases} F_a^{-1}f + F_b^{-1}(1-f) = \overline{F^{-1}} & \text{for } \vec{G} = 0 \\ (F_a^{-1} - F_b^{-1})S(\vec{G}) = \Delta(F^{-1})S(\vec{G}) & \text{for } \vec{G} \neq 0 \end{cases}, \tag{3}$$

where F is the physical parameter used for C_{11} and for ρ , the subindex "a" and "b" stands for the inclusions and the

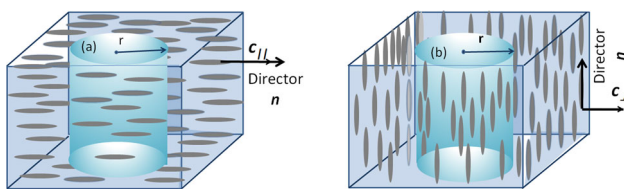


Fig. 1 A 3D representation of a unit cell of a square lattice composed of a solid cylinder and liquid crystal molecules. Director direction n is along the long axis of the cylinder (a), and director n is along the long axis of the cylinder (b)

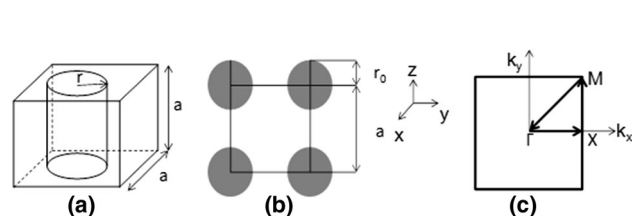


Fig. 2 Unit cell of a square lattice two-dimensional phononic crystal (a). Transverse cross section of a representative 2D phononic crystal (b) and Brillouin zone of 2D square lattice PCs (c)

host material, respectively. $S(\mathbf{G})$ term in the equation is the structure factor defined in two-dimensional system as

$$S(\vec{G}) = 2fJ_1(Gr_0)/(Gr_0), \quad (4)$$

where f is the filling fraction of the cylindrical rods with lattice constant a , $J_1(x)$ is the Bessel function of the first kind of order one, \mathbf{G} is the two-dimensional reciprocal lattice vector, and r_0 is the cylinder's radius. The acoustic wave equation then can be solved as an eigenvalue equation by applying the Bloch theorem. A software implementation and numerical calculation was carried out by the code written by Elford [33] with minor modifications.

3 Discussion

The computational model based on the PWE method and the physical parameters of the system have been given in the above section. Numerical results for the band structure are given in Fig. 3. Figure 3a, b shows the acoustic band structure for the homogeneous and the homeotropic orientations of the LC directors, respectively. To obtain Fig. 3a, homogeneously aligned 5CB liquid crystals are assumed to be perfectly parallel to the surface of the circular cross section of the cylindrical rod. The wave vector is in the plane of the planar section, and the longitudinal acoustic mode velocity c_{\parallel} is used. It is clear that complete acoustic band gaps are formed due to the overlapping of frequency bands in different directions of periodicity. On the other hand, in a similar manner to the previous system, homeotropically aligned LC molecules are assumed to be perpendicular to the circular cross section of the cylinder. The longitudinal wave velocity in this case is c_{\perp} , and the band structure corresponding to this mode is shown in Fig. 3b. It is evident that a similar band structure is obtained and, therefore, the widths of the full gaps in both figures are insignificant. This is not an

unexpected observation since the difference between the LA wave velocities $\Delta c = (c_{\parallel} - c_{\perp})$ is rather small. However, the frequency values of the gaps are shifted to the higher values of frequency when Fig. 3a, b are compared. The shifting levels are shown by black arrows in Fig. 3. From Fig. 3a, b, it can be deduced that a possible tunable phononic crystal structure can be obtained. This can be done by changing the acoustic wave velocity continuously with respect to the director vector. We may consider that as a quasilongitudinal mode, and one needs to know the sound velocity for each director orientation.

Figure 4 shows the corresponding phononic density of states (DOS) of the 2D phononic crystal as a function of frequency for perpendicular and parallel alignment of the NLC molecules. DOS for homogeneous orientation is given by the solid line, and DOS calculated for the wave vector aligned perpendicular to the directors is shown by the dashed line. Calculation of DOS was carried out by sampling k -points in the two-dimensional BZ. A sum of all bands over all frequencies yields the density of states as a function of frequency. DOS calculations are particularly important since some physical properties, such as thermal conductivity and specific heat, can be modified by changing the phonon density of states in a phononic crystal. Briefly, they provide insight into both microscopic and macroscopic properties. In Fig. 4, it is clear that there is a shift in the DOS states as a function of frequency, and the shift is more apparent at higher frequencies compared to lower frequencies.

