Simultaneous existence of phononic and photonic band gaps in periodic crystal slabs

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Abstract: We discuss the simultaneous existence of phononic and photonic band gaps in a periodic array of holes drilled in a Si membrane. We investigate in detail both the centered square lattice and the boron nitride (BN) lattice with two atoms per unit cell which include the simple square, triangular and honeycomb lattices as particular cases. We show that complete phononic and photonic band gaps can be obtained from the honeycomb lattice as well as BN lattices close to honeycomb. Otherwise, all investigated structures present the possibility of a complete phononic gap together with a photonic band gap of a given symmetry, odd or even, depending on the geometrical parameters.

OCIS codes: (130.0130) Integrated optic; (130.3120) Integrated optics devices; (230.0230) Optical devices; (230.1040) Acousto-optical devices; (230.5298) Photonic crystals.

References and links

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1. Introduction

Phononic crystals [1,2], constituted by a periodical repetition of inclusions in a matrix background, has received a great deal of attention during the last two decades [3]. Associated with the possibility of absolute band gaps in their band structure, these materials have found several potential applications, in particular in the field of wave guiding and filtering [4] (in relation to the properties of linear and point defects) as well as in the field of sound isolation [5]. Another issue of interest is based on the refractive properties of these materials for exploring phenomena such as negative refraction, focusing, self-collimation and beam splitting [6] as well as for the realization of metamaterials for controlling the propagation of sound [7]. Recently, the study of phononic crystal slabs has become a topic of major interest. Indeed some of us and other authors have demonstrated [8–14] that with an appropriate choice of the geometrical and physical parameters, these finite thickness structures can also exhibit absolute band gaps. This makes them suitable for similar applications as in the case of 2D phononic crystals with the additional property of confinement in the vertical direction.

In the photonic crystal counterpart, the medium is made up of periodic dielectric materials and can prohibit the propagation of electromagnetic waves in specific wavelength ranges [15]. Such infinite 2D periodic structures have opened up new features for controlling light, leading to the proposition of many novel devices [16]. Photonic crystal slabs retain, at least approximately, many of the desirable properties of 2D infinite photonic crystals but in the same time are much more easily realized at submicron length scales. Depending on the physical and geometrical parameters, the restriction to finite height of the structure recreates the band gap in the guided modes of the slab below the light cone [17–19].

Many papers have investigated the simultaneous existence of photonic and phononic band gaps and the confined phonon-photon interaction in 1D structures constituted by multilayer materials [20,21]. In 2D structures, many papers have investigated separately the existence of photonic and phononic band gaps, but relatively few works have been devoted to simultaneous control of phonons and photons [22–25] and most of these papers are dealing with the case of infinite 2D structures [22–24]. Maldovan and Thomas [22,23] have shown theoretically that phononic and photonic band gaps can be obtained in 2D square or hexagonal lattice crystals made up of air holes in a silicon matrix. Sadat-Saleh et al. [24] have

demonstrated the possibility to open phononic and photonic band gaps in complex arrays like multiple cylinders per unit cell in lithium niobate 2D structures. Experimental evidence of such a band gap phenomenon has been reported recently in 3D phononic and photonic crystal of amorphous silica spheres [26].

The aim of this paper is to investigate in detail the conditions of existence of simultaneous phononic and photonic band gaps in finite 2D crystals of various structures constituted by a periodic array of holes in a silicon slab. It should be noticed that the existence conditions of the band gaps are quite different in slabs of phononic/photonic crystals as compared to their 2D infinite counterpart. For instance, the existence of absolute phononic band gaps in a slab requires some conditions on the geometrical parameters, especially as concerns the thickness of the slab compared to the lattice period [8–14], and moreover the width of the band gaps are reduced as compared to the case of 2D infinite phononic crystals. On the other hand, in photonic crystal slabs, the band gaps should be searched below the light cone to insure the propagation of the waves along the slab and avoid the radiation of light into vacuum, while there is no reference to the light cone in infinite 2D photonic crystals. Therefore, we give here a first comprehensive study of the simultaneous existence of absolute phononic/photonic band gaps in crystal plates.

