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# Opening of simultaneous photonic and phononic band gap in two-dimensional square lattice periodic structure

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We discuss two points related to the simultaneous existence of phononic and photonic band gaps in a two-dimensional crystal constituted by a square array of holes drilled in a matrix. In a first part, using the case of a sapphire sample in the microwave range, we show that in addition to the phononic gap, an absolute photonic gap may be obtained making use of the high values as well as the anisotropy of the dielectric matrix elements in the microwave regime. In a second part, using the case of silicon in the telecom frequency range, we demonstrate that absolute photonic and phononic gaps may be obtained by making a combination of two crystals having slightly different filling factors. The calculations of the band structures and transmission coefficients were mainly computed using the finite difference time domain method. © 2011 American Institute of Physics.

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## I. INTRODUCTION

The mechanical and electromagnetic waves propagating in periodic structures can undergo dispersive effects that are not observable in conventional homogenous materials. Phononic crystals, which are periodic structures made of two materials with different mechanical properties can be used to control mechanical waves.<sup>1–5</sup> Similarly, photonic crystals are periodic structures made of different dielectric materials designed to control the propagation of electromagnetic waves.<sup>6,7</sup> Both of such periodic structures can obviously create phononic or photonic band gaps in which, respectively, the propagation of phonons or photons is prohibited.<sup>7–15</sup>

The control, localization, and guiding of light and sound is an interesting physical phenomena. An appealing novel research area here is the design of periodic structures that can control and localize both light and sound in the same spatial region at the same time. This could enhance the interaction between phonons and photons and can thus create nonconventional acousto-optical devices for the simultaneous control of electromagnetic and elastic waves.<sup>8,10,11</sup> A prerequisite of the existence of such interaction is the presence of the simultaneous control and localization of light and sound. It is then essential to have a periodic structure possessing both complete phononic and photonic band gaps, so called “phoxonic” band gap.

The existence of a complete phononic band gap in a periodic structure does not necessarily imply that it also possesses a complete photonic band gap and vice versa. A comprehensive search for periodic structures owing both band gaps is thus needed. Several authors investigated the opening of simultaneous band gaps making use commonly the lattice

geometry and the filling fraction.<sup>9,12</sup> In fact, Maldovan and Thomas<sup>9</sup> have reported that phoxonic band gap can be obtained in a two-dimensional (2D) periodic structure based on silicon substrates. Sadat-Saleh *et al.*<sup>12</sup> reported on the tailoring of phoxonic band gap on lithium niobate using notably heterometric hexagonal lattice. Further, Mohammadi *et al.*<sup>13</sup> have shown the opening of phoxonic band gap in square and honeycomb lattice based on silicon plates. Independently, Pennec *et al.*<sup>14</sup> dealt with the same problem in square, honeycomb, and more generally boron nitride lattices. Very recently, Papanikolaou *et al.*<sup>15</sup> reported on the opening of phoxonic band gap in three-dimensional (3D) metallodielectric cubic lattice. Experimental evidence of the existence of simultaneous band gap has been reported in a 3D periodic structure based on amorphous silica spheres.<sup>16</sup>

In this paper, we propose to study two problems related to the opening of simultaneous photonic and phononic band gaps in a 2D square lattice structure of periodic array of holes in a matrix. In the first case, the matrix is constituted by sapphire where we take advantage of the anisotropy of the dielectric tensor in the microwave regime to show the possibility of an absolute photonic gap for both TE and TM waves, together with an absolute phononic gap. In the second case, we use a silicon matrix in the telecom frequency range (optical wavelengths of 1550 nm) and show that, in addition to the phononic gap, it is possible to obtain an absolute photonic transmission gap by combining two crystals with slightly different filling factors. One motivation behind this work is to propose a simple periodic structure that can be easily prepared by conventional microtechnology tools with an acceptable fabrication tolerance. The transmission spectra for different polarizations of the incident (optical and acous-

