

One-dimensional photonic crystals with semiconducting constituents: the effects of the absorption mechanisms

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We have calculated the photonic band structure and the optical properties of two periodic layered systems, air/LiTaO₃ and air/InSb, with the dielectric constant of the semiconducting medium taking into account the phononic contributions. Intrinsic electron and hole densities are also considered for the InSb. In addition to the photonic gaps originated by the structural configuration and the dielectric contrast (gaps by diffraction), there exist photonic gaps of metallic (*polaritonic*) behavior that appear at two frequency regions, just above the transverse phononic frequency and below the effective plasma frequency. We have found that the absorption mechanisms give rise to inflexion points in some bands – the curve of dispersion returns without reaching the Brillouin zone limit. An infinite concentration of non-dispersive bands is found below the polaritonic gap when the absorption is neglected. However, with realistic absorption such infinite series of flat bands disappears, giving place to a finite number of dispersive bands.

Keywords: Photonic band gap; polaritonic; photonic structure; semiconductor.

En este trabajo presentamos un estudio sobre la Estructura de Bandas Fotónicas y las propiedades ópticas de dos sistemas multicapas distintos, aire/LiTaO₃ y aire/InSb, para los cuales la constante dieléctrica del medio semiconductor toma en cuenta las contribuciones fonónicas. Las densidades intrínsecas de electrones y huecos son consideradas para el InSb. Además de las bandas fotónicas prohibidas originadas por la estructura geométrica y contrastes dieléctricos (brechas por difracción) existen bandas fotónicas prohibidas debido a la naturaleza metálica (polaritónica) de los componentes semiconductores. Estas brechas existen en dos regiones de frecuencias, a valores mayores de la frecuencia de resonancia fonónica y para valores menores de frecuencia de plasma efectiva. Hemos encontrado que los mecanismos de absorción dan lugar a puntos de inflexión en algunas bandas los cuales no llegan al límite de la primera zona de Brillouin. Por otra parte, para el caso en que no existe absorción, hemos encontrado una concentración infinita de bandas no dispersivas. Estas bandas están por debajo de la banda prohibida polaritónica. Sin embargo, cuando se considera un sistema realista en donde se incluyen los efectos de absorción del material semiconductor, la dispersión en las bandas da lugar a un número finito de bandas.

Descriptores: Brecha de banda fotónica; semiconductores; estructura fotónica; polariton.

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Recently it has been demonstrated that the introduction of metallic or semiconducting materials as photonic crystal (PC) constituents can lead to new physical phenomena due to the possible coexistence of photonic gaps, phononic vibrations and plasmonic oscillations [1,2]; it means that the photonic band structure (PBS) of an otherwise pure dielectric PC could be enriched by the presence in the constitutive materials of an intrinsic optical phononic gap ($\omega_T < \omega < \omega_L$) and an intrinsic metallic gap ($\omega < \omega_p$). Examples of some new phenomena reported recently for PC's constructed with polar materials are the *node switching* (the nodes of the field pattern of the electromagnetic modes are polarization-dependent) and the *flux expulsion* (the frequency transition across a polariton gap edge induces an expulsion of fields from the polaritonic medium to the surrounding dielectric) [3].

Thus, it is possible to separate in two types the band gaps observed in PC's having a semiconducting component: in frequency ranges where the semiconductor's dielectric constant is real and positive, photonic gaps arise due to the dielectric contrast, lattice symmetry and filling fraction – they are gaps that result exclusively due to diffraction effects. On the other hand, at frequencies where the semiconducting dielec-

tric constant becomes complex, with negative real part, *polaritonic* band gaps appear. Because of the intrinsic dispersion of the semiconducting medium is naturally accompanied by losses, the band structure of these PC's is complex.

