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NUMERICAL STUDIES OF DISORDERED PHOTONIC CRYSTALS

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Abstract—Since the first demonstration of a complete photonic band gap by E. Yablonovitch in 1987 [1], photonic band gap materials have attracted a very significant interest in Electromagnetism but also in Solid State Physics. Doped photonic crystals that have a point defect (a local disturbance) have been extensively studied with the emergence of this new area of Physics. They present localized modes in the band gap and triggered many potential applications. Fewer papers have been devoted to strongly disordered photonic crystals that are periodic on the average. These structures are disturbed on the overall feature and the defect corresponding is referred to as extended. Analogue at a first glance to amorphous semiconductors, these materials could present interesting properties. Moreover, manufacture of photonic crystals is still a real challenge for the optical domain and undesirable extended defects can appear leading to a compulsory study of the tolerances of periodicity for such new materials.

1. INTRODUCTION

Photonic crystals are periodic structures in which optical properties can be tailored depending on the index contrast and the geometry of the elementary pattern [1–3]. The simplest photonic crystal is unidimensional and corresponds to a Bragg reflector. A two-dimensional photonic crystal can be a set of parallel identical cylinders (dielectric or metallic rods, holes in a dielectric material) periodically arranged in a homogeneous medium. A three-dimensional crystal can be for instance a set of identical spheres periodically arranged, but many other patterns have also been tested. By analogy with semiconductor materials, band structures can be calculated for photonic crystals using numerical methods and reveal band gaps for certain frequency ranges of the incident wave on the material. In the microwave domain, the first 3D photonic crystal referred to as the Yablonovite [4] was constituted by three series of cylindrical holes having three fold symmetry drilled at 35° from the normal to the surface and presented a full band gap whatever the direction and polarization of the incident field. 2D and 3D structures count a large number of potential applications for the microwave domain where they could be used as very efficient reflectors [5], antenna substrates, etc. In the optical domain highly attractive applications are considered, such as filters, optical switches, cavities, very efficient (low-threshold) laser diodes and light emitting diodes [1, 4, 6], superprism [7, 8], etc.

To be still consistent with this usual analogy between Electromagnetism and Solid State Physics, disordered photonic crystals can be either structures containing localized defects and may be the analogue of real crystal with point defect or structures containing extending defects. We will describe below the first type (point defects) of disordered

structures then the second type (extended defects).

In real crystals, typical point defects are atoms missing from the lattice or extra atoms inserted in the crystal lattice. The last decade have seen numerous studies on disturbed photonic crystals with point defects that correspond to a defect created locally within the structure in adding, moving or removing material [9]. A pioneer work by Anderson in 1958 [10] has been devoted on the study of the properties of disordered lattices and superlattices and has revealed that these structures can present light localization (energy trapped in the defected zone referred to as Anderson's localization). These structures were also called doped photonic crystals because they can modify locally the properties of the frequency response of the structure. Indeed, localized modes can appear in the band gap for such a structure. A simple explanation is generally used for a defect consisting in a cavity created by removing one or several cylinder/spheres in a two/three-dimensional photonic crystal: the cavity plays the role of a relay for the photons which can then penetrate the structure. Consequently, the localized state appearing inside the band gap corresponds to a resonance peak (mode) of the cavity [11–15] and can be enhanced using a periodic defect [16]. Moreover, according to some selection rules, linked to both symmetry of the incident field and of the structure, it is possible to control the occurrence of a mode [11, 13, 17, 18]. The control of the propagation of the light by these new materials is linked to the control of localized modes and has been extended to the study of propagation in waveguides [19]. Many numerical methods have been devised to analyze doped photonic crystals. Five of these methods are briefly outlined in the next section as they have also been used to study disordered structures of interest of this review paper. It is worth signaling another method that has been used to analyze doped photonic crystals: the Finite Element Method [20]. It is possible to calculate the S matrix (that contains the reflection and transmission coefficients) for undisturbed infinite photonic crystal using symmetric boundaries. For the basic method, the size required for a disordered structure is very large compared to the memory size of a computer even for a point defect. The only defect which was simulated so far with this method was a cavity of infinite width.

The second type of disordered photonic crystal experiences strong disturbances on the overall structure and may rather be compared to real crystals with extended defects. Extended defects are locations where atom positions are displaced over a large area and they have attracted a significant interest because fabrication of periodic structure is highly difficult especially for the visible domain where the size of the elementary pattern is submicrometric. As a consequence, the

study of tolerances of periodicity for photonic crystals is a crucial problem. In particular, the knowledge of the behavior of the band gap depending on a random variation of parameters like the index or the lattice constant mimicking fabrication imperfections is essential. Moreover, as for real crystals such as silicon, photonic crystals should be expected to present different behaviors when their periodicity is strongly disturbed by extended defects but maintained on the average. Many effects like light localization at edges of band gaps occur only when the disordered structure is large enough compared to the wavelength. Due to computer limitations, theses structures are not approachable numerically. One tip consists then in averaging on many small realizations of one disturbance [41]. As a result of a strong disturbance, band tails (instead of narrow peaks) usually appear at the edge of the band gaps [27, 39]. These effects can not easily be shown experimentally because i) they require dozens of experiments, ii) it is difficult to guarantee that only one type of defect is present in the actual structure. Therefore, numerical simulations are important to assess the effect of a particular type of extended defect on optical properties of a photonic crystal and allowable deviations during its fabrication.