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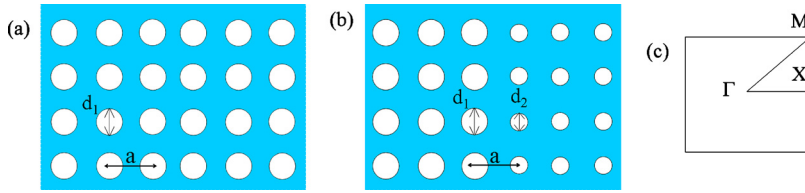


FIG. 1. (Color online) (a) 2D Periodic array of cylindrical Air-holes, of diameters  $d_1$ , in sapphire matrix arranged along a square lattice. (b) Schematic design of a coupled 2D crystals of cylindrical air-holes, of diameters  $d_1$  and  $d_2$ , in Si matrix arranged along a square lattice of the same period,  $a$ . (c) The irreducible Brillouin zone of the 2D square lattice.

tical) waves are calculated for a finite thickness sample and analyzed in relation with the dispersion curves of the modes in the infinite structure.

The paper is organized as follows. In Sec. II, we present briefly the geometry and the method of calculation of the band structure and the transmission coefficient in 2D phononic crystals. Sections III A and III B present discussion on several numerical results obtained, respectively, for the sapphire and silicon based structures.

## II. GEOMETRY AND METHOD OF CALCULATION

The phononic and photonic band structures and transmission coefficients are mainly calculated by using the finite difference time domain (FDTD) method. In addition, for some cases, the convergence of the band structure calculations is checked by the plane wave expansion (PWE) method. The sapphire sample, assumed as a simple 2D square-period array to open up simultaneous band gaps, is analyzed in the microwave range regime taking into account the dielectric-tensor anisotropy. Whereas the silicon sample, taken as a combination of two different periodic arrays to open up such band gaps with square lattice geometry, is analyzed in the telecommunication range (optical wavelengths of 1550 nm). Figure 1 gives the schematic representation of both of these structures.

## III. NUMERICAL RESULTS AND DISCUSSIONS

### A. Periodic structure based on sapphire

The cylindrical holes in sapphire have been thought as a potential structure to open phoxonic band gap owing to its high elastic and dielectric contrasts in some frequency ranges. We present and discuss here the computed photonic and phononic dispersion curves, as well as the transmission through finite 2D periodic structure.

The elastic wave propagates in the plane normal to the axis of air cylinders. We have calculated their dispersion relations for the decoupled transverse mode (out-of-plane shear vibrations) along the  $z$  axis and for the mixed modes (in-plane vibrations) which are in the  $(xy)$  plane. The transverse and longitudinal sound velocities in sapphire are, respectively,  $C_t=6.04$  km/s and  $C_l=11.09$  km/s, and its mass density is  $\rho=3986$  kg/m<sup>3</sup>.

The photonic calculations are performed in the microwave frequency range where the sapphire's dielectric tensor is anisotropic and the indices of refraction are high ( $\epsilon_{||}=11.5$  and  $\epsilon_{\perp}=9.3$ ). Obviously, the opening of a photonic band gap in near infrared frequency range is more difficult due to the low refractive index of sapphire in this range ( $n_{\text{sapphire}}=1.75$ ).

Figure 2 displays in the middle panels the phononic (lower row) and the photonic band structures of TE (upper row) and TM (middle row) polarizations for a square lattice array of infinite cylindrical air holes in the sapphire matrix for a filling fraction of  $f=0.66$ . The band structures are computed both with FDTD and PWE methods. We have used a dimensionless frequency  $\Omega=\omega a/2\pi c$ , where  $c$  is the light velocity in vacuum for electromagnetic waves or the transverse sound velocity in sapphire for elastic waves. The