It is easier to understand the refraction and reflection phenomena of certain waves in k -space since the law of conservation of momentum is met at reflection and refraction of waves. This can be best done by introducing the equifrequency surface (EFS) of the acoustic wave. This surface is obtained directly from the calculated eigenmodes inside the unit cell to form the dispersion surfaces of

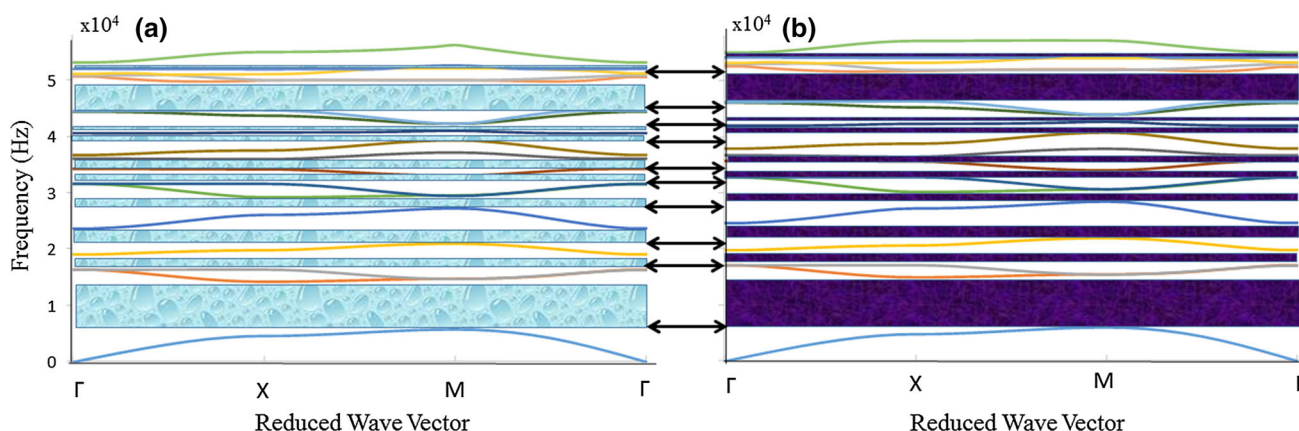


Fig. 3 Band structure of LiTaO_3 scatterers in 5CB LC with $f = 0.78$, and $r/a = 0.5$. The band structure on the *left* belongs to the rods in homogeneously oriented LC material (a), and the band structure on the *right* belongs to the same rod in homeotropically oriented 5CB LC host (b)

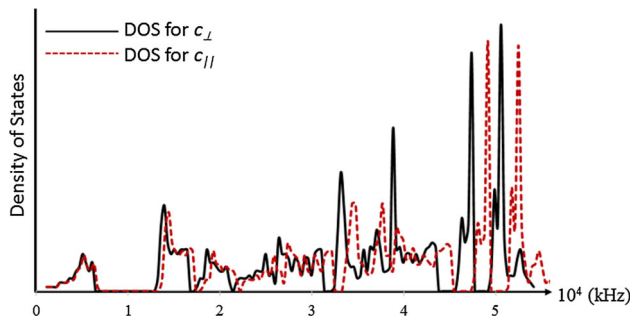


Fig. 4 Density of states (DOS) calculated for perpendicular and parallel alignment of the NLC molecules for the 2D phononic crystal system. DOS for homogenous orientation is represented by the *solid line*, and DOS calculated for the wave vector aligned perpendicular to the directors is shown by the *dashed line*

acoustic waves. Figure 5a, b shows the dispersion surfaces of the 2D PnC system for the first modes including homogeneous and homeotropic orientations of the host 5CB LC molecules. At first glance, there is almost no noticeable difference in both figures. The difference in dispersion curves in Fig. 6a, b is more virtually noticeable compared to Fig. 5a, b. However, all of these dispersion surfaces hold vital information because each point on the

surface gives the possible eigen solutions that consist of all the allowed wave vectors in the first Brillouin zone. It can be deduced that dispersion curves may be useful for quantitative information. Therefore, isotropic or anisotropic wave propagation of waves in PnC can be best analyzed by the equal frequency contour (EFC). Figures 5c, d and 6c, d show the EFCs of the waves at some different frequencies in the Phononic crystal. The contours in Fig. 5c, d are similar in shape and circular at first for points close to the center. However, the contours become non-circular at higher frequency values when the director vector is perpendicular to the cylinder axis. The deviation from circular shape is faster than homeotropic orientation. This deviation simply implies an anisotropic phase velocity of the longitudinal acoustic wave. Figure 5c, d shows that the contours are also non-circular, which means phase velocity depends on wave propagation direction. Moreover, all of these can be understood much better by a known approach known as the conventional approach.