Very recently, some studies have dealt with extended defect in a 2D and 3D disturbed photonic crystals [21–38] or in a much simpler 1D model [39, 40]. These studies have been presented using different numerical methods. However, depending on the problem tackled, not all methods are equivalent or suitable. In this paper, a review of these studies is presented and discussed. The purpose here is to focus on extended defects rather than point defects since the latter were extensively studied during the last decade.

2. NUMERICAL METHODS

In this part, we will review different numerical methods that have been devoted during the past decade to the investigation of properties of disturbed photonic crystals. Some of these methods permit to calculate transmission and reflection coefficients, which are experimentally attainable. The main methods are: 1) the Plane Wave Method [42], 2) the Finite Difference Time Domain (FDTD) method [43], 3) the Transfer Matrix Method (TMM) [44], 4) a rigorous scattering theory for 2D [45] or 3D [46, 47] photonic crystals and 5) the study of Diffraction Gratings [48, 49]. All of these methods can deal with metallic or dielectric structures and with 1D, 2D or 3D geometry.

2.1.1. The Plane Wave Method in Outline

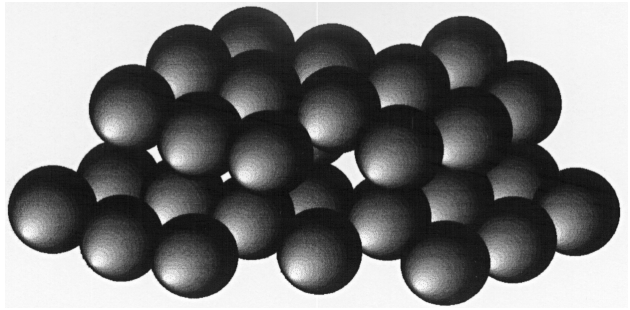
The plane-wave method is, in essence, the resolution of Maxwell's equations using an expansion of the electric field with discrete Fourier series expressed on the plane waves basis, which is possible when the medium is supposed to be periodic. This technique, well described in [42], was historically the first method used to calculate band structures of photonic crystals having a frequency independent dielectric function. It is directly emerging from Solid State Physics as an application of the Bloch's theorem to electromagnetic waves that can propagate inside the structure. It has been applied since to many calculations of band structures of 2D and 3D photonic crystals [50–57] although convergence is quite slow in some 3D cases [58] owing to the large fluctuation of truncated series approximating the actual dielectric constant and fields. The diamond lattice (one example of such a structure is depicted in Figure 1(a)) proposed for the first time by Yablonovitch [4], has widely been studied since this face centered cubic geometry has an advantageous full gap whatever applied incident field. Figure 2 presents the calculation of the band structure for the 3D photonic crystal of Figure 1(a), obtained with the plane wave method.

At a first glance, the plane wave method does not seem very suitable for studying disturbed photonic crystals as the count of plane waves escalates when the structure diverges from a periodic one. However, many structures having a point defect have already been studied with this method using a supercell technique. A convergence study is then necessary to verify that the coupling is weak between adjacent supercells. Recently, some papers have dealt with square, triangular and graphite 2D [24, 28, 34] or 3D [22, 29] extended defect in photonic materials by means of the plane wave method.

In any case, it is not possible to access to reflection and transmission coefficients with this method.

2.1.2. Disturbed Photonic Crystals Studied with the Plane Wave Method

A very recent study of 2D disturbed dielectric photonic crystals having an extended defect has been performed by Li et al. [34] using the Plane Wave method. Structures studied were square and triangular lattices of dielectric cylinders in air for an TM-polarization (**E** along the axis of cylinders). The TE-polarization study was ignored since the band gap is quite narrow for such a case. The authors have succeeded to deal with two typical types of randomness by the way of a supercell technique using a large number of plane waves: cylinder site displacements referred to as site randomness by the authors



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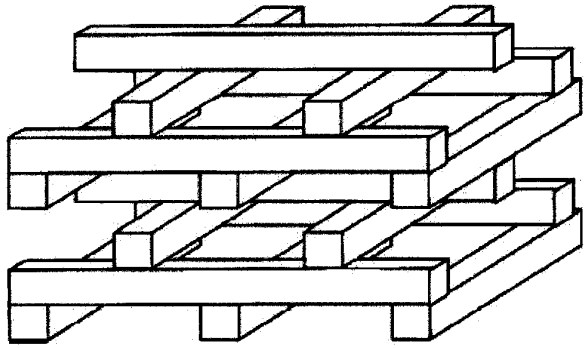


(b)

Figure 1. (a) A diamond lattice of spheres (from Joannopoulos et al. [2]) and (b) a stacked-bar structure (from Chutinan et al. [31]).