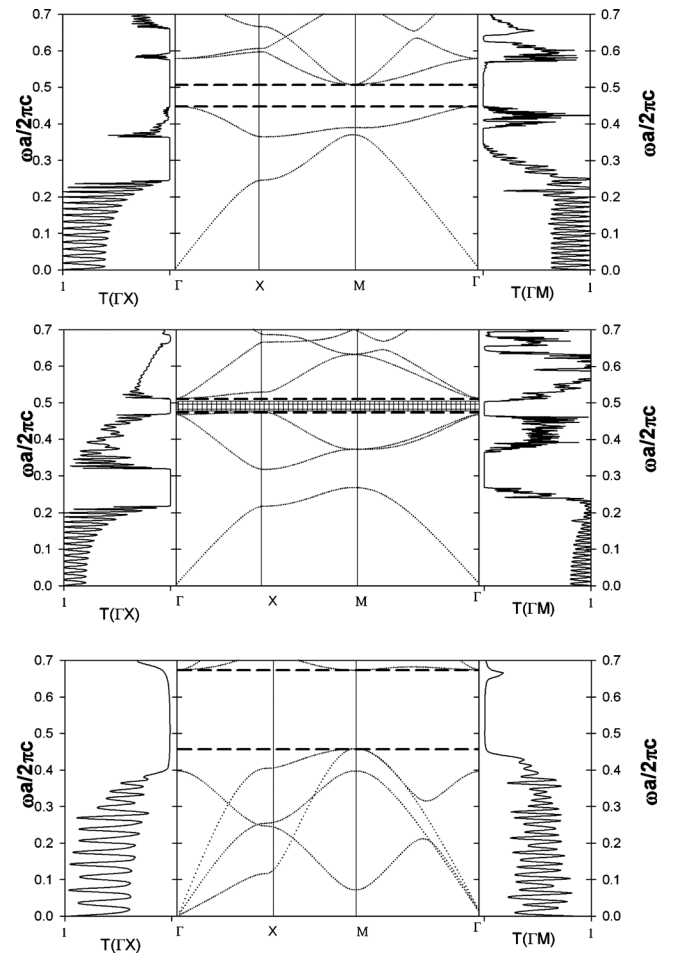


FIG. 2. Photonic and phononic band structures (middle panels) and the corresponding transmission coefficient (left and right panels) for a square lattice array of circular air holes in sapphire for filling factor  $f=0.66$  computed with PWE and FDTD methods. Band structures and transmission coefficients for the photonic TE polarization (upper row), photonic TM polarization (middle row), and phononic (lower row) are displayed in units of the normalized frequency  $\omega a/2\pi c$ , where  $c$  is the velocity of light in vacuum for electromagnetic waves and the transverse velocity of sound in sapphire for elastic waves. Left and right panels give the transmission coefficients through a finite 2D phoxonic crystal composed of  $N=16$  periods, vs the reduced frequency in the  $\Gamma X$  and  $\Gamma M$  directions, respectively. The dashed straight lines show the width of the gaps. The hatched region (lower row and middle panel) corresponds to the absolute phoxonic band gaps.