Detailed study of the interaction between ordinary and polaritonic gaps was made recently by Ribbing *et al.* [4]. For 1D PC's they found that the characteristics of the polaritonic gap in the reflection spectrum depend strongly on the material at the top layer in the finite sample (they used a SiO₂/Si multilayer). On the other hand, Huang *et al.* have formulated a complete theory for describing complex states of real frequency Ψ_ω (with complex wave vector) and real wave vector Ψ_k (with complex frequency) [3]. Within this theory the spatial and temporal decays – described with the real ω and real k configurations, respectively – in lossy PC's were found related by the group velocity. More recently Gantzounis and Stefanou studied the optical response of two and three dimensional polaritonic PC's [5,6]. For an array of cavities in polar semiconductor they found strong resonances involving flat-surface and cavity phonon polaritons.

In this paper we describe the optical properties of two lossy 1D polaritonic PC's. We have chosen LiTaO₃ and InSb

as semiconducting components. The dielectric medium is air. Our goal is to show the strong effects produced by the semiconductor losses on the PBS. Beyond the results previously presented by several authors, we shall demonstrate the occurrence of a PBS *collapse* at the frequency region near and inside the polaritonic gap (the losses destroy the interference mechanisms which are responsible of the PBS). We define this phenomenon as PBS collapse). Consequently, we think that various phenomena predicted by other authors (as the node switching and flux expulsion above mentioned) should be reconsidered. All our calculations (photonic band structures and transmission spectra) were made with the well-known transfer matrix method.

Let us begin by presenting the dielectric function $\varepsilon(\omega)$ of the two semiconducting materials under consideration. From Solid State Theory [10] we know that a good representation for $\varepsilon(\omega)$ of polar semiconductors in the infrared region that takes into account the phonon dispersion is

$$\varepsilon(\omega) = \varepsilon_\infty \left(1 + \frac{\omega_L^2 - \omega_T^2}{\omega_T^2 - \omega^2 - i\omega\gamma} \right), \quad (1)$$

where ω_L and ω_T are the longitudinal and transverse optical phonon frequencies and γ is the damping constant for phonons. Equation (1) shows that in absence of absorption the dielectric constant diverges at $\omega = \omega_T$ and becomes zero at $\omega = \omega_L = \omega_T \sqrt{\varepsilon_0/\varepsilon_\infty}$ where ε_0 and ε_∞ are the static and optical dielectric constants, respectively.

On the other hand, for frequencies at the far infrared region mobile electrons and holes can also contribute to the optical response of a semiconductor. Following the *plasma model* presented in Ref. 7 one can define the plasma frequencies ω_{pe} and ω_{ph} as $\omega_{pe,h}^2 = 4\pi n_{e,h} e^2 / m_{e,h} \varepsilon_\infty$, where $n_{e,h}$ and $m_{e,h}$ are the intrinsic concentration and mass of electrons and holes, respectively. With the plasma contribution in account, the dielectric function takes the form

$$\varepsilon(\omega) = \varepsilon_0 \left(1 + \frac{\omega_L^2 - \omega_T^2}{\omega_T^2 - \omega^2 - i\omega\gamma} - \frac{\omega_{pe}^2}{\omega(\omega + i/\tau_e)} - \frac{\omega_{ph}^2}{\omega(\omega + i/\tau_h)} \right), \quad (2)$$

where $\tau_{e,h} = m_{e,h} \mu_{e,h} / e$ are the collision times which are written in terms of the carrier mobilities $\mu_{e,h}$.

Equations (1) and (2) are appropriate for semiconducting materials of large and small electronic band gap, respectively. For wide band gap semiconductors electronic transitions demand lasers of high energy. Thus the creation of holes in the valence band by electron transitions into the conduction band can be ignored at the infrared region and the optical properties of these materials are mainly related to the longitudinal and transverse optical phonons. This is the case of ferroelectric materials as the Lithium Tantalate (LiTaO_3) which at room temperature and crystalline phase has a gap $E_g \sim 8$ eV [8], with optical phonon frequencies $\omega_L = 294.7$ THz and $\omega_T = 167.7$ THz [9].

On the other hand, electronic transitions between valence and conduction bands are easier in semiconductors of small gap. As an example we can mention the Indium Antimonide (InSb) of gap $E_g = 0.17$ eV [10]. Because of this small gap, electron and hole plasmas can coexist with phononic vibrations at frequencies of THz or beyond. The corresponding longitudinal and transverse frequencies are $\omega_L = 37$ THz and $\omega_T = 35$ THz.