and cylinder radius variations referred to as size randomness. The disordered system was approximated as a periodic system with a period large enough to guarantee negligible coupling between neighboring supercells. Typically, the supercell contained 5×5 unit cells for site randomness and 7×7 for size randomness. For site randomness, the position of each rod was randomly disturbed by executing a translation $\gamma_x a$ on x and $\gamma_y a$ on y, where a was the lattice constant and γ_x and γ_y were variables uniformly distributed over the interval $[-d_{xy}, d_{xy}]$ where d_{xy} characterize the random strength of the disordered system. An equivalent distortion of $\gamma_r a$ was applied on radii for the size randomness: the new radius for the i^{th} cylinder was given by $r_i = r_0 + \gamma_r a$ with a random strength of d_r. They calculated the density-of-states (DOS) for different realizations of disordered structures. Results were independent of the realization of the sample with a

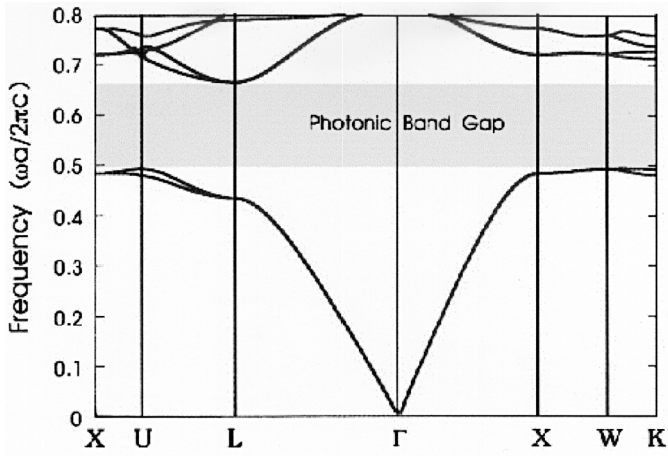


Figure 2. Photonic band structure of a 3D photonic crystal constituted of air spheres periodically arranged in a high dielectric material ($\varepsilon = 13$) with a diamond like geometry, calculated with the plane wave method. The x-axis indicates the directions of the wave vector varying across the irreducible Brillouin zone (from Joannopoulos, J. D., R. D. Meade, and J. N. Winn, *Photonic Crystals, Molding the Flow of Light*, Princeton University Press, 1995, reprinted by permission of Princeton University Press).

site randomness contrarily to that obtained with a size randomness, especially at strong disorders. More generally, results revealed that the sensitivity to disorder was more important with size randomness than with site randomness. Actually, as shown in Figure 3, band gaps tended to reduce very slightly even for a strong disturbance of the site displacement (typically a strength as large as half the cylinder radius was applied). On the contrary, band gaps reduced more than one-half for typical size randomness strength of about one-third the cylinder radius. They explained this behavior in showing that localization states responsible of band gaps reduction appeared far more easily even with weak size randomness than for a strong site randomness. In any case, the ground band gap was far more robust than the higher ones. This result was highly consistent with other theoretical efforts [22, 24, 28, 29] and was explained considering that the higher the frequency, the larger the ratio of disorder to minimum feature size.

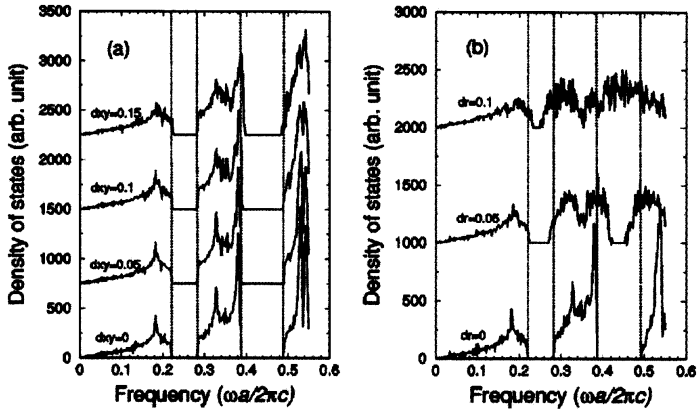


Figure 3. Density of state (DOS) of disordered crystals with (a) site randomness and (b) size randomness in various random strengths. The DOS was calculated for the E-polarization (**E** along the axis) of a square lattice of dielectric cylinders in air. The cylinders have a filling factor of 30% and a dielectric constant of $\varepsilon = 12.96$. Dotted vertical lines in (a) and (b) represent the band edges of a periodic crystal. For a clarity of view, the upper curves are offset alternately (from Li, Z. Y., X. Zhang, and Z. Q. Zhang, *Physical Review B*, Vol. 61, 15738, 2000, with permission of Phyical Review B).