Most of the calculations are performed with the Plane Wave Expansion (PWE) method and the convergence of the results is also checked in some cases with the use of the layered multiple scattering (LMS) method as well as the finite difference time domain (FDTD) method. Section 2 describes the geometries considered in this paper as well as the method of calculation. Section 3 presents the results for the most commonly used case of square lattice containing one or two cylinders per unit cell. Section 4 is devoted to the study of the honeycomb lattice and this array is generalized in section 5 to the case of boron nitride (BN) lattices containing two atoms per unit cell. The conclusions are summarized in section 6.

2. Geometry and method of calculation

Figure 1 represents the general cases of the centered square lattice with two atoms per unit cell and of the boron nitride lattice. By considering the lattice period a as the unit length, there are several geometrical parameters involved in the problem, namely the thickness h_{Si} of the Si slab, the filling fraction f and the ratio $\alpha = r_1/r_2$ of the radii of the two types of holes in the unit cell. The filling fraction of the air holes in the membrane is given by:

$$f = f_1 + f_2 = \frac{\pi(r_1^2 + r_2^2)}{a^2}$$

for the square arrangement and by:

$$f = f_1 + f_2 = \frac{\pi(r_1^2 + r_2^2)}{a^2 \frac{\sqrt{3}}{2}}$$

for the BN structure. The more common single square lattice is obtained in the structure of Fig. 1(b) for $\alpha = 0$. The boron nitride lattice, depicted in Fig. 1(c), includes the triangular ($\alpha = 0$) and the honeycomb ($\alpha = 1$) arrays as particular cases.

In all the band structures presented in the paper, the frequencies are given in the dimensionless unit $\Omega = \omega a/2\pi c$ where c is the transverse velocity of sound in silicon for elastic waves and the velocity of light in vacuum for electromagnetic waves.

According to the symmetry of the structure with respect to the middle plane of the slab, the modes can be classified into symmetric (even) and antisymmetric (odd) modes. In a previous work [12], we have demonstrated the existence of absolute phononic band gaps in square and honeycomb lattices of holes in a Si membrane provided the thickness of the slab is about half of the lattice period and the filling fraction is sufficiently high. In this work, we first concentrate on the existence of a complete phononic band gaps which are calculated for a

large variety of the geometrical parameters in the useful ranges (h_{Si}/a from 0.4 to 0.7, f from 0.3 to 0.7 and α from 0 to 1). Then, we search for the photonic band gaps (either complete or for one type of symmetry) in the same ranges of parameters. In general, the complete photonic band gaps occur only in a few cases which are difficult to obtain for all symmetries. Therefore, the full acoustic and optical band gap can be obtained in many situations with a complete phononic gap together with a photonic gap of a given (odd or even) symmetry. It is worth mentioning that in a real photonic crystal device the excitation of even or odd modes separately can be easily achieved by a proper selection of the polarization of the injected light. This means that, in principle, a photonic band gap occurring for a unique symmetry (odd or even) should be enough for most functionalities such as cavities, waveguides or splitters. Let us also mention that in the slab geometry, the photonic gaps have to be searched only below the light cone in vacuum. However, these gaps should preferably occur at dimensionless frequencies Ω below 0.5, otherwise they will be restricted only to a very small area of the Brillouin zone close to the light cone and are therefore not very interesting.
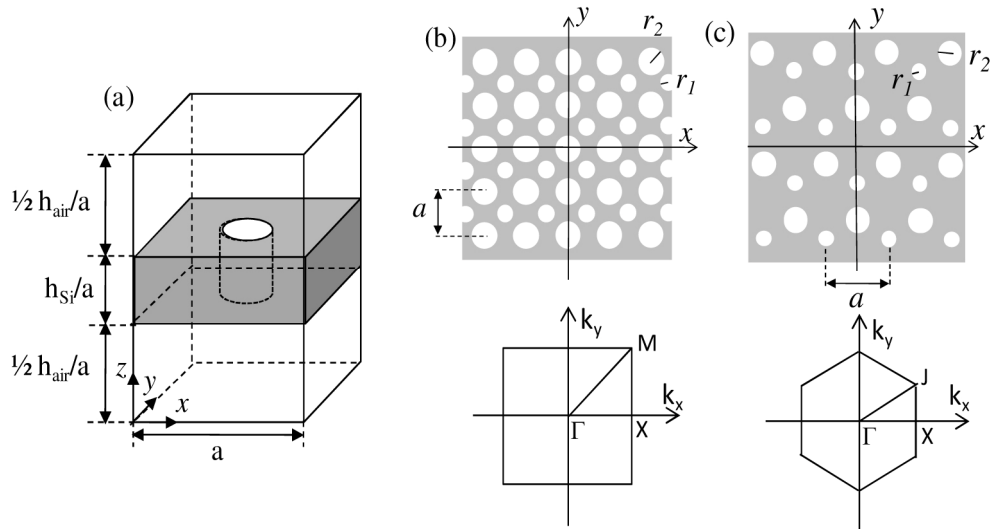