In what follows we shall present results for air/ LiTaO_3 and air/InSb 1D PC's involving Eqs. (1) and (2) in calculations. The numerical parameters associated to absorption that we use were published in Refs. 3 and 7. In order to know the polaritonic gaps in these materials, we begin presenting in Fig. 1 the real and imaginary parts of the two respective bulk dielectric functions. Note the existence of a relative wide polaritonic gap in LiTaO_3 with lower edge at 167 THz; 132 THz below the InSb presents, contrarily, a small polaritonic gap.

Qualitatively the main difference between both materials is the occurrence of a metallic-like gap at low frequencies (< 10 THz) in InSb.

As is expected these gaps will define in much the characteristics of the PBS of the two multilayers under consideration. For the air/ LiTaO_3 system we made calculations

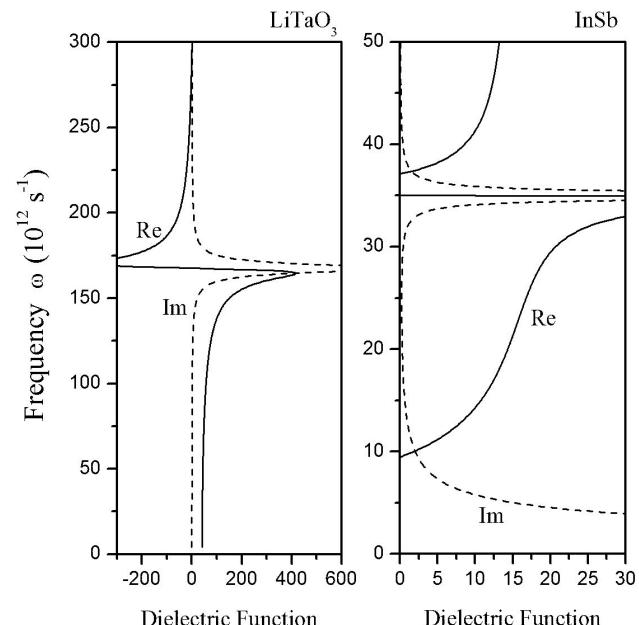


FIGURE 1. Dielectric functions of the two semiconductor materials considered in this paper as PC components.

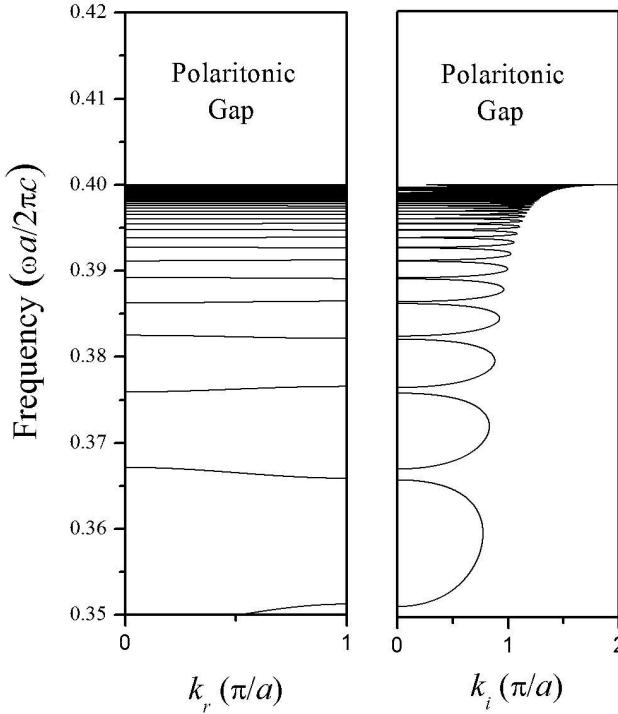


FIGURE 2. Resonant type solutions for the Air/LiTaO₃ 1D PC. This is an infinite number of planar bands. The bands are closer (the band gaps are smaller) as the frequency approaches to ω_T .

