Two Dimensional Triangular Lattice PhoXonic Crystal with Graphite Plate

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Abstract- We have shown the simultaneous existence of photonic and phononic band gaps in a two-dimensional triangular lattice crystal. Our calculations are focused on a structure formed of air inclusions on a Graphite plate. We introduce a cavity in the structure, which will lead to a simultaneous confinement of both optical and acoustic excitations. Photonic and phononic cavity modes are obtained, which implies the existence of permissible bands in the band gap due to the defect included in the structure.

Key Words: Cavity modes, optical and acoustic excitations, PhoXonic crystal.

1. INTRODUCTION

Photonic and phononic crystals are periodic structures with the same interests and consequences as semiconductors, namely the existence of forbidden bands in a certain range of wavelengths for the propagation of electromagnetic waves for photonic crystals and ultrasound for phononic crystals. The possibility of obtaining a crystal with a dual phononic and photonic band structure is studied theoretically for the first time by Maldovan and Thomas [1, 2, 3, and 4]. They are shown the simultaneous existence of photonic and phononic band gap in 2D crystals for a square or hexagonal network of air holes in a silicon matrix. This existence gives birth to new artificial crystals called phoXonic crystals, the X symbolizing introduced as a defect in the crystal. The localization of both excitations in the same cavity which leads to a strong phonon-photon coupling in a 2D Si phoXonic crystal is demonstrated recently [6, 7]. The acousto-optic interaction is a theme that has been introduced into the scientific community since the 1960's thanks to the theory of Leon Brillouin [8], who studied the coupling of a light wave, with a hypersonic wave. In this article, we study the simultaneous existence of phononic and photonic band gaps, in 2D triangular lattice constituted by a periodic network of deposited air inclusions on a Graphite plate. The choice of Graphite as a matrix component comes from the fact that it has a structure very close to diamond, or its resistance to high temperatures and high loads. Thanks to these properties, very low friction coefficients can be obtained even under very high loads.

The paper is organized as follows. In section 2, we first describe the geometry of the crystal. Then we present the calculation method. Section 4 presents the existence of simultaneous photonic and phononic band gaps. The existence of highly confined optical and acoustic waves inside a phoXonic cavity, created by removing one hole in the perfect structure is shown in section 5. The conclusions are summarized in section 6.

2. GEOMETRY USED

2.1 FILLING FACTOR

The fill factor denoted \( f \) corresponds to the ratio of the area of circular inclusions of radius \( r \) on the area of the unit cell of network parameter \( a \) such that;

\[
f = \frac{2\pi r^2}{\sqrt{3} a^2} \quad (1)
\]

In our calculations, the radius \( r \) of the cylinders is taken equal to \( 0.46a \), with “a” network parameter, this value seems to be a good candidate after several computations. This radius corresponds to a fill factor “f” of 0.77. It shows simultaneous complete and sufficiently large band gaps for the optical polarizations TE and TM, as well as the acoustic modes.

2.2 TRIANGULAR NETWORK

The crystal formed of a base or elementary pattern is modeled by a network of nodes distributed periodically in space.

Using the three basic vectors \( \vec{u}_1, \vec{u}_2 \) and \( \vec{u}_3 \), a 3D direct network can be described as follows;

\[
\vec{R} = a_1 \vec{u}_1 + a_2 \vec{u}_2 + a_3 \vec{u}_3 \quad (2)
\]

With, \( a_1, a_2, a_3 \in \mathbb{Z} \).

The definition of basic vectors \( \vec{v}_1, \vec{v}_2 \) and \( \vec{v}_3 \) of the reciprocal network is given by the relations (3), (4) and (5);

\[
\vec{v}_1 = 2\pi \frac{\vec{u}_1 \times \vec{u}_2}{\vec{u}_1 \cdot (\vec{u}_2 \times \vec{u}_3)} \quad (3)
\]

\[
\vec{v}_2 = 2\pi \frac{\vec{u}_1 \times \vec{u}_3}{\vec{u}_1 \cdot (\vec{u}_2 \times \vec{u}_3)} \quad (4)
\]

\[
\vec{v}_3 = 2\pi \frac{\vec{u}_2 \times \vec{u}_3}{\vec{u}_1 \cdot (\vec{u}_2 \times \vec{u}_3)} \quad (5)
\]

Table 1 presents the basic vectors of the direct and reciprocal networks for the structure of the 2D triangular
crystal. The geometric presentation of the triangular structure is illustrated in Figure 1.

The periodic structure consists of a triangular lattice of air holes in a Graphite matrix (C). Table 2 summarizes the acoustic and optical constants of the material.

Table 1: The triangular network with its basic vectors of direct and reciprocal networks.

