Planar defects in photonic crystals

1994 J. Phys.: Condens. Matter 6 6257

(http://iopscience.iop.org/0953-8984/6/31/025)

J. Phys.: Condens. Matter 6 (1994) 6257–6264. Printed in the UK

Planar defects in photonic crystals

V Karathanos†, A Modinos† and N Stefanou‡

† Department of Physics, National Technical University of Athens, Zografou Campus, GR-157 80, Athens, Greece

‡ Solid State Section, University of Athens, Panepistimioupolis, GR-157 84, Athens, Greece

Received 10 February 1994

Abstract. We establish the existence of an absolute frequency gap of the electromagnetic field in photonic crystals with tetragonal symmetry, and examine the dependence of the gap on the geometry of the structure. We calculate the transmittance through a slab of finite thickness of the material, and show that planar defects in the slab produce interface states of the electromagnetic field, at frequencies within the photonic gap, manifested by sharp resonances in the transmittance of these systems

1. Introduction

The optical properties of photonic crystals—composite media consisting of units arranged in a host material with a different dielectric function—have been discussed by a number of authors in recent years (see [1] and references therein), following the suggestion by Yablonovitch [2] that such media may have interesting applications in the field of optoelectronics. The first theoretical papers [3, 4] aimed at the calculation of the spectrum of eigenfrequencies of the electromagnetic (EM) field in a given medium, and as a result of these calculations we know, already, that photonic crystals with absolute gaps in the optical region of the spectrum are possible. It is the existence of these gaps (analogous to the energy gaps of electrons in semiconductors) which promise important technological applications. It turns out that ordinary semiconductors have a sufficiently high refractive index for this purpose, which is indeed fortunate, and one expects that the technology of actually manufacturing these crystals will be achieved in good time [1]. So far, verification of the theory comes from experiments in the microwave region and a scaling argument: the equations depend on the ratio of the lattice constant to the wavelength of the photon and not on the magnitude of one or the other of these quantities.

The experiments measure the reflection and transmission of light incident at an angle on a slab of the photonic crystal and, therefore, for a complete analysis of such experiments one should be able to evaluate these quantities. A method for doing this has been described by us in a previous paper [5]. Our method assumes that the crystal consists of non-overlapping spheres in a medium of different dielectric function. The formalism constitutes an extension of multiple-scattering techniques developed in relation to the theory of low-energy-electron diffraction by ordinary crystals. A method which avoids the specific assumption as to the shape (spherical in our method) of the scatterers has been published by Pendry *et al* [6].

In the next section we describe a crystal which exhibits an absolute photonic gap and examine the dependence of the gap parameters on the geometry of the crystal. We view the crystal, or a slab of it, as a succession of layers parallel to a given crystallographic plane. Each layer may consist of one or more planes of spheres, and in the case to be considered,

0953-8984/94/316257+08$19.50

it consists of two such planes. Within the formalism of [5] it is relatively easy to vary the distance between the layers normal to the surface and we have taken advantage of this possibility in order to examine the dependence of the gap parameters on this variation.

It is also easy, within the formalism of [5], to replace the spheres of one particular plane by spheres of different size or different dielectric constant and in this way to introduce into the system a planar defect. As a result, one obtains, as we shall demonstrate in section 3, a band of interface states of the EM field corresponding to frequencies within the frequency gap of the crystal, which in turn gives rise to sharp resonances of the transmission coefficient for light incident at a given angle on the slab of the material.

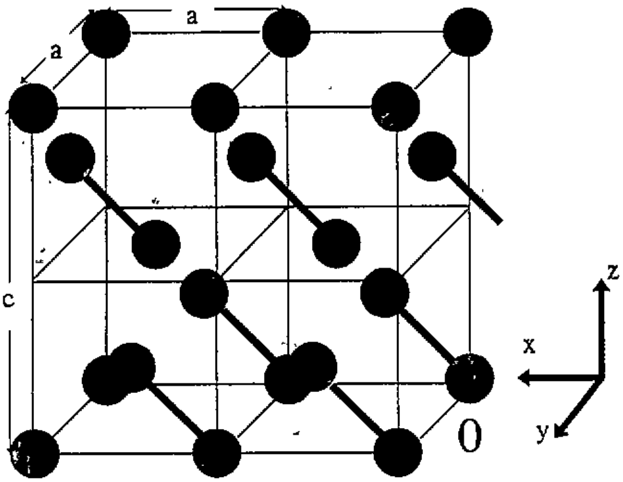

Figure 1. The crystal seen as a stack of layers parallel to the xy plane. Each layer consists of two planes of spheres.