Fig. 1. (a) Representation of the unit cell for the numerical calculations. Centered square (b) and Boron Nitride (BN) (c) lattices with two atoms per unit cell together with the corresponding Brillouin zones. h_{Si} and h_{air} are respectively the thickness of the Si slab and air in the super-cell considered in the course of the PWE computation. r_1 and r_2 are the radii of two types of holes in the unit cell of the lattice with period a.

The calculations are generally performed by using the PWE method with periodic conditions applied on each boundary of the super-cell [see Fig. 1(a)]. On the phononic side, the air thickness (h_{air}) can be reduced to a small slab since elastic waves cannot obviously propagate in vacuum. The air is modeled as a low impedance medium with very low density and very high velocity of sound. The convergence of the calculation is quite fast [12] and is achieved for a number of plane waves of 1215 for the square lattice and 1815 for the BN structures. Calculations have been checked using two other methods, namely the finite element (FE) and the finite difference time domain (FDTD).

On the photonic side, the thickness of the air slab has been chosen such that it enables to decouple the silicon slabs belonging to neighboring super-cells. Figure 2 shows the evolution of the dispersion curves as a function of the air thickness hair for a square array in the ΓM direction of the irreducible Brillouin zone for the following geometrical parameters: h_{Si}/a = 0.6 and r/a = 0.43.
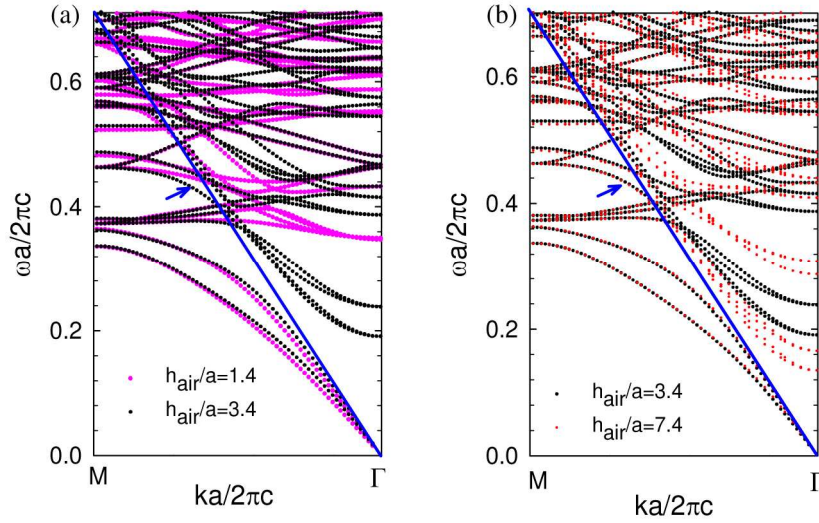
Fig. 2. Photonic dispersion curves for $h_{air}/a = 1.4$ (a) $h_{air}/a = 7.4$ (b) in comparison with $h_{air}/a = 3.4$ in the ΓM direction of the Brillouin zone for a silicon slab of holes in a square lattice for the geometrical parameters $h_{Si}/a = 0.6$ and $r/a = 0.43$. The blue solid line delimits the light cone.
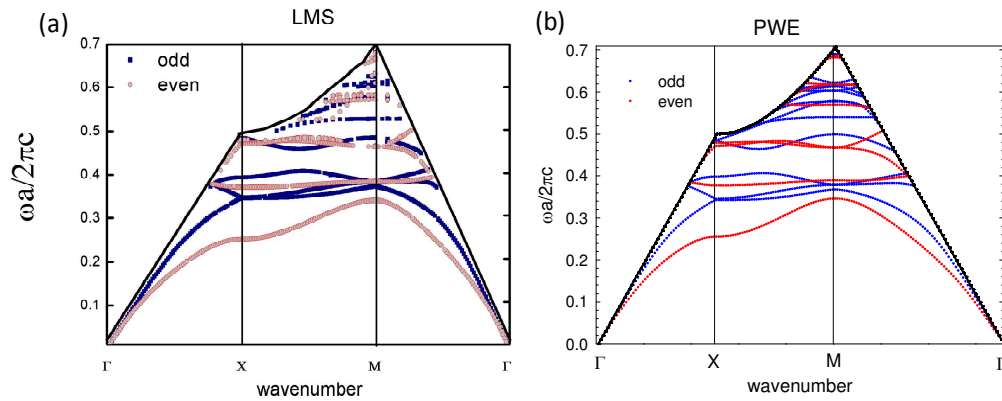