<table>
<thead>
<tr>
<th>Crystal structure</th>
<th>Network pattern</th>
<th>Direct network vectors</th>
<th>Reciprocal network vectors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triangular</td>
<td>Triangular</td>
<td>$u_1 = (a, 0)$</td>
<td>$v_1 = \frac{2\pi}{a} \left(1, -\frac{1}{\sqrt{3}}\right)$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$u_2 = \left(0, \frac{a}{2}, \frac{\sqrt{3}}{2}\right)$</td>
<td>$v_2 = \frac{2\pi}{a} \left(0, \frac{2}{\sqrt{3}}\right)$</td>
</tr>
</tbody>
</table>

Table 2: Elastic and optical constants of Graphite (C) used in numerical simulations. The refractive index $n$, the density $\rho$, the transverse velocity $c_t$ of sound along the direction of propagation [9, 10].

<table>
<thead>
<tr>
<th>Material</th>
<th>$\rho$ ($Kg / m^3$)</th>
<th>$c_t$ ($m / s$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Graphite</td>
<td>2.6988</td>
<td>2800</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3040</td>
</tr>
</tbody>
</table>

**3. CALCULATION METHOD**

The method used in our calculations is the finite element method; these elements present the result of the discretization of the domain of computation. The solutions sought for each finite element are developed on a set of basic functions. From a numerical point of view, the choice of basic functions is dictated by the necessary compromise between the degree of approximation of the solution and the number of degrees of freedom, related to the total cost of calculation [11].

The finite element method uses a mesh directly adapted to the studied geometry, which makes it possible to optimize the mesh while avoiding the use of a mesh excessively fine. Also, the finite elements allow meshing only areas with high gradient, particularly suitable for the calculation of unit cells of a crystal with very large and very small rays.

**4. PHOXONIC CRYSTAL**

4.1 IRREDUCIBLE ZONE OF BRILLOUIN

The first Brillouin zone of the triangular lattice is shown in Figure 1 on the left. According to Brillouin's definition, the area is determined by the smallest space within the mediating planes of the line segments joining a node of the reciprocal network to its neighbours. The normalization of a Brillouin irreducible zone corresponding to the triangular network can be written in the form given by equation (6), while adopting the designation given in Fig.1.

$$\Gamma M = \frac{1}{\sqrt{3}}; \Gamma K = \frac{2}{3}, KM = \frac{1}{3}$$  (6)

**4.2 REPRESENTATION OF THE BAND DIAGRAM**

Fig. 2 represents the acoustic and optical dispersion diagrams obtained for the triangular array in Graphite substrate. The calculation was made following the first zone of Brillouin of the triangular network $\Gamma - K - M - \Gamma$. It reveals a complete photonic band for transverse electric (TE) and transverse magnetic (TM) polarization, and two wide acoustic bands, which implies more chances to have the maximum possible of the modes of defects, and consequently, a confinement and interaction even more important.

Fig. 2: Optical band diagram TM (a), TE (b), and acoustic (c) of a network triangular in Graphite.

**5. DEFECT MODES IN PHOXONIC BAND DIAGRAMS**

5.1 SUPER CELL METHOD

The super cell in the case of a perfect crystal is formed of a set of adjacent unit cells. Indeed, repeating the super cell, by successive translations of basic vectors of the superstructure, reproduces the same crystal [12].

The band diagrams calculated by the super cell model are similar to those obtained by the unit cell, just that only the direction $\Gamma - K$ will be taken into consideration. Indeed, the cavity modes have a quasi-zero group velocity; therefore their resonant frequencies are identical regardless of the direction of propagation of the wave vector in the first Brillouin zone. The defect modes obtained are calculated in a super cell consisting of $9 \times 9$ air inclusions (holes) in Graphite. These have dimensions large enough to avoid coupling between adjacent cavities while taking into account a reasonable calculation time.

5.2 CAVITY MODES

The study of the confinement of electromagnetic and elastic waves in a phoxonic crystal requires the search for
modes of defects. These modes will be calculated by the method of the super cell, for a punctual defect corresponding to the omission of a hole of the structure cavity “L1”. These calculations are performed for the triangular Graphite network. Figure 3 shows 4 TE photonic modes, 5 TM photonic modes, and 6 phononic modes located in their band gaps.

![Figure 3: Distribution of optical and acoustic displacements of cavity modes. The total displacements are represented in color scale at the end of each presentation.](image)

6. CONCLUSION

In this paper, we have investigated the opening of phoxonic band gaps (simultaneous photonic and phononic) in a 2D infinite Graphite phoXonic crystal drilled with holes. We have shown that, the creation of a cavity inside the perfect crystal, leads to several localized photonic and phononic modes, which propose several possibilities to confine simultaneously phonons and photons and to enhance their interaction.

REFERENCES