2.2.1. The Finite-Difference Time-Domain (FDTD) Method in Outline

This method is formulated by discretizing Maxwell's curl equations over a finite volume. The space and time derivatives of the electric **E** and magnetic **H** fields are formulated by means of centered difference approximations. This method is very flexible and powerful because it can deal with active or passive structures applying the appropriate boundaries conditions to consider an infinite or finite material (thus corresponding to a real piece of material). Indeed, most of photonic crystals studied so far concerned passive structures. However, a new field has emerged recently with the introduction of active structures comprising electronic components such as PIN diodes in order to control electronically their electromagnetic properties [59, 60]. The FDTD method can take into account these components. The theory consists in discretizing the problem over a finite four-dimensional domain with appropriate boundary conditions enforced on the source, conductors and mesh walls, the Maxwell's equations are then approximated using the centered difference approximation on

both time and space first-order partial differentiations. Typically, the x-component of the electric field is given for a $(\Delta x, \Delta y, \Delta z)$ mesh by:

$$E^{n+1}_{xi,j,k} = E^{n}_{xi,j,k} + \frac{\Delta t}{\varepsilon \Delta y}\left(H^{n+1/2}_{zi,j+1,k} - H^{n+1/2}_{zi,j,k}\right) - \frac{\Delta t}{\varepsilon \Delta z}\left(H^{n+1/2}_{yi,j,k+1} - H^{n+1/2}_{yi,j,k}\right) \quad (1)$$

Similar expressions are obtained both for other components of $\mathbf{E}$ and for the magnetic field $\mathbf{H}$. In the formula (1), i, j, k are integers related to the space discretization with x, y, z space-coordinates, n to the time discretization, and ε is the dielectric constant.

The maximum time step that may be used is limited by the stability restriction of the finite difference equations:

$$\Delta t \leq \frac{1}{v_{\max}}\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}\right)^{-1/2} \quad (2)$$

where $v_{\max}$ corresponds to the maximum velocity of light in the computational volume.

As said previously, almost all types of passive or active structures (and linear or non-linear) can be dealt with this very powerful method. It is not limited to a plane wave incident field, which may be useful in the study of emitters embedded in photonic crystal as it would be the case for lasers. Another interesting feature of this method is the possibility of a dynamic resolution of Maxwell's equations and may permit to study dynamic behaviors of photonic crystals. It is worth noting the lack of a rigorous model for very specific structures such as thin wires. Limitations of the theory are then attained in that case. Moreover, this method is a time resolution that requires a Fast Fourier Transform operation to obtain the transmission with respect to the frequency. At a first glance, this method is advantageous since it does not require an inversion of a linear system, but the temporal approach can be a problem for calculating a quality factor of a cavity with a good resolution. For indication to the maximum size storage of the computer, it has already been successfully applied to calculate the transmission spectrum of a graphite 2D photonic crystal containing up to 90 dielectric rods having a diameter to wavelength ratio equal to 0.04 and a dielectric filling factor of 16.3% with highly accurate results (the reliability is obtained when compared to experimental measurements) [61] (Figure 4).

The interested reader is referred to the book of Taflove [43] for a very detailed explanation of the FDTD method.

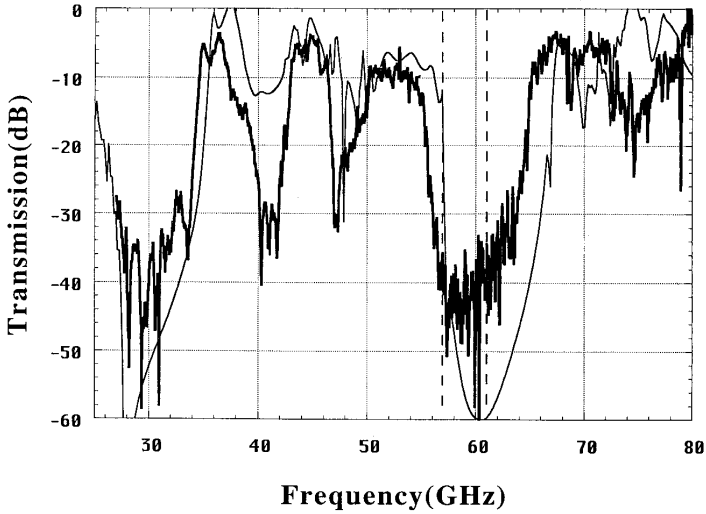
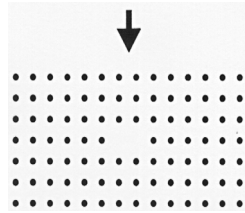


Figure 4. Transmission spectrum of a 2D graphite structure photonic crystal experimentally measured (thick curve) and numerically obtained (thin curve) by means of the FDTD method and for a TM-polarization for the Γ-K direction (perpendicular to the rods). The structure contained 90 alumina rods of dielectric constant $\varepsilon = 0$, and the dielectric filling factor was equal to 16.3%. Vertical dashed lines indicate the positions of the full photonic band gap (from Gadot, F., A. Ammouche, E. Akmansoy, T. Brillat, A. de Lustrac, and J.-M. Lourtioz, *IEE Proceedings Optoelectronics*, Vol. 145, 415, 1998, reprinted with permission of IEE).