The conventional approach is that a straight line from the central point (Γ point) to another point on a contour gives the direction of the phase velocity, while the direction of velocity of energy is presented by the normal

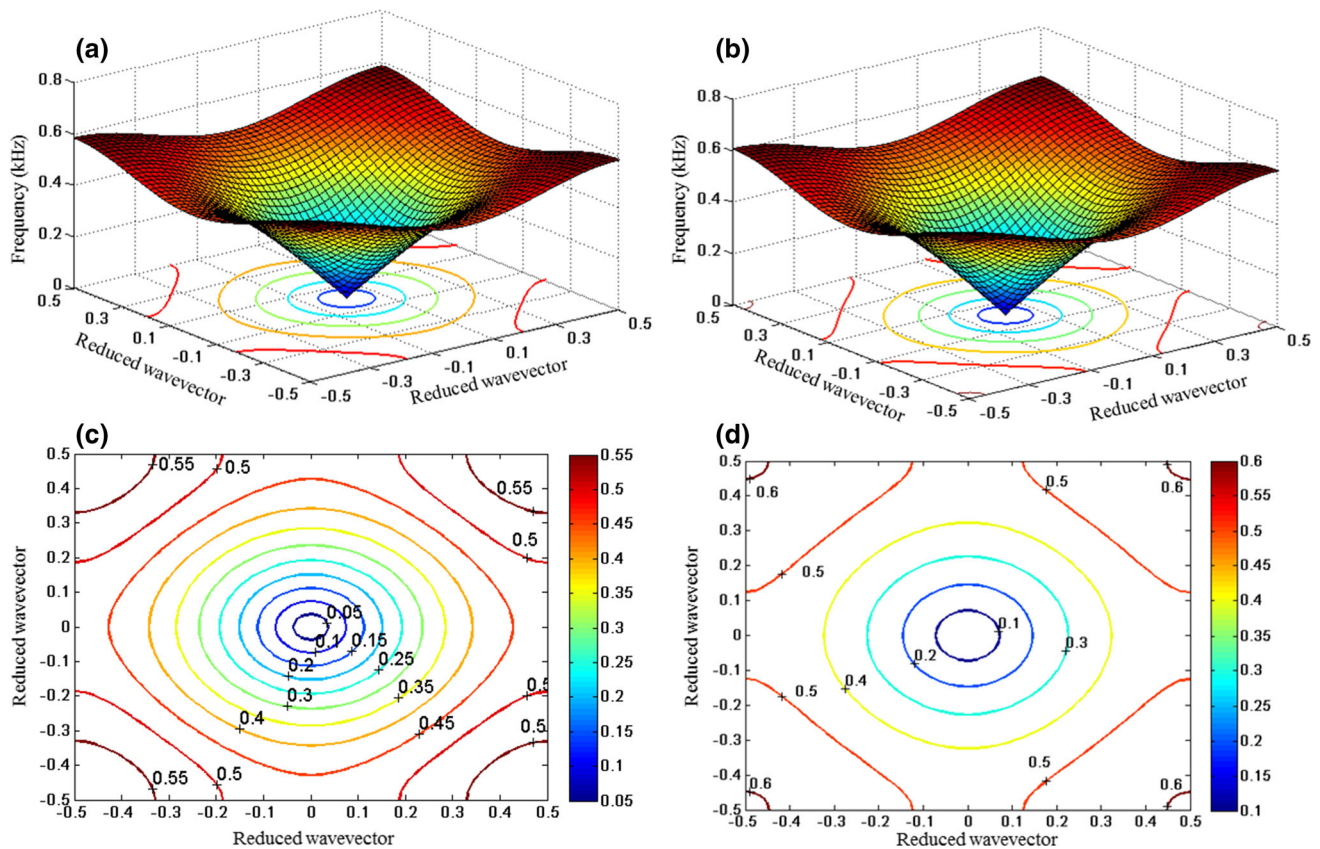


Fig. 5 **a** Dispersion, $\omega(k)$, relation for the first mode of the square PC, calculated for all k -vectors in the first Brillouin zone and **b** the equifrequency contours for the first mode