2. Photonic gaps in diamond-like structures

We view the crystal (see figure 1) as a stack of layers parallel to the xy plane. The periodicity of the layers parallel to this plane is described by a two-dimensional (2D) square lattice defined by the primitive vectors

$$a_1 = (a, 0, 0) \qquad a_2 = (0, a, 0)$$

and the two-point basis, at $(0, 0, 0)$ and $(a/2, 0, c/4)$, defines the two planes of a layer. The $(n+1)$th layer along the z axis is obtained from the nth layer by a simple translation described by the primitive vector

$$a_3 = (a/2, a/2, c/2).$$

The diamond structure is obtained by putting $c = a\sqrt{2}$. As we have already noted in the introduction, we used the ratio c/a as a variable parameter in our calculations. When the ratio c/a is different from $\sqrt{2}$ the structure changes from diamond to a centred tetragonal

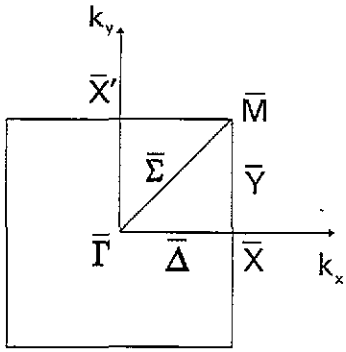

Figure 2. The surface Brillouin zone of the crystal (xy plane).

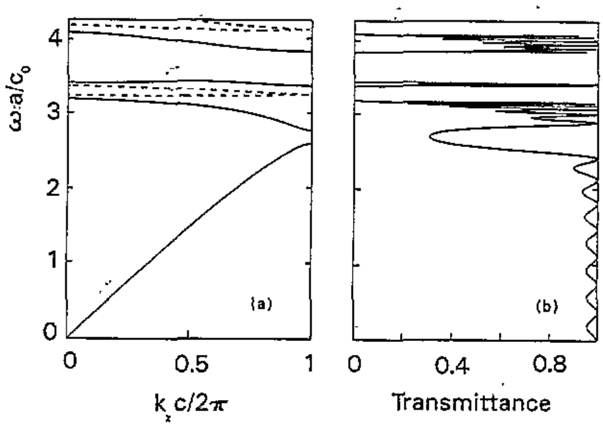

Figure 3. (a) Frequency bands, for $k_\parallel = 0$, in a crystal of tetragonal structure ($c/a = 1.7$) consisting of non-overlapping spheres ($\epsilon_M = 12.96$) in a medium of dielectric constant equal to unity. c_0 denotes the velocity of light. (b) Transmittance of light incident normally on a slab of the crystal consisting of eight layers.

lattice with the two point basis at $(0, 0, 0)$ and $(a/2, 0, c/4)$. In all cases the 2D reciprocal lattice and the surface Brillouin zone (SBZ) are the same. The latter is shown in figure 2.

We calculated the photonic complex band-structure for $\boldsymbol{k}_\parallel = (k_x, k_y)$ along the symmetry lines of the SBZ and at selected points elsewhere in the zone, in the manner described in [5]. For given $\boldsymbol{k}_\parallel$, we obtained the real frequency lines, $k_z(\boldsymbol{k}_\parallel, \omega)$, which are functions of ω, with real values of k_z over certain regions of ω and complex values elsewhere. The sections of real $k_z(\boldsymbol{k}_\parallel, \omega)$ of these lines correspond to the normal modes of the EM field, which are, of course, propagating Bloch waves in the given (infinite) crystal. We remember that the reduced $\boldsymbol{k}$ zone corresponding to this crystal is given by $\boldsymbol{k} = (\boldsymbol{k}_\parallel, k_z)$, with $\boldsymbol{k}_\parallel$ in the SBZ and $-|b_3|/2 < k_z \leqslant |b_3|/2$ where $b_3 \equiv 2\pi \boldsymbol{a}_1 \times \boldsymbol{a}_2/\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)$. Values of $\boldsymbol{k}$ outside this zone lead to the same set of normal modes.