2.2.2. Disturbed Photonic Crystals Studied with the FDTD Method

A comparison between experimental measurements and FDTD method calculations of the transmission spectrum has been recently addressed [38] in the case of extended defects in metallic photonic crystals for the microwave domain. This work indicated the tolerances of metallic structures to three generic types of disorder: site, angular and size displacements. The 2D structures were finite-sized (constituted of 7×14 rods) as experimental structures and results obtained with the FDTD model fitted very well to experimental results. It was showed that band gaps and localized states of doped 2D metallic photonic crystals were particularly insensitive to site displacement (Figure 5) and inclination variations while for the size variation localized states tend to appear at the edges of the band gap. These results are consistent with the results of Li et al. [34] who resolved the site



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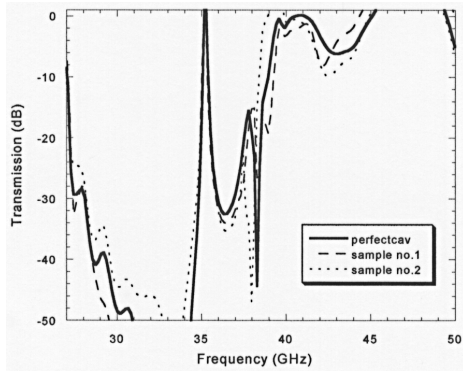

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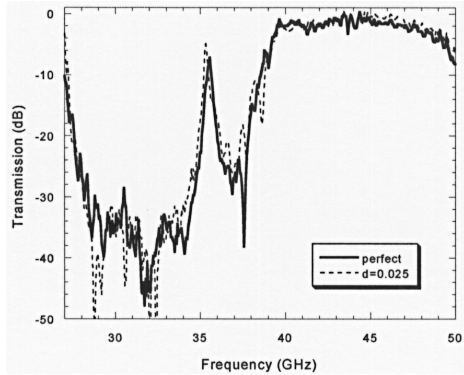

(c)

Figure 5. (a) Doped square 2D metallic photonic crystal studied in [38], rods had a radius of 1.5 mm and the lattice constant was 6 mm; (b) FDTD calculations of the transmission spectrum for a strength of disorder d_{xy} equal to 0.025 both for two different samples and for the perfect case; and (c) experimental data (from Guida, G., T. Brillat, A. Ammouche, F. Gadot, A. de Lustrac, and A. Priou, *Journal of Applied Physics*, Vol. 88, 4491, 2000, reprinted by permission from the Office of the Publisher, American Institute of Physics).

displacement dielectric case with the Plane Wave method. Hence, behaviors for a true band gap of dielectric and metallic periodic materials seem to be similar with respect to a site and size displacement disorder.

2.3.1. The Transfer Matrix Method in Outline

In this section, the salient points of the Transfer Matrix Method (TMM) are reviewed. The method is a layer by layer calculation of the field. It begins with Maxwell's equations where the field contains the time only in the factor $\exp(-i\omega t)$. Written in terms of $(\omega, \mathbf{k})$ space we have,

$$\mathbf{k} \times \mathbf{E} = +\omega \mathbf{B} \tag{3}$$

$$\mathbf{k} \times \mathbf{H} = -\omega \mathbf{D} \tag{4}$$

For the first equation we make use of the following approximation to discretize Maxwell equations on a cubic mesh of unit dimensions (a, b, c):

$$k_x \approx (-ia)^{-1}(\exp(ik_x a) - 1) \tag{5}$$

and for the second,

$$-k_x \approx (-ia)^{-1}(\exp(-ik_x a) - 1) \tag{6}$$

and similarly for y and z. A transfer matrix approach is made viable by retaining some components, (E_x, E_y, H_x and H_y), and Fourier-transforming back into real space. After some manipulations the equations may be expressed in a matrix form,

$$F(\mathbf{r} + \mathbf{c}) = \sum_{r'} \widehat{T}(\mathbf{r}, \mathbf{r}') F(\mathbf{r}') \tag{7}$$

where

$$F(\mathbf{r}) = \begin{pmatrix} E_x(\mathbf{r}) \\ E_y(\mathbf{r}) \\ H_x(\mathbf{r}) \\ H_y(\mathbf{r}) \end{pmatrix} \tag{8}$$

Since $\mathbf{r}$ and $\mathbf{r}'$ lie within one layer ($z = z'$), and $\widehat{\mathbf{T}}$ is the real space transfer matrix, Eq. (7) permits a layer by layer calculation of the field propagating in the z-direction. The reflection R and transmission T coefficients may be found from the components of $\widehat{\mathbf{T}}$ for plane waves incident on a layer. Alternatively, when $\widehat{\mathbf{T}}$ represents a unit cell, by applying Bloch's theorem in the z direction, the band structure can

be obtained from the eigenvalues of $\widehat{\mathbf{T}}$. Various investigations in the literature have demonstrated the application of TMM for a wide range of PBG materials [62–66].

The interested reader is referred to the original reports [44, 67, 68] for a detailed explanation of the method that has widely been used for the study of PBG structures.

2.3.2. Extended Defect Studies with the TMM Method

Sigalas et al. [30] and Chutinan et al. [31] have used this method very recently to analyze effects of extended defects on band gaps of a finite thickness slab of 3D photonic crystals. The former study dealt with the very interesting diamond symmetry both with spheres and connected wires (it was previously suggested that a connected structure may present wider band gaps) having random site displacements, while the second dealt with a stacked-bar (Figure 1(b)) structure having various types of disorder (misalignment of stripe position, deviation of intersecting angle, variation of layer thickness and variation of stripe width).

As for the plane wave method, authors were obliged to use a supercell technique. Then, their structures were of infinite width and effects of the actual finite width of the material were neglected.