Fig. 3. Photonic dispersion curves for a silicon slab of holes in a square lattice for the geometrical parameters $h_{Si}/a = 0.6$ and $r/a = 0.43$ computed with (a) the layered multiple (LMS) method and (b) the plane wave expansion (PWE) method.

By increasing the thickness of air separating two neighboring slabs, one can observe in Fig. 2(a) a decrease of the dispersion branches located above the light cone towards lower frequencies as far as the air thickness increases. Below the light cone, where the branches correspond to the guided modes of the photonic silicon slab, most of the branches remain unchanged except one of them highlighted with a blue arrow. Actually, the latter branch introduces a limitation on the existence of a photonic band gap and its convergence needs to be checked carefully. As seen in Fig. 2(b), the convergence of this specific branch is achieved for an air thickness of $h_{air}/a > 3.4$ while the branches over the light cone still continue to move to lower frequencies. One mention also that the number of plane waves have been adapted to each thickness of the unit cell to achieve a good convergence (2673 for h_{air}/a equal to 1.4, then 3645 and 7047 for h_{air}/a equal to 3.4 and 7.4 respectively). In the rest of the paper, the air thickness has been chosen equal to $h_{air}/a = 7.4$ to insure the stability of the whole branches under the light cone and the calculations have been performed with a number of plane waves equal to 7047. In Fig. 3, the previous PWE result [Fig. 3(b)] is compared to the dispersion

curves calculated on the same photonic structure using another numerical method, i.e. the layered multiple scattering (LMS) method [27,28] [Fig. 3(a)], with a quite good agreement. Calculations have also been checked using finite difference time domain (FDTD) with the same conclusions.

3. Square lattice

We first present the case of the simple square lattice ($r_1 = 0$, $r_2 = r$, $\alpha = 0$). Figure 4 reports the evolution of both phononic and photonic gaps for each symmetry, even (red) and odd (blue), as a function of the filling factor f and for a set of silicon plate thicknesses h_{Si}/a in the range [0.4, 0.7].