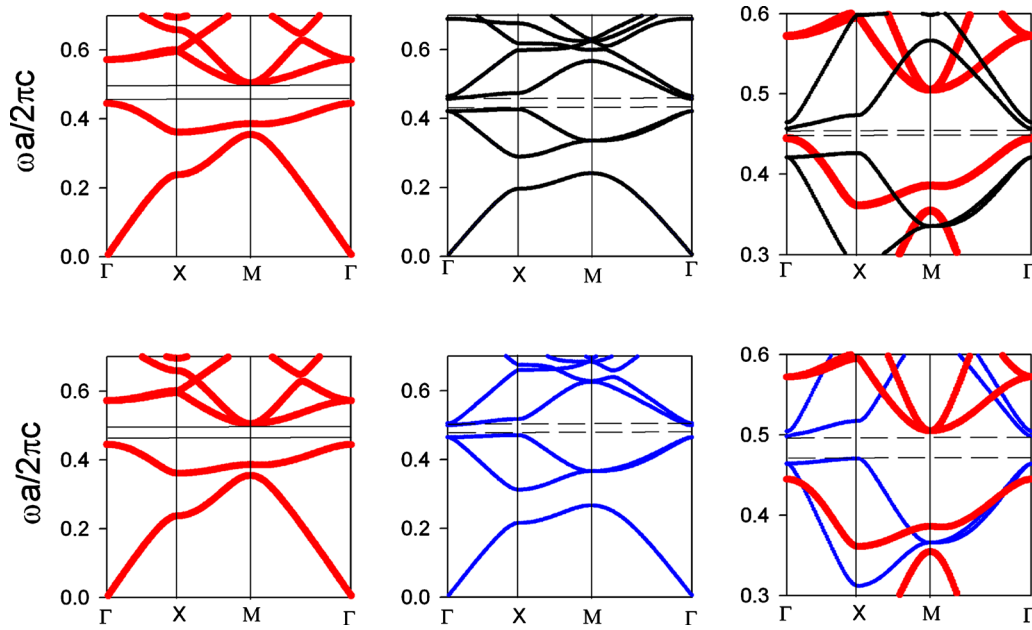


FIG. 3. (Color online) Photonic band structures of TE (left panels) and TM (middle panels) polarizations for a square lattice array of circular air holes in isotropic (upper row) and anisotropic (down row) sapphire for filling factor  $f=0.66$  computed with PWE and FDTD methods. The magnification of the superposition of the band structures for these 2D structures are presented in the right panels exhibit an absolute photonic gap in the reduced frequency range delimited by the dashed horizontal lines.  $\omega a/2\pi c$  is the normalized frequency, where  $c$  is the velocity of light in vacuum.

dashed-straight lines show the width of the gaps for each value of the wave vector inside the reduced Brillouin zone delimited by the lines  $\Gamma XM$  and for each polarization of the electromagnetic (TE or TM) or acoustic waves. The gaps extend from  $\Omega=0.4478$  to  $0.5072$  (TE),  $\Omega=0.4667$  to  $0.5109$  (TM), and from  $\Omega=0.4569$  to  $0.6721$  (acoustic). One can notice the existence of a common frequency region (hatched region in the middle row and middle panel) corresponding to the absolute simultaneous photonic band gaps. This omnidirectional gap for total reflection extends from  $\Omega=0.4667$  to  $0.5072$ .

Due to the large contrast between the elastic parameters of sapphire and air, the absolute gap of the 2D phononic crystal extending from  $\Omega=0.4569$  to  $0.6721$  is rather wide compared to another system such as Hg/Al.<sup>17</sup> Moreover, in the microwave frequency range, the significant dielectric anisotropy of sapphire allows the coincidence of the omnidirectional gaps associated with the TE and TM polarizations. This is not possible in isotropic crystals such as silicon or if we consider sapphire as an isotropic medium. To emphasize this point, we calculated in Fig. 3 the photonic band structures of sapphire periodic crystal without taking account of its dielectric anisotropy. These band structures clearly indicate that the natural dielectric anisotropy of sapphire plays a key role in the opening of a common photonic band gap for both TE and TM polarizations.

In order to study the light and sound transmission through a finite 2D structure, we now consider a finite 2D phoxonic crystal composed of  $N=16$  periods. In the left and right panels of Fig. 2, we present the transmission coefficients, computed with FDTD method, with the reduced frequency  $\Omega$ , respectively, in the  $\Gamma X$  and  $\Gamma M$  directions. Due to the finiteness of the 2D structure, the transmission never becomes exactly equal to zero but can decrease to almost van-

ishing values in some frequency ranges. For each polarization of the electromagnetic and the acoustic waves, the agreement is good between the band gaps appearing in the dispersion curves (middle panels) and in the transmission coefficients (left and right panels). Such agreement asserts fine convergence of the results obtained with FDTD and PWE methods. The region of reduced frequency in which the transmission rate is almost vanishing is indicated by the dashed straight lines to show the width of the gaps.