Sigalas et al. [30] investigated the localization length formally defined by:

$$l = -\frac{2La}{\langle \ln T \rangle} \tag{9}$$

where La is the thickness of the slab of the disordered photonic crystal, and $\langle \ln T \rangle$ is the logarithmic average of the transmission over different configurations. The localization length has been introduced in the study of random medium and is a length representative of the thickness of material necessary to localize light (stop light propagation). In [30], this quantity has then a feature similar to the transmission of the material studied. Calculations of Sigalas et al. revealed that the rods' case is more robust than the spheres' case due to the connectivity of the rod structure that exists for any amount of disorder. The authors suggested that these strongly disordered photonic crystals can not be compared to disordered type IV semiconductors for which the electrons are always locally influenced by a quasi perfect tetrahedral atomic symmetry even though atoms have random positions. This evidences that a comparison with amorphous materials should be approached with extreme carefulness.

Concerning calculations for the stacked-bar structure [31], dealing directly with the transmission spectra, the sensitivity to disorder was

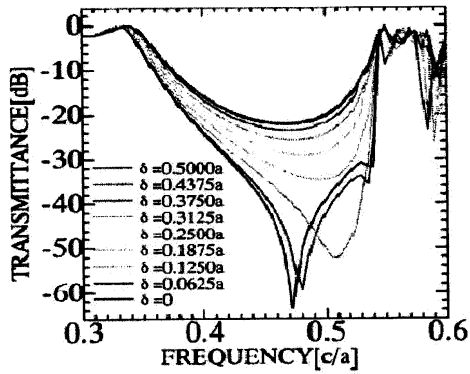

Figure 6. Transmission spectra of a normally incident wave for polarization in which the electric field is parallel to the x-axis, when δ varies from 0 to $0.5a$, a being the period in the y direction of the stacked-bar structure. The refractive index, width and thickness of a stripe were 3.309, $0.25a$ and $0.3a$ respectively. The deepness of the band gap increases as δ decreases (from Chutinan, A. and S. Noda, *Journal of the Optical Society of America B*, Vol. 16, 1398, 1999, reprinted with permission of the Optical Society of America).

dominated by the stripes misalignment provided that it was parallel to the propagating direction of the incident field. Figure 6 presents transmission spectra through eight layers of a stacked-bar structure (corresponding to two periods), in the stacking direction and for different stripes misalignment defects quantified by δ. The authors suggested that behaviors of the transmission spectra with respect to the disorder can be understood considering the insensitiveness of the electromagnetic wave to the existence of perpendicular dielectric rods.

2.4.1. A Rigorous Scattering Theory

A rigorous scattering theory [45] permits to deal with a certain type of 2D photonic crystal consisting in a finite number N of parallel cylinders made of a perfectly conducting or dielectric material of optical complex index v. The method consists in the resolution of a linear system which unknowns are coefficients of the diffracted field. To establish the linear system, the actual incident field on a cylinder is written as the sum of the conventional incident field and of the fields diffracted by the other cylinders. For any arbitrary rod, the field at a point P in the vicinity of this rod can be written in the form of the sum of a local incident field $E_n^i(P)$ and a local diffracted field $E_n^d(P)$ expressed by a Fourier-Bessel

expansion. The local incident field $E_n^i(P)$ is then generated not only by the actual incident field $E^i(P)$ but also by the field scattered by the other rods in the direction of the n^{th} rod. Using Graf's formulae [69] and the S-matrices of the rods (providing for each rod a simple relation between the coefficients of the incident field and the coefficient of the field diffracted by the rod), it is possible to access to the linear system linking the coefficients of the local incident field to the coefficients of the local diffracted field. Finally, after resolution of the linear system, the field scattered at infinity by the set of N parallel cylinders can be obtained using:

$$E^d(P) = g(\theta)\frac{\exp(ikr)}{r^{1/2}} \tag{10}$$

deriving from the asymptotic expression of the Hankel function, and where $g(\theta)$ depends only on the angular θ coordinate and on coefficients of the diffracted field.

The intensity at infinity (also called bistatic differential cross-section) is defined by:

$$D(\theta) = 2\pi|g(\theta)|^2 \tag{11}$$

and for lossless cylinders an energy balance criterion can be used to verify the validity of the results obtained [45].

The reader can find in [41, 70, 71] various tests of validity of the results. Using Mie's theory, it is possible to adapt this method to deal with a 3D photonic crystal constituted of spheres placed in the space [46, 47, 72].

Dielectric constants and shapes of rods are described in a S-matrix and can be randomly varied together with the positions using this method. Alternatively, all type of incident wave can be tackled provided that it is expressed on a Fourier-Bessel expansion. The main limitation is the type of 2D photonic crystal which is then necessarily a set of parallel cylinders (dielectric or metallic and with arbitrary shapes) or necessarily a set of spheres for the 3D case. This method combines very good relative accuracy (better than 1%) with rapid computation. Structures of a few hundred cylinders have already been studied. Sabouroux et al. [73] have recently realized a 2D dielectric photonic crystal with an hexagonal geometry. Their measurements in the microwave domain of the transmission spectrum showed a very good agreement with calculations obtained with this numerical method (Figure 7).

