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Published in:
Journal of Applied Physics

Link to article, DOI:
10.1063/1.4944600

Publication date:
2016

Document Version
Publisher's PDF, also known as Version of record

Link back to DTU Orbit

Citation (APA):

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Citation: Journal of Applied Physics 119, 114502 (2016); doi: 10.1063/1.4944600
View online: http://dx.doi.org/10.1063/1.4944600
View Table of Contents: http://scitation.aip.org/content/aip/journal/jap/119/11?ver=pdfcov
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Optical and acoustic sensing using Fano-like resonances in dual phononic and photonic crystal plate

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(Received 11 November 2015; accepted 8 March 2016; published online 21 March 2016)

We perform a theoretical study based on the transmissions of optical and acoustic waves normally impinging to a periodic perforated silicon plate when the embedded medium is a liquid and show the existence of Fano-like resonances in both cases. The signature of the resonances appears as well-defined asymmetric peaks in the phononic and photonic transmission spectra. We show that the origin of the Fano-like resonances is different with respect to the nature of the wave. In photonic, the origin comes from guided modes in the photonic plate while in phononic we show that it comes from the excitation of standing waves confined inside the cavity coming from the deformation of the water/silicon edges of the cylindrical inclusion. We finally use these features for sensing and show ultra-sensitivity to the light and sound velocities for different concentrations of analytes.

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I. INTRODUCTION

The extraordinary optical transmission, known as EOT, has been introduced in 1998 by Ebbessen through a work based on a metallic film patterned with periodic cylindrical holes.1 Following this original work, many papers have discussed the physical origin of this effect2–5 considering the competition between three kinds of fundamental physical properties, namely, the Surface Plasmon Polariton (SPP) excitation, the Fabry Pérot resonances in the apertures, and the modes guided through the metallic crystal plate. All these effects can couple separately or together with the external incident radiation. Similarly, the demonstration and the description of Fano resonances in dielectric photonic crystal plates under normal illumination have been provided in terms of Bragg scattering and guided resonant plate modes.3–5 A few years later, this unexpected phenomenon has been demonstrated in phononic crystal, considering air-borne acoustic periodic structure under normal incidence. Papers have been devoted to one-dimensional acoustic gratings with sub-wavelength slits6,7 or 2D periodic slabs drilled with air holes.8–10 Just a few works report on the reverse situation, i.e., when the embedded medium is solid and the interfacial membrane is made of air. This situation has been discussed in 2D structure with bulk elastic waves and in phononic membrane with incident Lamb waves.11,12 Khelif et al. investigated theoretically the propagation of elastic waves in a phononic crystal plate consisting of piezoelectric inclusions placed periodically in an isotropic host material.13 In these papers, the origin of the modes is discussed according different resonances coupling with the diffractive waves. The ones that are currently admitted to govern the acoustic properties of the plates under normal excitation are the lattice resonances in periodic arrays, Fabry-Pérot modes of the hole cavities, localized eigenmodes, and elastic Lamb modes.

Recently, a new topic merged, turned toward the existence of simultaneous phononic and photonic band gaps. The phoxonic band gap has been demonstrated for example, in silicon crystal membranes with periodic array of air holes14,15 or in periodic arrays of silicon pillars on thin homogeneous SiO2 plate.16 The introduction of defects inside dual photonic and phononic crystals gave the opportunity to trap both photons and phonons in the same cavity for the purpose of enhancing their optomechanical interaction.17–19

Our goal is to estimate the potentiality of a phoxonic crystal plates to be an efficient tool for sensing simultaneously the light and sound velocities of liquids in a same structure. From the point of view of sensing applications, some authors have studied the normal transmission of optical waves through a plate perforated periodically with holes and measured the shift of a well-defined feature in the spectrum with the refractive index of the embedding liquid.20–23 A similar concept has been applied by Cunningham as direct biochemical assay technique24 and further developed as label-free imaging of cell attachment with photonic crystal enhanced microscopy.25 Phononic crystals plates have recently been introduced as a new sensor platform with normal incidence of sound26 as well
as phononic crystal sensor featuring a liquid filling air inclu-
sions\(^{27}\) or cavity defect.\(^{28}\) Salman \textit{et al.}\(^{29}\) demonstrate nu-
merically the determination of ethanol concentration through a
linear waveguide in a two dimensional phononic crystal of
water cylinders in a mercury host. Oseev \textit{et al.}\(^{30}\) have shown
the determination of gasoline properties with a phononic crys-
tal cavity sensor. By the way, a microfluidic resonator has
been opto-mechanically actuated using non-solid phases of
matter.\(^{31}\) A theoretical investigations of a new sensor platform,
the phoXonic sensor, was reported recently for in-plane waves
in 2D infinite periodic crystal.\(^{32}\)