In figure 3(a) we show the frequency bands for $\boldsymbol{k}_\parallel = 0$, of a crystal with tetragonal structure ($c/a = 1.7$) consisting of spheres of dielectric constant $\epsilon_M = 12.96$ and radius $S = 0.265a$ in a host of dielectric constant equal to unity. They correspond to the real k_z sections of the real frequency lines $k_z(\boldsymbol{k}_\parallel = 0, \omega)$. The transmittance of light incident normally on a slab of the crystal consisting of eight layers is drawn next to the frequency band-structure (figure 3(b)) in order to establish the relation between the two: the transmittance practically vanishes or is very small for frequencies within gaps and is non-zero for frequencies within bands that couple to the incident field. The small transmittance for frequencies within the lowest gap is due to the fact that the imaginary part of the $k_z(\boldsymbol{k}_\parallel = 0, \omega)$ which determines the attenuation is quite small in this case leading to an attenuation length comparable with the thickness of the slab. The broken lines in figure 3(a) correspond to normal modes of the EM field in the crystal which are not activated by the incident radiation and, therefore, do not allow for the transmission of light. For an explanation of this phenomenon see [5].

We have obtained the frequency bands for points along the symmetry lines of the SBZ and other points as well. From these we obtained the frequency gaps for each $\boldsymbol{k}_\parallel$ and eventually the projection of the photonic band-structure on the SBZ shown in figure 4. The shaded areas correspond to frequency gaps, i.e. regions of frequency where propagating EM waves cannot exist in the crystal. We see that for the given structure there is a region of frequency within which no propagating wave is allowed in the crystal whatever the value of $k_{\|}$. This absolute gap extends over a region $\Delta\omega_G$ around the midgap frequency ω_{MG}.

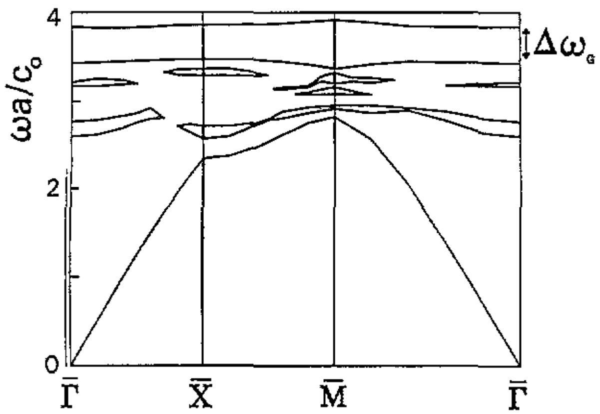

Figure 4. Projection of the photonic band-structure on the SBZ. The gaps in the frequency spectrum are represented by the shaded areas. We observe the existence of an absolute gap of width $\Delta\omega_G$.

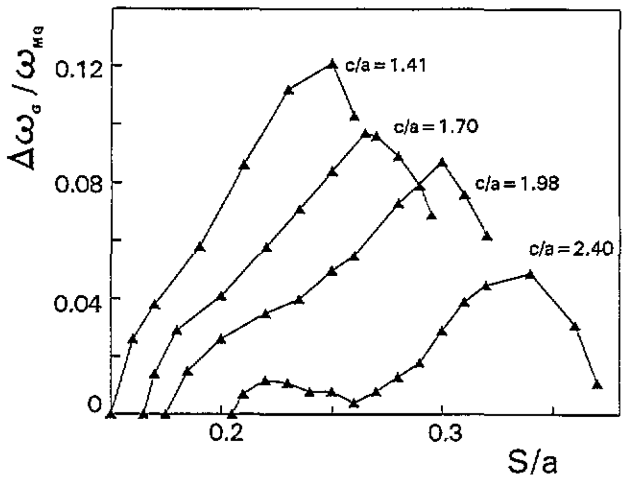

Figure 5. Variation of $\Delta\omega_G/\omega_{MG}$, of the absolute gap, with c/a and S/a.

We have done the same calculation for different values of the ratio c/a and for different values of S/a. The results are shown in figure 5. We see that for given c/a the ratio $\Delta\omega_G/\omega_{MG}$, which characterizes the gap, has a maximum when plotted against S/a, and that this maximum gets larger as we approach the diamond structure.