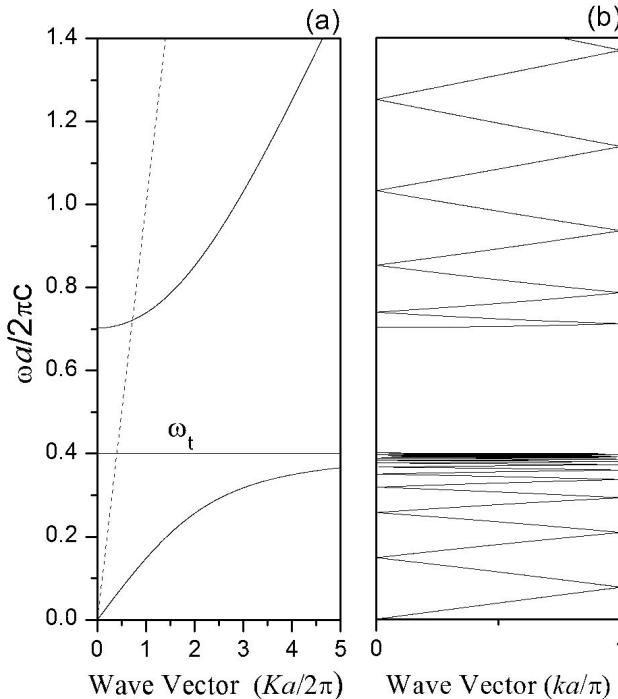


FIGURE 3. a) Dispersion relation of the optical phonons in LiTaO₃. The wave vector K takes values from zero to infinite. b) Projection of the dispersion relation on the 1D Brillouin Zone. The Bloch wave vector k goes from zero to π/a .

with structural parameters $a = 4.5\mu\text{m}$ and $f = 0.5$, the lattice parameter and the filling factor, respectively. Ignoring

absorption effects, the photonic bands in the region of low frequencies takes the form of those for an ordinary dielectric PC. The most interesting behavior occurs near the polaritonic band gap edges. Figure 2 shows the existence of a quasi-planar band series just below ω_T (in order to incorporate the lattice parameter we introduce the reduced frequency $\Omega = \omega a/2\pi c$. Thus, in Fig. 2 $\Omega_T = \omega_T a/2\pi c = 0.4$). This result can be easily understood; in bulk semiconductors the dispersion relation $k(\omega)$ of optical phonons below the polaritonic gap increases monotonously with decreasing positive slope and converges asymptotically to Ω_T [10], (See Fig. 3a). By following the idea of a band structure associated to a *vacuum* lattice, we can over impose a 1D periodic lattice on the infinite homogeneous semiconductor. Consequently the phonon dispersion curve can be projected into the corresponding first Brillouin zone; of course, no band gaps below the polaritonic gap will appear – the medium continues being homogeneous – but a series of bands more and more planar are observed as the frequency approximates to Ω_T , (see Fig. 3b). Then, when the air layers are introduced to form the 1D PC the gaps due to the periodicity appear affecting slightly the curvature of these bands. (This interpretation has been ignored by other authors when they have described similar photonic bands)[3].

On the other hand but still for the air/LiTaO₃ system, at frequencies just above the upper gap edge the bands behave