In this paper, we discuss in details the novel concept of
dual phononic and photonic plate for sensing the light and
sound velocities of biochemical analytes, under normal inci-
dence. The structure is composed of a silicon crystal plate
drilled with air holes. The whole device is immersed in a liq-
uid. The goal is to define a highly sensitive phxonic sensor
sensitive simultaneously to the optical and acoustic index of
refraction of the fluid. Such ultra compact structure then rep-
resents a label-free, affinity-based acoustic and optical nano-
sensor, useful for biosensing applications.

The outline of the paper is described as follows. In
Sec. II, we first define the geometrical and physical parame-
ters of the structure before coming to the presentation of the
finite difference time domain (FDTD) method used for the
calculation of the photonic and phononic transmission coeffi-
cient. We investigate in Section III the phononic and pho-
tonic transmission of an incident wave launched normally to
the drilled plate embedded in the liquid. Section IV is
devoted to a discussion on the choice of the geometrical pa-
rameters and how they affect the trend of the well-defined
features in the transmission coefficients with the acoustic
and optical properties of the analyte. This study allows the
design of a high sensitive phononic/photon crystal sensor.
Finally, the conclusions are drawn in Section V.

II. GEOMETRICAL PARAMETERS AND METHOD OF
CALCULATION

We study the normal transmission through a periodically
perforated silicon plate with a lattice constant, \(a\), a hole ra-
dius, \(r\), and a thickness \(h\) (Figure 1(a)). The plate is totally
immersed in a liquid. Silicon is considered as a cubic mate-
rial with the elastic constants \(C_{11} = 16.57 \times 10^{10}\) (N/m\(^2\)),
\(C_{44} = 7.962 \times 10^{10}\) (N/m\(^2\)), \(C_{12} = 6.39 \times 10^{10}\) (N/m\(^2\)),
and with a mass density \(\rho = 2331\) kg/m\(^3\). From the optical
point of view, silicon behaves as an isotropic medium with a ref-
RACTIVE index \(n = 3.5\). The embedded medium is firstly cho-
SEN as water with acoustic wave velocity \(c_{\text{water}} = 1490\) m/s
and optical refractive index 4/3.\(^{33}\)

All photonic and phononic transmission curves presented
in the paper have been obtained with the help of homemade
3D finite difference time domain (3D-FDTD) codes. The
FDTD approach has been first used extensively with success to
study the propagation of electromagnetic waves through pho-
tonic band gap materials.\(^{33}\) Later on, the FDTD method has
been extended to phononic crystals.\(^{34}\) This method solves ei-
ther the electromagnetic or the elastic wave equations by dis-
cretizing time and space and by replacing derivatives by finite
differences in the equations of motion. As compared to other
numerical method such as plane wave expansion (PWE), it
presents the advantage of allowing simulation of mixed pho-
monic structures, composed of both fluids and solids.

Figure 1(b) represents the elementary unit cell used for
the calculation. For instance, we build a sample in three parts
along the direction of propagation \(y\). Perfect matching layers
(PML)\(^{35}\) are imposed at the free ends of the homogeneous
regions to avoid the reflective waves. The crystal is consti-
tuted of cylindrical inclusions of finite height along the
\(z\) direction, arranged periodically on a square lattice in the
\((x, y)\) plane. The lattice is periodically infinite along \(x\) and \(y\).
The input signal is launched from the left of the unit cell, per-
pendicularly to the plate. The transmitted signal is then
recorded at the end of the second homogeneous region and
integrated along the \((x, y)\) plane. Accordingly, the space is dis-
cretized in all directions with a mesh interval of \(a/30\) in pho-
tonic and \(a/40\) in phononic for a good convergence of the
calculation. The equations of motion are solved with a time
integration of \(t = 2^{19} \times dt\) in both photonic and phononic calcu-
lations. To yield the transmission coefficient, the outgoing sig-
nal, recorded as a function of time, is Fourier transformed and
normalized to the Fourier transform of a signal propagating
through a homogeneous liquid. The transmission curves are,
in general, presented as a function of a normalized frequency
\(\Omega = o a/2 n c\), where \(o\) is the angular frequency (in s\(^{-1}\)), and
c is either the velocity of light in vacuum for the electromagnetic
waves or the transverse velocity of sound in bulk silicon.