2.4.2. Extended Defects Studied with the Rigorous Scattering Theory

This method was employed in studies on doped photonic crystals consisting of point defect in periodic structures [71]. This technique

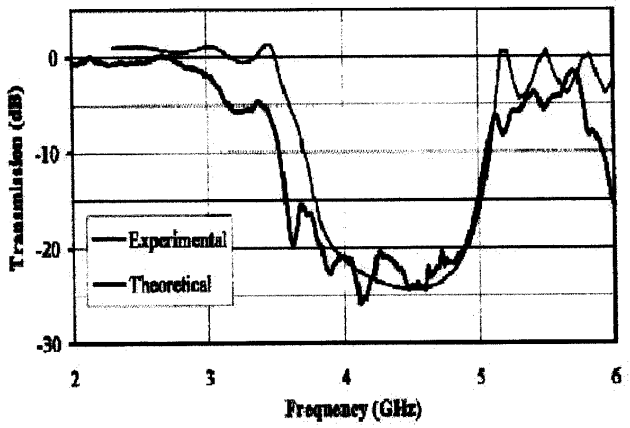

Figure 7. Transmission spectrum for a 2D dielectric photonic crystal having an hexagonal symmetry and made of 80 rods of dielectric constant ε equal to 6 and a 5 mm radius. The shift between experimental and numerical results was explained by a dependency on the dielectric constant on the frequency (reprinted from Sabouroux, P., G. Tayeb, and D. Maystre, *Optics Communications*, Vol. 160, 33, 1999, with permission from Elsevier).

has also been applied to the study of extended defects [41, 27] for disordered 2D dielectric and metallic photonic crystals experiencing a random variation of the rods location. In the metallic case, the study has permitted to prove for the first time that the large forbidden band gap extending from zero to the cut-off frequency ω_p was not related to the periodicity but to the metallicity of the rods (Figure 8). Indeed, a strong perturbation in positions of rods does not generate a noticeable distortion in the overall response of the structure to an electromagnetic wave. In previous works [74–77], ω_p was regarded either as been analogue to a type of plasma frequency associated with the motion of electrons in the continuous medium (in solid state physics) or as the shortest frequency which fits between the rows of wires (electromagnetic theory). The behaviour of metallic crystals that are effective media at very low frequencies was then explained by a frequency dependent dielectric constant described for a 2D square lattice array of perfectly conducting rods by:

$$\varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2} \tag{12}$$

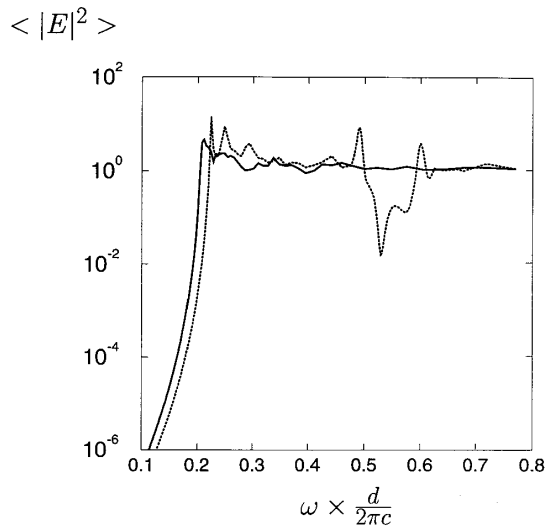

Figure 8. Mean of the energy penetrating a square 2D photonic crystal (dotted line) and an average over 6 different realizations of this crystal but strongly disordered with site displacements of strength $d_{xy} = 0.5$ that corresponds to the maximum value possible (reprinted from Guida, G., *Optics Communications*, Vol. 156, 294, 1998, with permission from Elsevier).

with the plasma frequency obtained with:

$$\omega_p = \frac{c}{d}\sqrt{\frac{2\pi}{\ln(d/2a)}} \tag{13}$$

where d corresponds to the period of the 2D photonic crystal and a to the radius of the metallic rods.

It has been shown [27, 76] that these formulae, which are valid only for extremely low frequency, are indeed a proper approximation even for the resonance domain (i.e. for a period d having the same order of magnitude as the wavelength) where localized states can actually appear.

However, although this rigorous scattering theory is highly suitable for a low frequency study, it was not used at high frequencies owing to the limitation of the computer memory storage. Indeed, this problem was not linked to the method but to the finite size nature of the structures. The mean of the electric energy penetrating the structure was calculated for a frequency range sufficiently large to cover the plasmon band gap and the first "true" band gap of the structure

but not the band gaps beyond. Typically, calculations were limited to $\omega d/2\pi c = 0.8$. A thorough study should check that all band gaps have the same behaviour that the first true band gap, that is to be linked to the periodicity and to tend to disappear for a very strong site displacement.