We now briefly discuss the existence and the behavior of the simultaneous photonic and phononic omnidirectional reflection band as a function of the geometrical parameters involved in our structure, namely, the filling fraction of air and the number,  $N$ , of unit cells in the 2D structure. We present in Fig. 4 for the sake of brevity only, the variation in the band gap width as a function of the filling fraction  $f$  for the photonic waves of TE [red (a)] and TM [blue(b)] polarizations, and for the phononic waves [black(c)]. Figure 4(d) is just a magnification of the variation in the common TE and TM photonic band gap versus  $f$ . This panel shows the frequency domain in which the propagation is prohibited for both polarizations when the band gaps of panel (a) and (b) are superimposed. Interestingly, these common photonic band gaps (white area) for both TE and TM polarizations and phononic band gaps (c) of the 2D sapphire periodic structure coexist at the same range of filling fraction, i.e.,  $0.64 < f < 0.74$ .

However, the opening of photonic band gap in near infrared frequency range is very difficult due to the low refractive index of sapphire in this range ( $n_{\text{sapphire}}=1.75$ ). If the incident optical wave belongs to this range of frequency, part of the incident wave of TE or TM polarization, can be transmitted through the 2D structure. This limitation about the existence of absolute simultaneous photonic and phononic



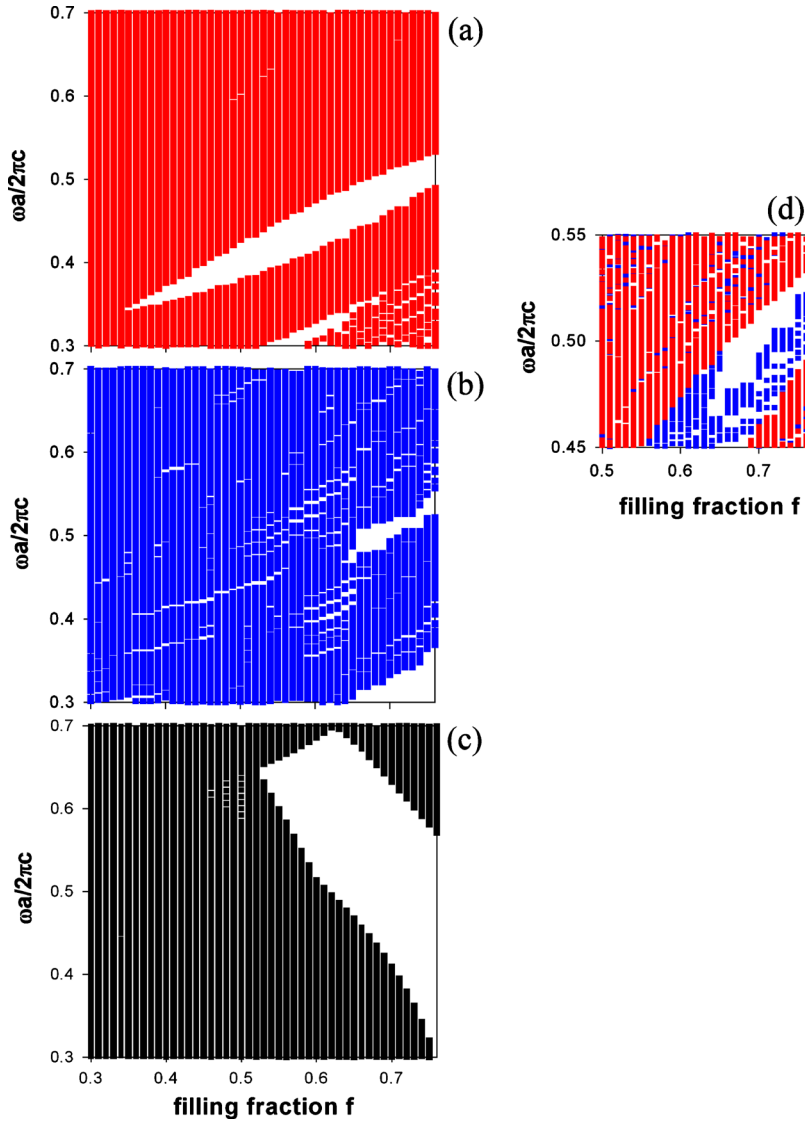


FIG. 4. (Color online) Distributions of the TE [red (a)], TM [blue(b)] photonic, and phononic [black(c)] band gap as a function of the filling fraction  $f$  in a simple square lattice array of circular air holes in sapphire. The normalized frequency  $\omega a/2\pi$  is defined as in Fig. 1. The shaded and white areas respectively correspond to the pass bands and the gaps of the 2D phoxonic crystal. In figure (d), the white area corresponds to the common TE and TM photonic which corresponds also to the absolute phoxonic band gap vs  $f$ .

band gap comes from the photonic waves, since the phononic gap is relatively broad and already exists for values of filling fraction  $f$  of the order of 0.5. In others words, the ability of 2D (air holes in sapphire matrix) structure to behave like a perfect phoxonic mirror in some range of reduced frequency (or wavelength) imposes a limitation on the choice of the domain of optical frequency.