III. DUAL PHOTONIC AND PHONONIC
TRANSMISSIONS

A. Photonic calculations

We present Figure 2 the photonic calculations for an inci-
dent wave launched perpendicularly to the plate when the em-
bedded medium is water (refractive index \(n_{\text{water}} = 1.33\)). The
transmission spectrum consists of sharp resonant features on a
smooth Fabry-Pérot background. The physical origin of these

FIG. 1. (a) Three-dimensional schematic representation of a normal transmis-
sion through a silicon periodic plate embedded in a liquid. (b) Elementary unit
cell used for the FDTD calculation of the photonic and phononic transmission.

On each \(y\)-boundaries of the unit cell, perfect matching layers (PML) are
applied, while on the \(x\)-boundaries, periodic boundary conditions (PBC) insure
the periodicity of the crystal. The phononic/photonic crystal plate of thickness
\(h\) has a lattice parameter \(a\) and a radius \(r\).
resonant features is known\textsuperscript{3,4} and can be understood by considering the Bragg scattering provided by the photonic crystal lattice which folds the modes of the dielectric plate into the first Brillouin zone. This brings modes above the light line, at the $C$ point of the Brillouin zone, allowing them to be coupled to by normal light illumination.

In the purpose of this study, we note that, with the geometrical parameters fixed to $r/a = 0.15$ and $h/a = 0.25$, the transmission curve (Figure 2(a)) leads to a well-defined and isolated peak/dip $\alpha$ at the reduced frequency 0.42 with an asymmetric shape. The map of the electromagnetic field at the frequency of the dip $\alpha$ is presented in Figure 2(b). One can see that the electromagnetic field is strongly confined and spread over the whole plate, both inside the water hole and the silicon matrix. As reported in the literature,\textsuperscript{3,4} such a mode is referred as a guided resonance mode of the dielectric plate and comes from the excitation at $k// = 0$ of the symmetric modes of the periodic plate.

The peak $\alpha$, well-isolated in the transmission spectrum, presents a high quality factor due to its asymmetric shape. Such a peak is suitable for the photonic sensing purpose. In the transmission curve, the peak $\alpha$ is followed by another dip, $\beta$ at $a/\lambda = 0.55$. However, the variation of the transmissions frequencies as a function of the radius $r$ ($h/a = 0.25$, Figure 2(c)) shows that the second peak is the consequence of the superposition of two others, $\beta$ and $\gamma$, which gather at low radius values. The evolution of the three modes $\alpha$, $\beta$, and $\gamma$ has been reported as a function of the height $h$ of the plate, for, respectively, a small radius ($r/a = 0.15$, Figure 2(d)) and a larger one ($r/a = 0.35$, Figure 2(e)). All frequencies increase (resp. decrease) as far as the radius (resp. height) increases, in good agreement with the corresponding optical effective index variation. It remains from this parametric study that, depending on the thickness of the plate and the radius of the holes, the structure presents several sharpen and isolated peaks in the transmission spectra then offer the opportunity to be used for sensing application.

### B. Phononic calculations

Figure 3(a) represents the acoustic transmission for a wave launched normally to the plate and when the embedded medium is water of density $d_{\text{water}} = 1$ and acoustic wave velocity $c_{\text{water}} = 1490 \text{ m/s}$. The transmission curve shows a well-defined asymmetric peak (A) at the reduced frequency
0.235. This kind of peak/dip feature is known as Fano-like or hybridized modes as introduced in Ref. 36.