In this geometry, a complete phononic and photonic band gap is found only when $h_{Si}/a = 0.4$ and for a high value of the filling factor f = 0.7 (black vertical arrow). Unfortunately, from the photonic side, this gap appears in a very restricted region of the Brillouin zone ($\Omega = [0.553, 0.658]$), near the M point, just below the light cone. It means that this solution is not really interesting. To cover the full directions of the Brillouin zone, the reduced frequency value should be lower than 0.5. With this condition, there is no overlap between the photonic gaps of both symmetries.
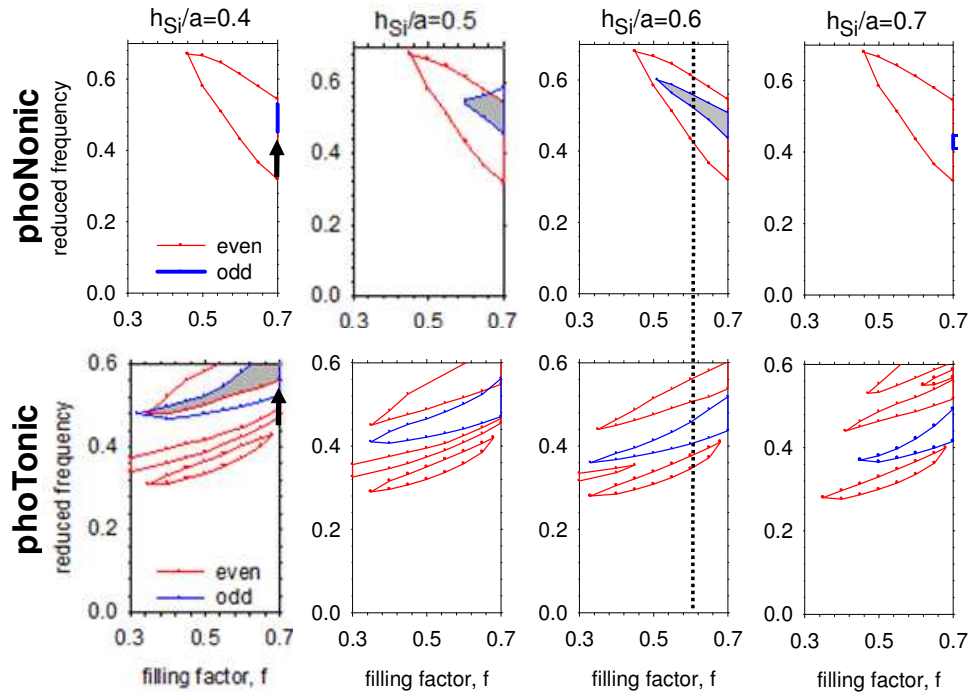

Fig. 4. Simple square lattice: evolution of phononic and photonic gaps of even (red) and odd (blue) symmetries as a function of the filling factor f for different values of the thickness of the silicon slab h_{Si}/a. The grey areas correspond to absolute band gaps.

The choice of a phononic and photonic crystal can be made by searching a structure that exhibits an absolute phononic band gap though a photonic gap of a given symmetry only. Figure 4 shows that in the phononic side the limitation comes from the odd modes which only display narrow gaps occurring for a thickness of the plate $h_{Si}/a = [0.5, 0.6]$ and for filling factors f≥0.6. In this thickness range, there are photonic gaps (either even or odd) at frequencies below 0.5.

For the square lattice structure one example of phononic and photonic band gaps for either symmetric (even) or antisymmetric (odd) optical modes can be chosen for the set of parameters ($h_{Si}/a = 0.6$, f = 0.65, r/a = 0.455) (see the black vertical dotted line in Fig. 4). In

view of telecom applications, the photonic band gap wavelength has to be chosen close to 1550nm. Then, the actual geometrical parameters become a = 701nm, h_{Si} = 421nm and r = 315nm for the odd gap and a = 590nm, h_{Si} = 350nm and r = 265nm for the even gap. For these structures, the mid-gap acoustic frequency falls at 4.2GHz and 5.0GHz respectively. With these parameters, the separation between neighboring holes becomes respectively 70nm and 60nm and makes this periodic crystal geometry technologically realizable.

We have generalized our study to the case of a centered square lattice containing two cylinders per unit cell. However, we have found that this new geometry cannot give rise to any more suitable choices of the phononic and photonic crystal. In particular, the limitation discussed above, about the odd phononic modes, remains. The odd phononic gap progressively closes when α increases from 0 to 0.2 which limits the photonic possibilities in the purpose of full acoustic and optical band gap investigations.

As an example, Fig. 5 gives the evolution of the phononic and photonic band gaps for each symmetry as a function of α = r_2/r_1, for a thickness h_{Si}/a = 0.6 and a filling factor f = 0.65. It is worth noticing that no more favorable situations can be found when the square lattice contains two different cylinders in the unit cell.
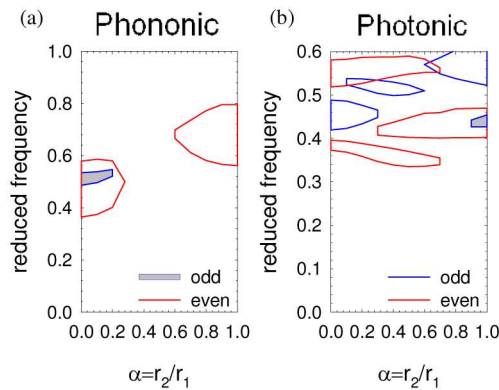

Fig. 5. Square lattice with two cylinders per unit cell: evolution of the phononic (a) and photonic (b) band gaps according to the symmetries even (red) and odd (blue) as a function of α = r_1/r_2, assuming the geometrical parameters h_{Si}/a = 0.6 and f = 0.65.