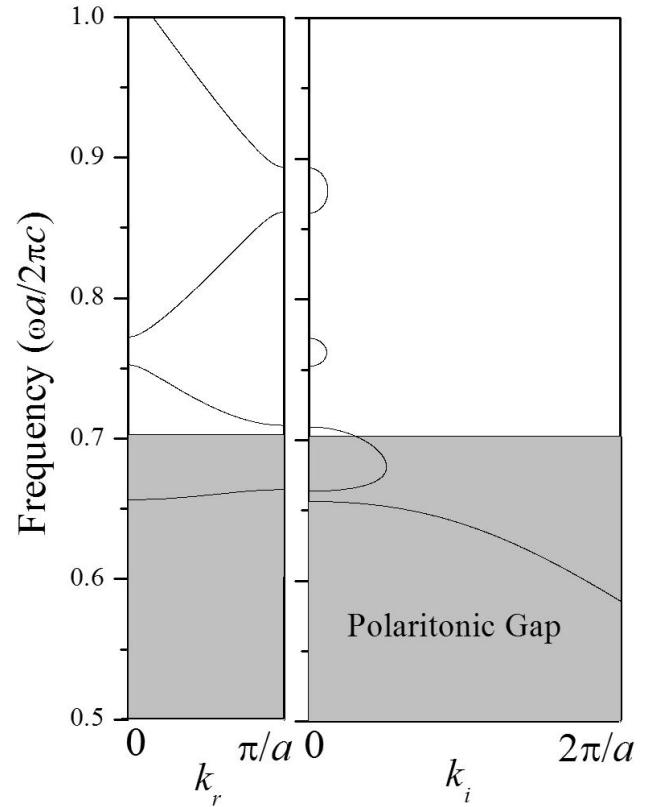


FIGURE 4. Nonabsorbent band structure at frequencies near the upper polaritonic gap edge for the Air/ LiTaO₃ PC. In contrast to what it happen at the lower gap edge (see Fig. 2), here resonant solutions do not exist.

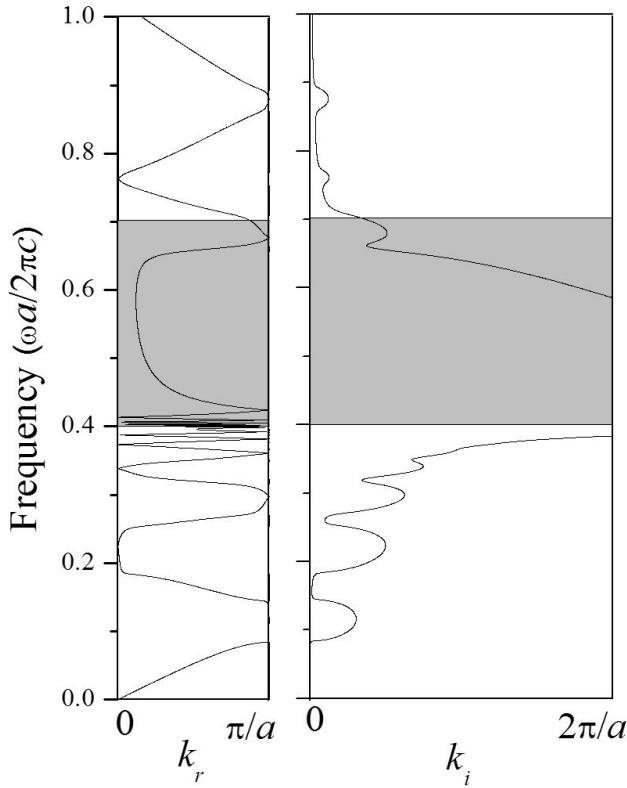


FIGURE 5. The complex band structure of a realistic absorptive Air/LiTaO₃ PC. Note that resonances penetrate slightly into the polaritonic gap.

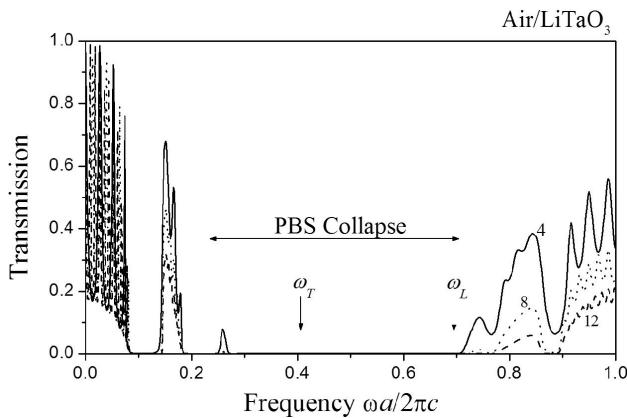


FIGURE 6. The photonic band structure *collapse* of the Air/LiTaO₃ PC. Transmission of light through PC samples of 4, 8 and 12 unit cells are shown. Note that above the second gap and below the polaritonic gap, practically for the three samples, the wave transmission is insensitive to the band structure.

completely different (See Fig. 4). Resonance-type solutions (flat bands) are not observed. Again the reason of this behavior is found in the own characteristics of the optical phonons in the bulk semiconductor in which the curve of phononic dispersion changes monotonously with increasing slope as K increases (See Fig. 3). At $K=0$ the curve begins at frequency $\Omega \sim \Omega_L$ with slope almost zero. For higher frequencies this

curve converges asymptotically to the light-line of the homogeneous medium of dielectric constant ε_∞ . Again by inserting the air layers to form the 1D PC the periodicity projects this curve into the Brillouin Zone and the gaps by diffraction appear.