The origin of the asymmetric peak A in the transmission spectrum is discussed with respect to the component $|U_z|$ of the displacement field at the frequency of mode A, considering the cross section in the $(y, z)$ plane, cutting the water hole along his diameter. The mode A is strongly localized at the four extremities of the cylindrical inclusion (dark points) before decreasing all around in the water. The Figure 3(c) shows the same calculation in 3D to highlight the decreasing of the field. In other worlds, it means that the field is localized at the circular edge of the cylindrical inclusion and is at the origin of a confined mode inside the cavity. The asymmetric peak/dip A, observed in the transmission curve calculation, is then the consequence of the coupling between the propagative incident wave and the cavity mode, leading to the Fano-shape resonance in the transmission spectrum.

IV. PHONONIC/PHOTONIC SENSOR

A high efficient phononic/photonic sensor should present a transmission reply which displays very sensitive features to the acoustic and optical velocity of the infiltrating analyte. The preliminary condition is to get isolated features (peaks or dips) in order to allow the sensing of the probed parameter on a sufficiently broad frequency range. One can see from the evolution of the asymmetric phononic peak A (Figure 4) that no conditions are required on the geometrical parameters to respect this condition as far as the thickness is lower than $h/a = 1$. It means that the limitation on the structure should come from the photonic side. As seen in Figure 2(c), considering the peak $z$, all radii can be chosen for the average thickness $h/a = 0.25$. In the following, we first start with a small ($r/a = 0.15$) and large radius ($r/a = 0.35$) with $h/a = 0.25$ and proceed to the estimation of the sensor efficiency in both case.

The efficiency of the sensor has been tested by changing the physical parameters of the embedded analyte, namely, the acoustic and optical velocities. In phononic and photonic, we have considered a same set of mixtures made of ionic liquid 1-Methyl-3-octylimidazolium Chloride with Methanol at different molar ratio $x$. The density $\rho_{\text{liq}}$, speed of sound $v_{\text{liq}}$, and refractive indexes $n_{\text{liq}}$ of the analyte, obtained from Ref. 37, are reported in Table I as a function of $x$.

Figures 5(a) and 5(b) show the behavior of the phononic and photonic transmission coefficients considering, respectively, the acoustic velocity and refractive index of the analyte. In both cases, the two asymmetric peaks, A in phononic
and in photonic, shift in frequency with the different liquids. In photonic, when the refractive index increases, the reduced frequency “a” decreases (Figure 5(b)). In phononic, when the longitudinal velocity decreases, which corresponds to an increase of the acoustic refractive index, the reduced frequency of dip A decreases as well. As a conclusion, the phononic and photonic behavior is the same: when the refractive index increases, the eigenmode wavelength is red-shifted.

The sensitivity of the sensor has been estimated in the telecommunication range which is reached when the period of the crystal is taken equal to 640 nm. With the objective of the dual sensor, the choice of the geometrical parameters, especially the pitch “a,” is done in the way to get the properties in a frequency range that can be easily captured in both acoustic and optical spectra. The only way to respect this condition is to choose a lattice parameter at the submicron scale that leads to GHz frequency in phononic and \(\lambda_{\text{m}}\) wavelength in photonic.

With this lattice parameter, and when the embedded medium is filled with water, the wavelength of modes \(\alpha\) occurs at 1533 nm while the frequency of mode A is at 2.13 GHz.

We report Figure 6(a) the evolution of the phononic frequencies as a function of the longitudinal velocity of the analyte and in Figure 6(b) the evolution of the photonic wavelengths as a function of the refractive index. In both case, the sensitivity corresponds to the slope of the curve which is linear and defined by, in phononic

\[
S_{\text{phononic}}^{i} = \frac{\Delta f_{i}}{\Delta c_{\text{liq}}} \text{ (MHz/m/s)},
\]

and in photonic

\[
S_{\text{photonic}}^{j} = \frac{\Delta \lambda_{j}}{\Delta n_{\text{liq}}} \text{ (nm/RIU)},
\]

where RIU is the Refractive Index Unit.

Another way widely used in photonic\(^{38}\) to characterize the sensing capabilities is given by the calculation of the figure of merit (FoM), which is the way to take into account the thickness of the peaks through the quality factor

\[
\text{FoM}_{\text{phononic}}^{j} = \frac{S_{j} \times Q_{j}}{f_{j}} \text{ (RIU)}^{-1},
\]

where \(Q_{j} = \frac{\lambda_{j}}{\Delta \lambda_{j}}\) is the photonic quality factor of mode j.