4. Honeycomb lattice

Figure 6 represents, for the honeycomb lattice (r_1 = r_2 = r, α = 1), the evolution of the phononic and photonic band gaps for each symmetry as a function of the filling factor f and for different values of the thickness of the silicon plate h_{Si}/a.

From the phononic side, the honeycomb array is more suitable than the square lattice. Both odd and even gaps are larger and open at lower filling factor. Moreover, one can notice that the absolute phononic band gap exists in the whole investigated range of h_{Si}/a from 0.4 to 0.7. The odd gaps are in general included in the even gaps except at low filling factor. The limitation comes this time from the photonic side. For the latter, the odd gap exists in the full range of the filling factor and for all the studied values of h_{Si}/a whereas the even gap is present for $h_{Si}/a \leq 0.5$ and progressively closes when the filling factor increases. Nevertheless, a complete phononic and photonic band gap, represented with a grey area in Fig. 6, occurs provided the thickness of the slab is in the range h_{Si}/a = [0.4-0.5]. Assuming that the dimensionless photonic frequency gap should be lower than 0.5 to cover all directions of the Brillouin zone, one can define as an example a set of parameters (h_{Si}/a = 0.5, f = 0.45, r/a = 0.249) (black vertical dashed line) which leads to a complete phononic and photonic band gap. Then, by assuming that the photonic midgap occurs at the telecommunication wavelength of 1550nm, we find the following geometrical parameters: a = 687nm, h_{Si} = 330nm and the hole radius r = 171nm. The separation between neighboring holes is then 55nm, which is quite

acceptable for the technological fabrication of the sample. With this lattice parameter, the phononic mid-gap frequency occurs at 4.9GHz.

Although the above example displays simultaneously a complete phononic and photonic band gap, the latter remains relatively narrow. Now, we can discuss more general situations exhibiting a full phononic gap but a photonic gap of a given symmetry only. One can notice that the photonic band gaps of even symmetry are obtained for the low values of the slab thickness, typically $h_{Si}/a \leq 0.5$ and can be chosen for several filling factors. As an example, the reduced parameters ($h_{Si}/a = 0.4$, $f = 0.45$, $r/a = 0.249$) lead to a band gap of even photonic symmetry (red vertical dashed line). One can also design structures with an odd photonic gap provided the thickness of the slab $h_{Si}/a \geq 0.5$ in order to insure the dimensionless frequency be lower than 0.5. Many filling factors, higher than 0.35, are suitable and one example is given by the following parameters ($h_{Si}/a = 0.7$, $f = 0.45$, $r/a = 0.249$) (blue vertical dashed line).
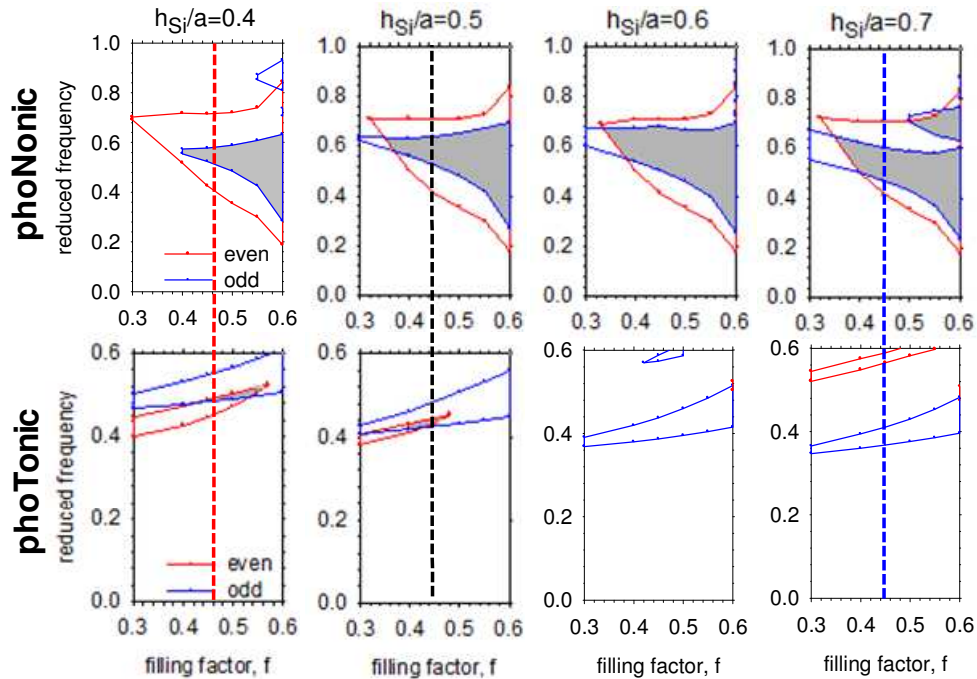
Fig. 6. Honeycomb lattice: evolution of the phononic and photonic even (red) and odd (blue) gaps as a function of the filling factor f for different values of the thickness of the silicon slab h_{Si}/a. The grey areas correspond to absolute band gaps.