As an example in microwave domain, let us assume the following geometrical parameters:  $a=1$  cm and  $f=0.66$ . Then, the photonic gap extends from  $1.4 \times 10^{10}$  to  $1.52 \times 10^{10}$  Hz, while the phononic gap falls in the range of 276–406 kHz.

## B. Periodic structure based on silicon

We put forward here another approach allowing the opening of simultaneous band gap within a simple square 2D crystal, with the optical gap falling in the near infrared frequency range. We thus aim to obtain a domain of reduced frequency in which the transmission of light waves is inhibited even for a telecommunication frequency. According to our previous works on one-dimensional phononic or photonic band gaps materials,<sup>18,19</sup> one solution to obtain omnidi-

rectional band gap consists of associating two 2D periodic structures of air holes in a silicon matrix that is chosen appropriately in such a way that the superposition of their band gaps displays a useful overlap. This means that in some frequency range, the minigap of one 2D structure overlaps with the others bands and vice versa. We have investigated several physical and geometrical parameters for such coupled 2D structures. One interesting solution among fewer others that give rise to an omnidirectional phoxonic band gap, is to combine two 2D structures of air holes in a silicon matrix. These two structures should have the same periods and different filling fractions  $f_1=0.64$  and  $f_2=0.60$ . The photonic [TE (blue), TM (red)] and phononic (black) band structures of each 2D structure are displayed, respectively, in the left and middle panels of Fig. 5. The magnified superposition of the band structures for these 2D structures in the right panels of Fig. 5 clearly exhibits a broad absolute phoxonic gap in the reduced frequency range  $0.4 < \Omega < 0.425$  (delimited by the dotted horizontal lines). One can expect that in this reduced frequency domain, all optical or acoustical waves generated in vacuum will be totally reflected. In practice, the coupled 2D structure is of finite width and we need to evaluate the