In parallel, one can define an equivalent figure of merit in phononic as follows:

\[
\text{FoM}_{\text{phononic}}^{i} = \frac{S_{i} \times Q_{i}}{f_{i}} \text{ (m/s)}^{-1},
\]

where \(Q_{i} = \frac{\lambda_{i}}{\Delta \lambda_{i}}\) is the phononic quality factor of mode i.

### Table I

<table>
<thead>
<tr>
<th>Molar ratio, (x)</th>
<th>Density (\rho_{\text{liq}}) (kg/m(^2))</th>
<th>Longitudinal sound velocity (c_{\text{liq}}) (m/s)</th>
<th>Refractive index (n_{\text{liq}})</th>
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<tr>
<td>1.000</td>
<td>786.64</td>
<td>1103</td>
<td>1.3268</td>
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</tbody>
</table>
Table II summarizes the results of the sensitivities and FoM calculated for the radii $r/a = 0.15$ and $r/a = 0.35$, with a thickness of the plate of $h/a = 0.25$. One can see that the phononic sensitivity and FoM are almost the same while in photonic the mode $x$ presents higher sensitivity and FoM for the larger radius. We also report the calculations for a thicker plate ($h/a = 0.5$). In both cases, phononic and photonic sensitivities and FoM decrease. One can conclude that the higher efficiency of the dual sensor is obtained for thin plate and large radii (hacked line in Table II).

V. CONCLUSIONS

This contribution shows the dual existence of optical and acoustic enhanced resonances inside silicon phononic and photonic (phoxonic) crystal plate under normal incidence of light and sound. These resonances lead to asymmetric peaks with Fano-like shape in the phononic and photonic transmission spectra for which the origin is totally different. In photonic, the asymmetric resonance comes from the coupling of the incident wave with a guided resonant mode of the dielectric plate. In phononic, the incident wave couples with a mode confined in the holes and due to the water/silicon edges deformation of the cylindrical inclusion. The geometrical parameters of the phononic/photonic crystal have been adapted to define structures in which the peaks of transmission are well-defined and sufficiently isolated from each other. We then showed that this structure can be used as a sensor for separately sense the sound and light velocity of unknown liquids with a high sensitivity to the acoustic/optical parameters of the infiltrating liquid. We demonstrate that the dual phononic and photonic sensor behaves in the same way: an increase of the refractive index velocity leads to a red shift of the eigenmode. We showed that a higher sensitivity and FoM are obtained for larger radius and thinner plate. We then proposed a new class of phononic/photonic sensors which have the possibility to probe light and sound velocity of unknown liquid through a same structure with high sensitivity. Future work will deal with finding the optimal wave-length/frequency scale. Optical sensors including photonic crystal sensors typically work at a few μm whereas only a few acoustic sensors apply the respective GHz frequencies. When going for liquid sensing, a major challenge must be considered which may introduce a frequency limit, viscous damping. Shear waves strongly decay within a few wavelength distance, whereas dissipation of longitudinal waves depends on bulk ($\mu$), and shear viscosity ($\eta$), the ratio of specific heats ($\gamma$), thermal conductivity ($\kappa$), and density ($\rho$) of the fluid. Experimental data of simple liquids are available for frequencies up to 200 MHz. Recently, Holmes et al. have analyzed Millipore water by an acoustic spectroscopy and have proven an expression for the dissipation term in the longitudinal wave number ($\gamma$)

$$\gamma = \frac{\omega^2}{2\rho c^3} \left[ \mu + \frac{4}{3}\eta + \frac{(\gamma - 1)\rho}{c_p} \right].$$

Finally, such structures can also open the way to enhance the phonon-photon interactions with the simultaneous confinement of the phononic and photonic waves. Through the confinement and the interaction between optical and acoustic waves inside mixed phoxonic crystals, we expect the enhancement of the properties of dual sensors.

22B. Cunningham, P. Li, B. Lin, and J. Pepper, Sens. Actuators, B 81, 316 (2002).