2.5.1. Diffraction Grating Theory

The Diffraction Gratings Method, based for instance on an integral formulation [48] or a rigorous coupled-wave method [49], permits one to calculate the S matrix linking the incoming waves to the outgoing waves for a stack of identical or different gratings. This matrix then provides the reflection and transmission coefficients of the total structure. The integral formulation uses a Rayleigh expansion of the field between two successive gratings. A linear combination of plane waves is then obtained with coefficients calculated using the integral formulation of gratings. The rigorous coupled-wave method is a modal theory that consists in determining a set of eigenvalues and eigenvectors of a propagation matrix containing information on the propagating waves in the stack of gratings. The S matrix is then obtained from the eigenvectors. These very classic methods are limited to the study of partially disordered photonic crystals with a defect consisting of the lack of one or more layers of perfect gratings and provide a very good agreement with results obtained with other numerical methods [78]. However, it is possible to use a supercell technique to deal with a strongly disordered structure as done by Asatryan et al. [32, 35]. The interested reader can find a very detailed review of efficient methods using the electromagnetic theory of gratings in the book of Petit [79], a general presentation of modal theory was given by Li [80] and the differential and integral theories applied to non periodical structures were given by Giovannini et al. [81].

It is worth noticing at this stage that methods [82, 83] based upon grating theories, not described here, are able to compute the dispersion curves of the Bloch modes. These methods then permit to calculate band structures as the plane wave method does and can often be more powerful as regards accuracy, memory requirements and computation time.

2.5.2. Extended Defects Studied with the Diffraction Grating Theory

Asatryan et al. [32, 35] used recently a method similar to the Diffraction Grating Theory to analyze properties of a disordered 2D photonic crystal generalizing the Rayleigh method to incorporate many cylinders per unit cell of the grating. Studied structures were constituted

of cylinders of random refractive index [32] and random geometry [35]. Random geometry included randomness of radii, random site displacement and random thickness of each layer constituting the photonic crystal. They compared the optical transmittance properties obtained to the absorption spectra of amorphous semiconductors. Both responses exhibit tail-like features near the band gap edges. Indeed, the optical transmission spectra do not reveal any isolated narrow peak associated with localized states when the structure is disordered. Spectra exhibit instead extensions of the band pass that can be interpreted as a gathering of several peaks due to disorder resulting in band tail near the edges of the bandgap.

3. CONCLUSION

Deviations from the periodic structures that may arise during a fabrication process are the analogue to extended defects in real crystals. They have been of interest since the earliest photonic band gap structure realizations. However, first conclusions on the effect of these deviations on band gap sizes and localized states appeared only very few years ago with the use of adapted numerical methods to permit a statistical analysis. The main methods encountered in the literature are described in this paper and limitations are indicated. All methods presented very accurate results when compared to experimental results. They can deal with any type of incident field provided that it is expressed on the required basis expansion, except for the plane wave method. Indeed, the calculation of a band structure is independent of the incident field: the plane wave method then only provides the possible propagating modes of the structure.

As a conclusion, the choice of a numerical method among the main usual methods presented here, depends on the problem tackled. To obtain a band structure rapidly with an efficient and quite easy to implement method, it is highly recommended to use the plane wave method. A less obvious method would be based on a grating theory. To calculate the reflection and transmission coefficients of a photonic crystal of finite size experiencing a sophisticated defect, the rigorous scattering theory is advised. This theory is able to model the real defect without any "tip" (like a supercell technique) and provides results without any approximation. However, with this method the structure must correspond to a set of parallel cylinders or holes for the 2D case and to a set of spheres for the 3D case. In any case, a modal theory (like the rigorous scattering or a rigorous coupled-wave method) is far more efficient than for instance temporal methods to calculate the Q-factor of a cavity in a photonic crystal. If one is interested in

comparing numerical simulations with experimental measurements, the FDTD and TMM methods have already revealed very reliable results permitting a direct calculation of transmission spectra. The advantage of the FDTD compared to the TMM is the possibility to also study a finite structure that is a real piece of material as for experiments as the rigorous scattering theory does. For future works, the FDTD should be more and more used as it can integrate quite easily active components into photonic band gap materials that seem the advantage so far of this method compared to the rigorous scattering theory. To study strongly disordered photonic crystals, a supercell technique is required for the TMM, the Diffraction Grating Theory and the Plane Wave Method as these methods were first developed to deal with periodic structures only. However, this technique is a distorted way to deal with disordered structures using numerical theories designed for periodic structures. In that respect, it is recommended to address the problem by the mean of a rigorous theory that provides the solution without approximation. The other methods briefly described here do not need a supercell. However, thanks to the steady advances in computers, the size storage is less and less an obstacle to calculate with a supercell technique.

Numerical studies have been devoted to the calculation of band structures, localization length or transmission spectra for various types of deviations and various types of photonic crystals from 1D to 3D. Sensitivity to disorder strongly depends on the parameter altered. For example, random site displacement generally leads to slighter reduction of the band gap than random size displacement. Analyses of field maps have permitted to reveal occurrence of localized states that appeared easily depending on the type of disorder applied. However, the extensive study of the behavior of localized modes (occurring for instance when a cavity is created) in extended defect is another crucial point that remains mainly unexplored. Allowable deviations depend on the application envisaged and it is obvious that for a very specific application requiring very sharp band edges only a very weak deviation is acceptable.

In the future, some works should be made in order to analyze the sensitivity to disorder of the very peculiar properties of photonic crystals such as the superprism phenomenon, the negative dielectric constant and the negative magnetic permeability. Moreover, the emergence of controllable photonic crystals that are active structures obtained in inserting for instance PIN diodes in the lattices to control band gaps and localized modes will also present extended defects.

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