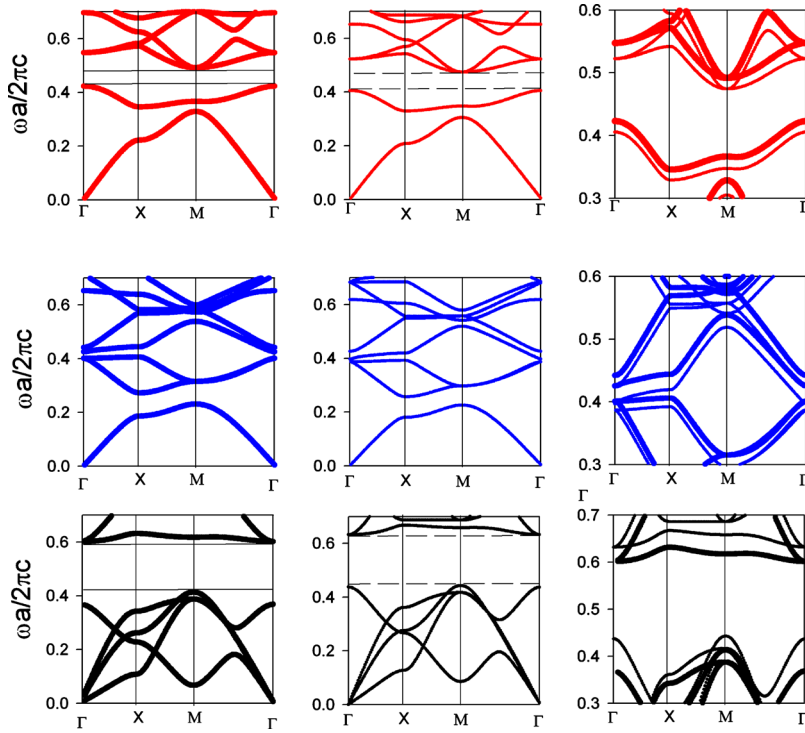


FIG. 5. (Color online) Photonic [TE (upper row) and TM (middle row)], and phononic (lower row) band structures of two different square lattice arrays of circular air holes in silicon for filling factor  $f=0.64$  [left panels (thick lines)] and  $f=0.6$  [middle panels (thin lines)]. The right panels, respectively, represent the overlap of the band gaps displayed in left and middle panels. The dotted horizontal lines delimited the frequency range, in which the propagation of light will be prohibited through a structure resulting from a combination in tandem of the two 2D phoxonic structures.  $\omega a/2\pi c$  is the normalized frequency, where  $c$  is the velocity of light in vacuum for electromagnetic waves and the transverse velocity of sound in silicon for elastic waves.