As Fig. 4 shows, surprisingly a single small band exists inside the polaritonic gap. The mid-frequency of this curve is $\Omega_s \sim 0.66$. We know that within the polariton gap only modes with fields decaying exponentially inside the LiTaO₃ layers can exist. Thus this band has to do with modes of fields evanescent inside the semiconducting layers but oscillatory in the air layers.

In order to explore the properties of the Air/LiTaO₃ system in a more realistic context we now include the absorption effects. Figure 5 shows the corresponding band structure (we are using $\gamma = 5.9$ THz) [9]. As is expected the bands near the polaritonic gap become absorbents. A finite imaginary wave vector indicates that the amplitude decays as the wave propagates through the PC - the higher the imaginary vector, the shorter the wave penetration. For example for the third allowed band centered at $\Omega = 0.26$ we found the imaginary wave vector $k_i \sim \pi/7a$; thus the penetration distance is $z \sim 2.2a$. It means that light with this frequency impinging on a finite PC sample will be absorbed almost completely already at the third cell.

The same as for the nonabsorbent approximation discussed above, the existence of (very absorbent) bands inside the polaritonic gap can be explained analyzing the dispersion relation of the bulk optical phonons in presence of absorption. As is well known in such case the lower phononic curve goes back crossing the phononic transverse resonance; then, by increasing the frequency, the curve almost reaches $K = 0$ returning again, crossing the longitudinal resonance. For higher frequencies the curve follows the corresponding dispersion curve of the non absorbing approximation. Thus the band structure shown in Fig. 5 results from the projection of this continue dispersion curve into the Brillouin zone. Then the air layers introduce diffraction effects that lead to the creation of appreciable band gaps only at frequencies below and above away from the polaritonic gap.

The effects of absorption are crucial in practical applications. Figure 6 shows the transmittance profiles for PC samples of 4, 8 and 12 unit cells. Note that only the two lower bands and the two higher bands allow energy transmission for the thicker samples. In fact already for 4 cells the PBS *collapses* at frequencies near and inside the polaritonic gap. So, it is useless to perform experiments sensitive to transmission near the polaritonic band edges.

We now describe the absorption effects in the air/InSb 1D PC. For frequencies near and inside the polaritonic gap (which is rather small) the physics is the same that in the previous case. Therefore we focus the discussion on the bands inside or near the metallic-like gap. Figure 7 shows that below the effective plasma frequency $\Omega_p = 0.2$, defined by the frequency at which the real part of the InSb dielectric constant becomes zero (crossing from negative to positive val-