5. Boron nitride lattice

To discuss the general trends in the BN lattice, we illustrate in Fig. 7 the evolution of the gaps from triangular ($\alpha = 0$) to honeycomb ($\alpha = 1$) for two thicknesses of the slab $h_{Si}/a = 0.5$ and $h_{Si}/a = 0.6$ and for a filling factor $f = 0.45$.

In the phononic side, the largest gaps are obtained towards the honeycomb lattice ($\alpha = 1$) and then the odd gaps are in general included in the even ones. However, for $h_{Si}/a \geq 0.6$, an odd gap can appear for all BN lattices (from triangular to honeycomb) whereas the even gaps remain open only towards the honeycomb lattice. In the photonic side, an odd gap exists for all BN lattices. The largest gaps of even symmetry occur towards the triangular lattice at frequencies around or below $\Omega = 0.4$. Nevertheless, the even modes can also display a narrow gap towards the honeycomb lattice (when $\alpha > 0.8$) provided the thickness of the slab is relatively small ($h_{Si}/a \leq 0.5$). In the latter case, this gap is included inside the odd one and gives

rise to a complete phononic and photonic band gap, as already discussed in the case of the honeycomb lattice. No more complete photonic band gaps are found from the BN structures.

Based on the above discussion, the choice of a phononic and photonic crystal can be made by searching a structure that exhibits an absolute phononic band gap though a photonic gap of a given symmetry only. With this limitation, many possibilities exist in the frame of BN lattices as illustrated in Fig. 7. Indeed, the following discussion shows the limits of the geometrical parameters for the simultaneous existence of an even and an odd photonic gap at two different frequencies. First, the existence of the absolute phononic gap requires a filling factor f greater than 0.4 and $\alpha \geq 0.5$. In the photonic side, the thickness of the slab should be taken above $h_{Si}/a = 0.5$ in order to keep the odd gap in the frequency range below $\Omega = 0.5$ (otherwise the gap occurs only in a very restricted range of the Brillouin zone close to the light cone). Finally, a sufficiently wide gap of even symmetry requires $\alpha \leq 0.8$.