3. Interface states due to planar defects

In the remaining part of this paper we look at the optical properties of a slab of the crystal when a planar defect exists within the slab. The planar defect may arise either because the spheres of a particular plane are different from those in the rest of the slab, or because of the introduction of a layer of host material at some position in the slab, this being equivalent to separating the slab into two halves and moving the two apart, along the z direction. In figure 6 we show the transmission coefficient of light incident normally on a slab which

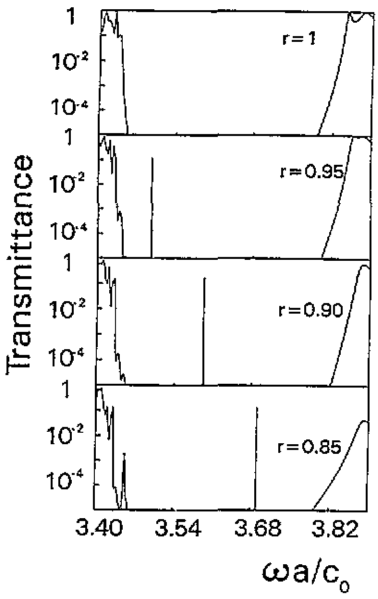

Figure 6. Transmission coefficient of light incident normally on a slab of nine layers. The spheres of the second plane of the fifth layer have a radius S_i which differs from the radius S of all other spheres in the slab, $S_i = rS$.

has the tetragonal structure ($c/a = 1.7$) of figure 1. The slab consists of nine layers of spheres and all spheres have the same radius $S = 0.265a$, except those of the second plane of the fifth layer (we count as first the layer on which the light is incident) which have a smaller radius S_i. We refer to this plane as the impurity plane. All the spheres in the slab, including those of the impurity plane, have the same dielectric constant $\epsilon_M = 12.96$. The dielectric constant of the host material equals unity. We see that a sharp resonance in the transmittance curve appears within the gap and that this moves to higher frequencies the smaller the radius of the impurity spheres. We infer from this, the existence of interface states of the EM field (states localized on the impurity plane) with reduced wavevector $k_{\parallel} = 0$, whose eigenfrequency within the photonic gap corresponds to the above resonance. It appears that a reduction in the region of higher dielectric constant within the unit cell of the photonic crystal pushes out of the lower band of frequencies and into the gap one or more states (normal modes) of the crystal. If we had an isolated impurity sphere, a 'pushed-up' state would have been localized on that impurity. In this respect the phenomenon is analogous to the introduction of acceptor-type impurities into a semiconductor, where the introduction of a 'less attractive' centre in place of an existing one, leads to the splitting of a state off the valence band. In our example we do not have isolated impurity spheres but an impurity plane, and we expect a band, or bands, of interface states to be associated with it. Moreover we expect a dispersion of these bands because of multiple scattering within the plane. This is indeed the case as seen from figure 7. The dispersion curves of this figure were obtained from corresponding transmittance curves of light incident on a slab of the crystal at an angle corresponding to certain $k_{\parallel}$. The bands denoted by 's' are activated by incident light which is s-polarized (the electric field is parallel to the plane of the spheres), and the band denoted by 'p' is activated by p-polarized incident light (the electric field lies in the plane of incidence and has a component normal to the plane of the spheres).

We have also calculated the transmittance of light through a slab consisting of eight layers separated into two halves (four layers in each) and pushed a distance d apart along the z direction. The space created between the two halves is taken by host material. The results of our calculations are shown in figure 8. The sharp resonances in the transmittance

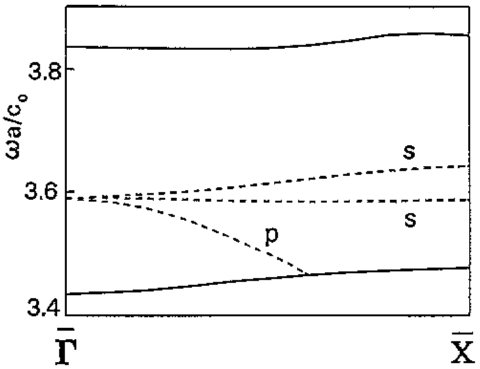

Figure 7. Bands of interface states (localized on the impurity plane of a nine-layer slab) along the $\bar{\Gamma}\bar{X}$ symmetry line. These are shown by broken lines. The solid lines represent the edges of the frequency gap. The slab is constructed as in figure 6 with $r = 0.9$.