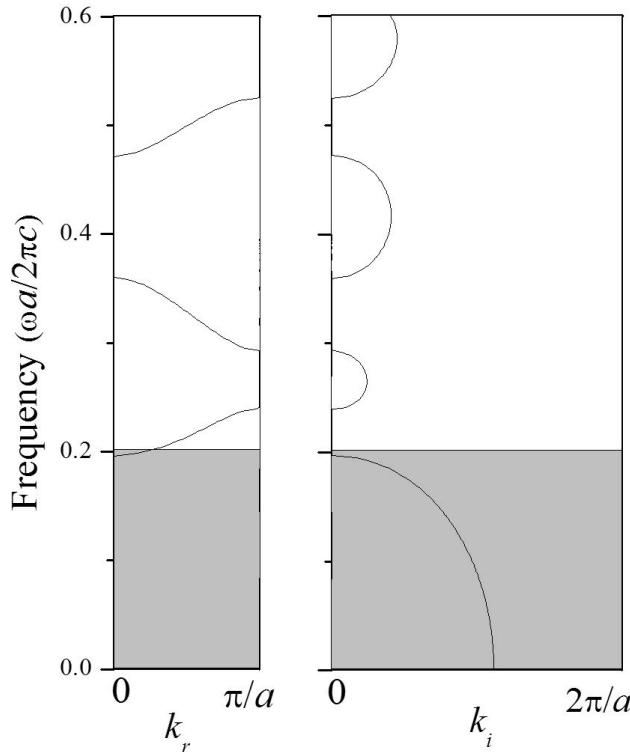


FIGURE 7. The complex photonic band structure for the Air/InSb nonabsorbent photonic crystal. The lattice parameter and the filling factor are $a = 40 \mu\text{m}$ and $f = 0.5$. Note that the maximum imaginary wave vector is reached at the static limit.

ues), without absorption only an imaginary wave vector exist. The first allowed band begins at Ω_p .

What could be the most interesting behavior occurs when absorption is included: inside the gap the maximum of the imaginary wave vector moves to a finite frequency (not zero) and the real wave vector shows a *backbending* effect (See Fig. 8). All the band structure becomes complex. Figure 9 shows that acceptable behavior of this multilayer as a PC is found in two frequency regions. For example a very good window could be the range $0.38 < \Omega < 0.62$. The *worst* frequency regions are those inside or near the polaritonic and metallic-like gaps.

It is important to remark the effect of losses on the photonic band inside the metallic-like gap. We note that in the limit of very low frequencies the diffraction condition is diminished by the absorption - absorption breaks in part the formation of stationary waves. For this reason in Fig. 8 the imaginary wave vector goes down at frequencies below than 0.05 on the scale of the figure. However, in spite of this reduction, k_i remains sufficiently high avoiding transmission of electromagnetic energy in finite samples as is shown in Fig. 9. This breaking of diffraction can be also inferred from the behavior of the real wave vector component. For frequencies below the point of bending (0.015 in the scale of Fig. 8) the lossy PC supports the formation of an allowed band (of very small slope). By increasing the frequency the diffrac-

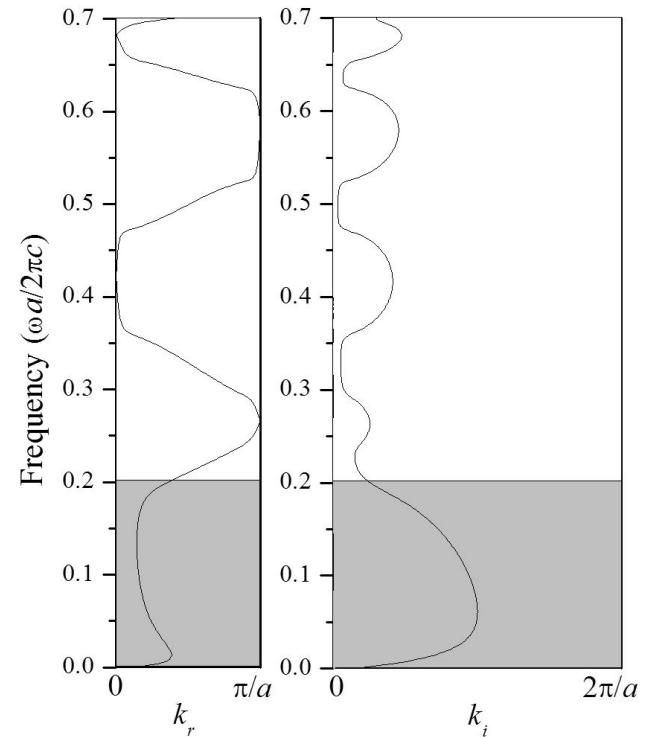


FIGURE 8. The complex photonic band structure for the Air/InSb absorbent photonic crystal. The imaginary wave vector becomes finite for all the allowed bands; due to the absorption the waves decay as they penetrate into the PC.