As an example, the reduced parameters for a phononic and photonic crystal can be chosen as ($h_{Si}/a = 0.6$, f = 0.45, $\alpha = 0.6$) (see the black vertical dotted line in Fig. 7). In telecom applications, the corresponding structure can be defined with the geometrical parameters a = 637nm, h_{Si} = 382nm, r_1 = 115nm and r_2 = 192nm for the odd photonic modes and a = 491nm, h_{Si} = 295nm, r_1 = 89nm and r_2 = 148nm for the even one. These lattice parameters lead to phononic mid-gap frequencies of 5.15GHz and 6.68GHz respectively.
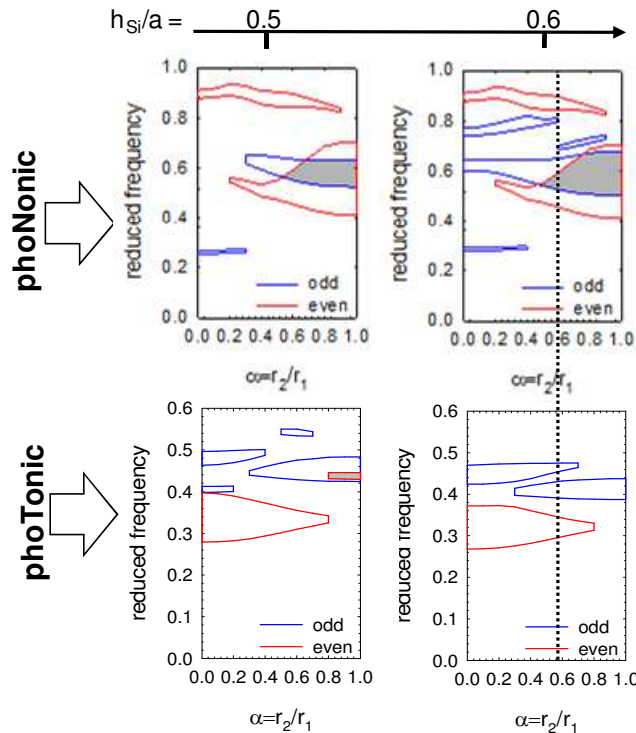

Fig. 7. Boron Nitride lattice: Phononic and photonic band gaps with f = 0.45 and for two thicknesses h_{Si}/a of the slab. The odd (blue) and even (red) modes are shown separately. The grey areas represent the domain of α where there are complete phononic and photonic gaps of both symmetries.

Table 1 summarizes the main structures suitable to exhibit an absolute phononic band gap together with photonic band gaps either for both or for only one type of symmetry. Of course, the choice of the lengths for the practical realization of the structure depends on the frequency range of interest for specific applications.

6. Conclusion

In this work, we have theoretically investigated the possibilities to open phononic and photonic band gaps in silicon slabs drilled with circular air holes. This is totally new with respect to similar works performed in 2D infinite structures [22–24] since the existence conditions for the absolute phononic/photonic gaps are quite different in the case of a slab as compared to the case of a 2D infinite structure. We have studied both phononic and photonic band gaps in different lattices and found that simultaneous absolute band gaps can be obtained with the honeycomb lattice as well as in a small domain of the BN lattices close to honeycomb. Nevertheless, for all geometries (square, honeycomb and boron nitride lattices) the simultaneous confinement of both elastic and electromagnetic energy is possible, provided the incident wave is polarized. Of course, these results are independent of the scale of the structure. We have specified some numerical parameters by assuming that the optical wavelengths are in the range of telecommunication (wavelengths around 1550 nm). This leads to acoustic frequencies that fall in the gigahertz regime. Phononic and photonic crystal slabs hold promises for the simultaneous confinement and tailoring of sound and light waves with potential applications to acousto-optical devices and highly controllable photon-phonon interactions. Other properties such as linear and point defects will be investigated in subsequent works.

Table 1. *Summary of the most suitable phononic and photonic crystals and the corresponding band gaps frequencies.*

Array	α	f	r_i/a	h_{Si}/a	Phononic band gap	Photonic band gap odd modes	Photonic band gap even modes	Observations
Square	0	0.7	0.47	0.4	[0.439, 0.544]	[0.553, 0.658]		- Complete phononic and photonic gap - In the neighborhood of M - High value of f
Square	0	0.65	0.45	0.6	[0.472, 0.534]	[0.410, 0.495]	[0.361, 0.400]	- Photonic gap of a given symmetry only
Honey comb	1	0.45	0.249	0.48	[0.525, 0.626]	[0.434, 0.454]		- Complete phononic and photonic gap
Honey comb	1	0.45	0.249	0.7	[0.468, 0.611]	[0.368, 0.410]	/	- Photonic gap of an odd symmetry only
Honey comb	1	0.45	0.249	0.4	[0.503, 0.588]	/	[0.445, 0.492]	- Photonic gap of an even symmetry only
Boron Nitride Ex.	≥0.6 ≤0.8 0.6	≥0.4	$r_1 = 0.181$ $r_2 = 0.302$	≥0.5 0.5	[0.521, 0.602]	[0.390, 0.432]	[0.291, 0.343]	- Photonic gap of a given symmetry only