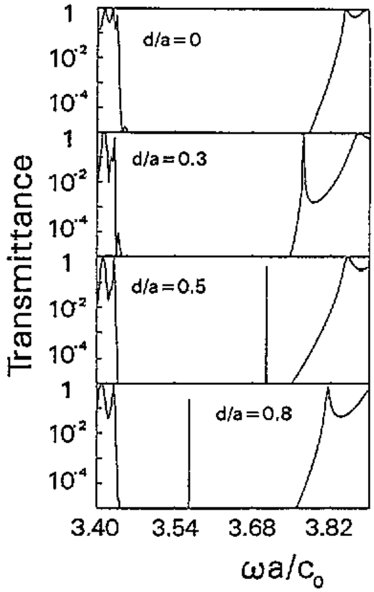

Figure 8. The transmission coefficient of light incident normally on a slab of eight layers separated in two halves and pushed a distance d apart along the z direction. The space created between the two halves is taken by host material.

curve are due, in this case, to modes of the EM field localized within the host layer. We observe that in this case the resonance frequency goes down as the width of this layer increases. The host layer acts as a 'potential well' with the two half-slabs on either side of it acting as mirrors to the photon field. A comparison between figures 6 and 8 suggests that in the case of the impurity plane the EM field in the resonance mode resides mostly within the impurity spheres (a region of high dielectric constant) in contrast to the host-layer resonance where, obviously, the field resides almost entirely within the host layer region ($\epsilon = 1$). In figure 9 we show the dispersion of the corresponding interface bands along the $\bar{\Gamma}\bar{X}$ and $\bar{\Gamma}\bar{X}'$ directions. We note that the structure under consideration does not have the symmetry of the structure described in figure 1. In particular, rotation by 90° about the z axis followed by reflection with respect to an xy plane is not a symmetry operation for the new structure. This means that the transmittance curve for incident light with $\boldsymbol{k}_{\|}$ along the $\bar{\Gamma}\bar{X}'$ direction is not the same as that with $\boldsymbol{k}_{\|}$ along $\bar{\Gamma}\bar{X}$. Similarly, the dispersion curves along the $\bar{\Gamma}\bar{X}$ and $\bar{\Gamma}\bar{X}'$ directions are different. The dispersion curve marked 's' is activated by s-polarized light, incident with $\boldsymbol{k}_{\|}$ along the $\bar{\Gamma}\bar{X}'$ direction. The curve marked 'p' is activated by p-polarized light, incident with $\boldsymbol{k}_{\|}$ along the $\bar{\Gamma}\bar{X}$ direction. The symmetry broken by the host layer is such that, had we chosen to cut the slab between the two planes of a layer, rather than between two layers of the crystal (as defined in section 1), we would have obtained similar results, but with $\bar{\Gamma}\bar{X}$ and $\bar{\Gamma}\bar{X}'$ directions interchanged.

We thought it worthwhile to compare the above results for the photonic crystal with the corresponding results for a stratified medium, i.e. a 1D periodic array of layers, homogeneous in the xy plane. The optical properties of such systems have been studied extensively [7] and we know that an absolute photonic gap can not exist in such systems. However, for a given value of $\boldsymbol{k}_{\|}$, corresponding to an angle of incidence on a slab of the material,

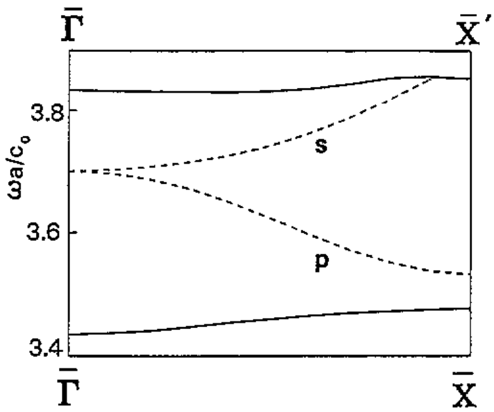

Figure 9. Bands of interface states, localized within the host layer region of the slab defined in figure 8 when $d = 0.5a$. The bands are shown by the broken lines. The solid lines represent the edges of the frequency gap.