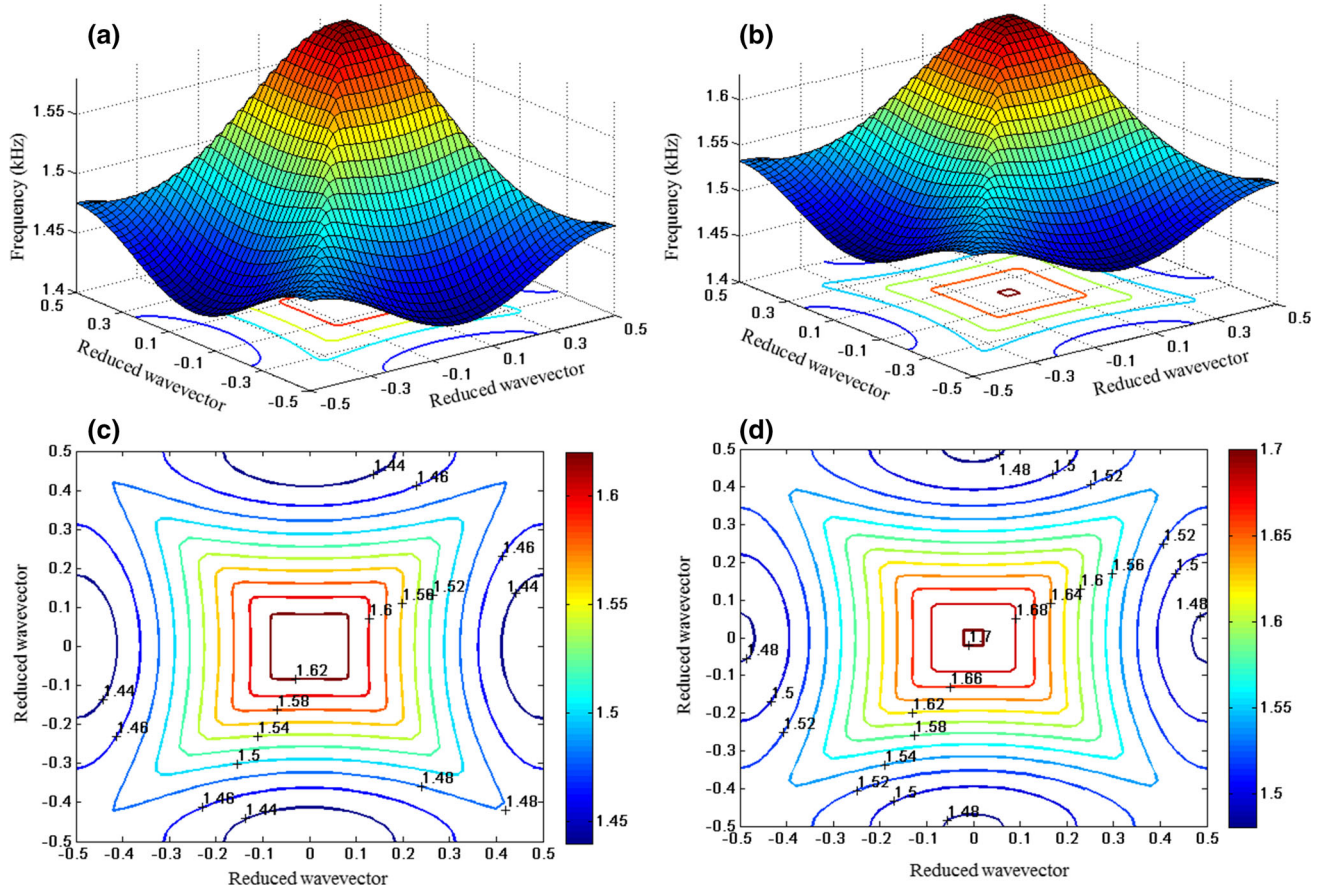


Fig. 6 **a** Dispersion, $\omega(k)$, relation for the second mode of the square PC, calculated for all k -vectors in the first Brillouin zone and **b** the equifrequency contours for the second mode

direction on the contour. Therefore, deviation from circular contour accounts for the different directions of phase and energy velocities.

4 Conclusions

In conclusion, we have studied the propagation of longitudinal waves perpendicular to the infinite periodically aligned inclusions. The conventional PWE method applied to a two-component system consisting of solid cylinders in a liquid matrix with slightly different acoustic parameters was studied and compared. Summarizing, we demonstrated the existence of acoustic band gaps of a two-dimensional phononic crystal containing a 5CB NLC and lithium tantalate (LiTaO_3). Also, we showed the existence of possible tunability of the acoustic band gaps based on the orientation of the LC molecules. Longitudinal acoustic waves propagating parallel (\parallel) and perpendicular (\perp) to the nematic liquid crystal (NLC) director n gives two different band gap structures. These gaps are structural ones, but they have relative differences in the band gap widths.

Furthermore, band gap features coexist in the same structure. These two examples show that introducing LC material into phononic crystal systems may be an effective approach for creating and tuning band structures.

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