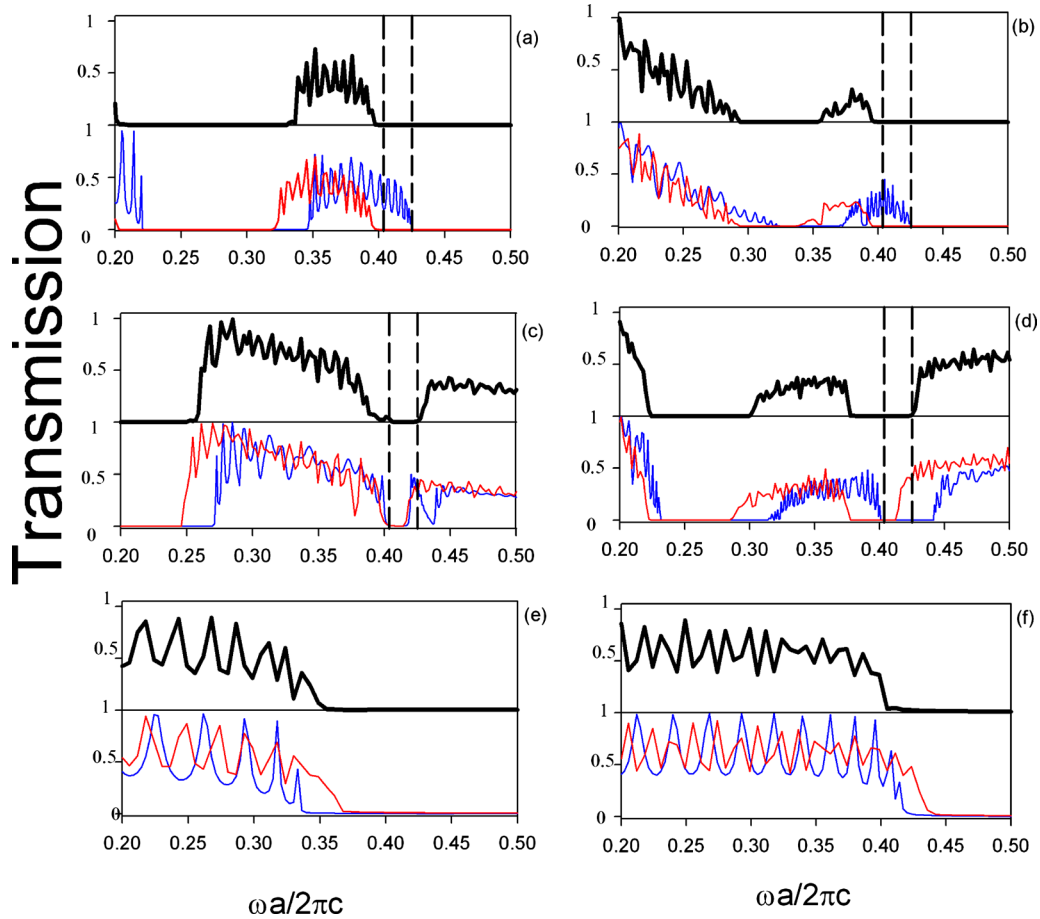


FIG. 6. (Color online) Transmission spectra through 2D phoxonic crystal of a square lattice array of circular air holes in Silicon for filling factors  $f_1=0.64$  and  $f_2=0.6$  (thin lines), and through the coupled 2D phoxonic structure (thick solid lines) computed with FDTD method. (a,b), (c,d), and (e,f), respectively, give the transmission for the photonic TE, photonic TM polarization, and phononic waves vs the normalized frequency  $\omega a/2\pi c$  defined as in Fig. 5. Left and right panels give the transmission coefficient in the  $\Gamma X$  and  $\Gamma M$  directions, respectively. The horizontal dashed straight lines indicate the edges of the common omnidirectional photonic band-gap.

capacity of the structure to prohibit the transmission of the waves. An illustration for the occurrence of the omnidirectional phoxonic gap is presented in Fig. 6. Therein we give, the power transmission through each of the above 2D structure separately (thin red and blue curves), and through the coupled 2D structure (thick solid curves), which means the real transmission through the coupled arrays. Each 2D square lattice structure contains  $N=8$  periods.

Figures 6(a)–6(f), respectively, give the transmission coefficients of the photonic of TE and TM polarizations and phononic waves versus the normalized frequency  $\omega a/2\pi c$ . The left and right panels of Fig. 6 give the transmission coefficient in the  $\Gamma X$  and  $\Gamma M$  directions, respectively. One can notice that in the common absolute photonic band gap of reduced frequency range  $0.4 < \Omega < 0.425$  (delimited by the vertical dashed straight lines), the waves are prohibited from propagation in one or in the other 2D structure, and therefore the calculated transmission through the coupled 2D system falls down to zero. From an application point of view, for instance to create a microcavity inside the phoxonic crystal, the defect should be surrounded by two shells constituted, respectively, by each type of the two structures.

#### IV. CONCLUSION

In this paper, we theoretically investigated the opening of simultaneous photonic and phononic band gaps in a simple square periodic array of holes drilled in sapphire and silicon substrates. The first novel aspect introduced here concerns the use of sapphire substrate as a potential material for tailoring simultaneous band gaps in microwave frequency regime. Second, such band gap in optical communication wavelength ranges may be conceived by combining two different periodic arrays. These results are of great interest in view of the achievement of phoxonic band gap materials as the tolerance in the fabrication technology increases with simple square lattice of filling fraction varying between 0.6 and 0.68.

In terms of potential applications related to both systems proposed in this work, first, for sapphire-based structure, one of the most promising applications concerns the using of such structure as a sensor notably in high temperature environment, since sapphire can withstand such harsh

conditions.<sup>20</sup> Second, concerning silicon-based structure, the light emission in silicon in view of fabrication of a silicon laser for instance, can be one of most attractive and challenging purpose to target in a close future.

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