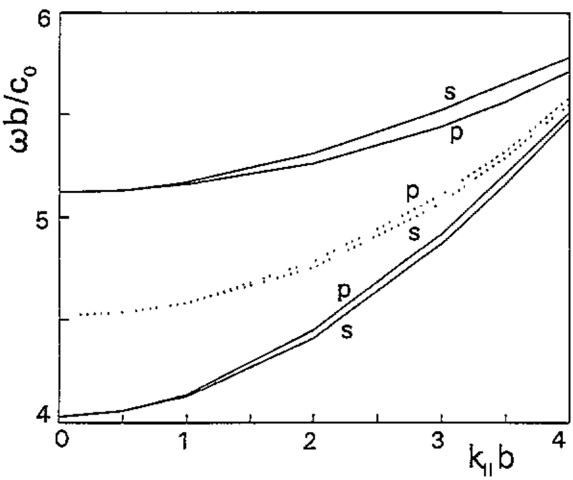

Figure 10. The frequency gap as a function of $k_\parallel$. The solid lines represent the edges of this gap for s- and p-polarized light. The dotted lines show interface states localized on an impurity layer within a slab of the material.

a gap may exist. This is demonstrated in figure 10. The unit-cell layer, of thickness b, of the system under consideration consists of two sublayers of thickness $d_1 = 0.15b$ and $d_2 = 0.85b$ and dielectric constants $\epsilon_1 = 12.96$ and $\epsilon_2 = 1$ respectively. The solid lines in this figure represent the lower and upper limits of the frequency gap as a function of $k_\parallel$ for s- and p-polarized light. The dotted lines show resonance frequencies within the gap, which appear when the fifth layer of a nine-layer-thick slab is replaced by an impurity layer with $d_1 = 0.23b$, $\epsilon_1 = 12.96$ and $d_2 = 0.77b$, $\epsilon_2 = 1$. The existence of a resonance is inferred from the corresponding transmittance curve in the same way as for the composite crystal. It is obvious that the main difference between the stratified medium and the photonic crystal derives from the existence of an absolute gap in the latter, which, expressed in different words, means that the gap in the photonic crystal does not vary dramatically with $k_\parallel$ as is the case for the stratified medium. The dispersion of the resonances within the gap is also very different in the two cases.

Finally, we should mention that by introducing an impurity plane with a unit cell commensurate to the surface cell of the given slab but much larger, i.e. a supercell with a single impurity sphere in it, one obtains states of the EM field with frequencies within the gap which are practically localized on isolated spheres. Such states, localized on isolated impurities, have been discussed by Johannopoulos *et al* [8].

References

[1] Yablonovitch E 1993 *J. Phys.: Condens. Matter* **5** 2443

[2] Yablonovitch E 1987 *Phys. Rev. Lett.* **58** 2059
Yablonovitch E and Gmitter T J 1989 *Phys. Rev. Lett.* **63** 1950

[3] Leung K M and Liu Y F 1990 *Phys. Rev. Lett.* **65** 2646
Zhang Z and Sapathy S 1990 *Phys. Rev. Lett.* **65** 2650
Ho K M, Chan C T and Soukoulis C M 1990 *Phys. Rev. Lett.* **65** 3152

[4] Chan C T, Ho K M and Soukoulis C M 1991 *Europhys. Lett.* **16** 563
Yablonovitch E, Gmitter T J and Leung K M 1991 *Phys. Rev. Lett.* **67** 2295

[5] Stefanou N, Karathanos V and Modinos A 1992 *J. Phys.: Condens. Matter* **4** 7389

[6] Pendry J B and Mackinnon A 1992 *Phys. Rev. Lett.* **69** 2772
Pendry J B 1994 *The Journal of Modern Optics* **49** 209

[7] Born M and Wolf E 1975 *Principles of Optics* (Oxford: Pergamon) p 51

[8] Yablonovitch E, Gmitter T J, Meade R D, Rappe A M, Brommer K D and Joannopoulos J D 1991 *Phys. Rev. Lett.* **67** 3380
Meade R D, Brommer K D, Rappe A M and Joannopoulos J D 1991 *Phys. Rev.* B **44** 13 772