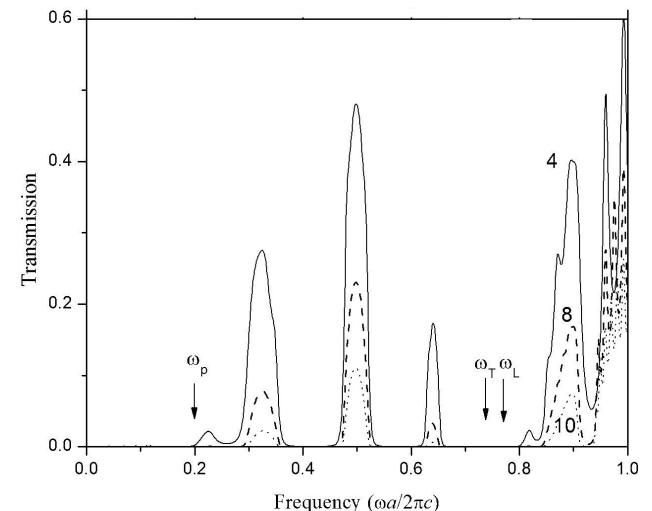


FIGURE 9. Transmission spectra for finite Air/InSb PC samples of 4, 8 and 10 cells. The first allowed photonic band with frequencies just above ω_p practically disappears for the three samples. However the PC has a good response in the range $0.25 < \omega a/2\pi c < 0.6$ for samples of 4 and 8 cells.

tion effects become more and more significant. As if it had reached the zone limit, the curve goes back in such way that the band structure for higher frequencies (but still inside the gap) almost recuperates the form of the non absorbent case.

At the light of this result and other we can conclude that absorption (diffraction) has the most significant weight in the interplay diffraction-absorption at low (high) frequencies inside the metallic-like gap.

Due to the strong absorption this interplay could be seen as an interesting and curious result because it is hard to detect experimentally the backbending effect. However for surface physics the effect could take relevance. As is well known the diffraction mechanisms are responsible of the fields confinement at the PC surface. Thus any perturbation of diffraction should be reflected in the surface response. Consequently the surface polaritonic waves in the low frequency region could acquire new structure and support novel leaky mechanisms.

In summary, we have investigated the role played by the losses in polaritonic PC's. For the two system studied we have described the collapse of the band structure corresponding to the otherwise dielectric PC – the same polaritonic PC but ignoring the absorption effects. Transmission calculations demonstrate that only reduced frequency ranges pre-

serve the quality of a PC with allowed and forbidden bands well defined. Consequently these polaritonic PC's could be used for applications in short ranges of frequencies. On the other hand, as is expected the loss mechanisms affect the conditions for creation of stationary oscillations; consequently the band gaps in the PC are modified. Particularly inside the metallic-like gap the interplay absorption-diffraction leads to a backbending behavior of the photonic band. This effect could be of interest for surface physics of PC's. Finally, we remark that any application or new physics reported for lossy polaritonic PC's must be reconsidered because we have found with the most realistic parameters available in the literature that absorption practically erases the photonic band structure at frequencies nearby the polaritonic band gaps.

Acknowledgments

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1. A. Rung and C.G. Ribbing, *Phys. Rev. Lett.* **92** (2004) 123901.
2. Kerwyn Casey Huang, P. Bienstman, J.D. Joannopoulos, K.A. Nelson, and Shanhui Fan, *Phys. Rev. B* **68** (2003) 075209.
3. Kerwyn Casey Huang *et al.*, *Phys. Rev. B* **69** (2004) 195111.
4. C.G. Ribbing, H. Högström, and A. Rung, *Appl. Opt.* **45** (2006) 1575.
5. G. Gantzounis and N. Stefanou, *Phys. Rev. B* **72** (2005) 075107.
6. G. Gantzounis and N. Stefanou, *Phys. Rev. B* **75** (2007) 193102.
7. A.S. Sánchez and P. Halevi, *J. Appl. Phys.* **94** (2003) 797.
8. Shigemi Kohiki, Massao Arai, Hideki Yoshikawa, and Sei Fukushima, *Phys. Rev. B* **57** (1998) 14572.
9. Kerwyn Casey huang, M.L. Povinelli, and J.D. Joannopoulos, *Appl. Phys. Lett.* **85** (2004) 543.
10. C. Kittel, *Introduction to Solid State Physics* (Sixth Edition, Wiley, New York, 1986)