

AN INTRODUCTION TO PHOTONIC BAND GAP (PBG) MATERIALS

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Abstract—This paper introduces photonic band gap (PBG) materials that are periodic dielectric or metallo-dielectric materials conceived to control the propagation of electromagnetic waves. Firstly, the principle of these materials is explained. Doped PBG materials are then presented with their main properties and applications. New phenomena like super-prism or super-lens are also introduced. A review of different numerical methods used to study photonic band gap materials and to analyze their properties is given next. Manufacturing processes are then briefly described and foreseen applications are presented. Finally, the new field of the controllable photonic band gap materials is introduced.

1 Introduction

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1. INTRODUCTION

Originally photonic band gap materials were introduced with the goal to control the optical properties of materials. Indeed, the last century has seen our control of the electrical properties of materials using semiconductors (to tailor the conducting properties of certain materials). Photonic band gap materials offer the same control for the electromagnetic properties of the materials. Using the formal analogy between Schroedinger's and Helmholtz's equations of propagation, Eli Yablonovitch [1] had the idea in 1987 to built artificial periodic structures playing on the permittivity in order to control totally the propagation of the light. The concept of a photonic band gap (PBG) material was born. To test this idea, he realized a prototype with a three-dimensional diamond hole lattice in Plexiglas. With this material he demonstrated the capability of the PBG material to control the propagation of an electromagnetic wave. Simultaneously the concept of strong localization of photons in disordered dielectric superlattices was proposed by S. John [2]. One of the most important properties of the photonic band-gap materials is the emergence of localized defect modes in the gap frequency region when a disorder is introduced to their periodic dielectric structure [3,4]. In addition to the purely scientific interest in these strongly localized eigenstates of photons, several applications to optical devices are expected. For example, as was pointed out by Yablonovitch, the single-mode light-emitting diode that utilizes spontaneous emission through a localized defect mode in a photonic band gap may have such properties as good temporal and spatial coherence, high efficiency, low noise, and high modulation rate. Another example is the waveguides composed of defects introduced into regular photonic band-gap materials, for which quite a high transmittance for the guided modes through sharp bends was theoretically predicted. This feature originates from the nonexistence of the electromagnetic modes outside the waveguides, and is a striking contrast to a large loss at the sharp bends observed

for ordinary optical waveguides. This feature may be quite useful for optical microcircuits.

First photonic band gap materials were realized with dielectric materials. However, different research groups have progressively introduced more complicated structures. For instance, in the microwave domain metallo-dielectric material was often used. Metallo-dielectric PBG materials are constituted of a periodic arrangement of metallic parts (rods for instance) either in air or embedded in a more complicated dielectric structure. They have some properties very different from purely dielectric PBG crystals. They have a gap down to very low frequencies. These materials have many advantages in this frequency domain: easy fabrication, robustness, conformability and low cost. More recently, controllable PBG materials were proposed at microwave and optical frequencies [4, 5]. Metallo-dielectric materials also allow the insertion of electronic devices in the core of the material leading to controllable structures. The reader could also find in the literature the electromagnetic gap (EMG) material calling for metallo-dielectric structures. However, we do not use this terminology here to not confuse the reading.

Sometimes metallo-dielectric photonic band gap materials, which are for instance reserved to the centimeter and millimeter wavelengths, are called electromagnetic gap (EMG) materials. But some of these structures may be used at higher frequencies, in the infrared or sub-millimetric domain for example. Also purely dielectric structures may be used at lower frequencies. Therefore the distinction between PBG and EMG materials is not evident. Another common name is photonic crystals (PC). This name may assign any structures that interact with the light. We use indifferently PBG or PC name in the following sections.

Many applications have been proposed for these materials, in optics or in the microwave domain. In optics several authors have proposed high-Q microcavities and low threshold lasers, novel types of filters, low-loss bent waveguides, novel LEDs, optical fibers [6–15]. In the microwave domain numerous applications of metallo-dielectric PBG have been investigated, such as reflectors and substrates for antennas, high impedance surfaces, compact uniplanar slow-wave lines, broad band filters [16–26]. The following is devoted to an introduction to photonic crystals and their emerging applications. The reader is referred to [15] for other reviews on many aspects of PBG materials.

2. PBG PRINCIPLE

PBG materials have a periodic arrangement of the permittivity. By analogy with semiconductor physics where a crystal lattice corresponds to a periodic arrangement of the atomic potential [27], PBG materials are also called photonic crystals (PC). The periodicity of the permittivity plays the same role for the photons that propagate inside the structure than the atomic potential for the electrons. Leading further this analogy, the geometry and the index contrast of the photonic crystal determinate many of its optical properties as it does for conduction properties of semiconductors. Playing on these two parameters, we can obtain frequency ranges for which light propagation is forbidden in the material and others ranges for which light can propagate. These frequency ranges are also scale dependent. Reducing the size of the elementary cell of the periodic lattice shifts the whole frequency range to higher values. The consequence of this property is the possibility to transpose a photonic crystal design from the microwave domain to infrared or visible range. For example a PBG material for the 1–5 GHz frequency domain will have a typical elementary cell size of a few centimeters and is very simple to realize experimentally. The same photonic crystal, designed to operate in the infrared domain has a cell size of about $1\ \mu\text{m}$ and $0.1\ \mu\text{m}$ to operate in the visible domain. This frequency range is usually calculated either by using an analogy with the band structure for which the Y -axis, representing the energy data, is swapped for the frequency or by calculating the spectrum that is the reflection coefficient of a finite layer of photonic crystal. Figure 1 shows band structures for a one-dimensional, a two-dimensional and a three-dimensional PBG materials respectively. The forbidden bands are shaded on this figure. The first function of a 3D PBG material is then a lossless isotropic mirror for one or several frequency ranges. A 2D PBG material behaves as a mirror only in two directions as revealed by Figure 2 and a one dimensional material has only one favored wave propagation direction. The same material is theoretically transparent for the complementary frequency bands.

In the microwave domain, metallic lattices have very interesting properties like, for example, a forbidden band from zero frequency to a frequency f_p called plasmon-like frequency (Fig. 3) [28]. This frequency corresponds to the largest wavelength of the field that fits the metallic grid. An allowed band follows this first forbidden band. The coupling of resonances of the different cavities of the crystal forms this band. Then the width of the band is linked to the number of the cavities and to the strength of their coupling. The number of

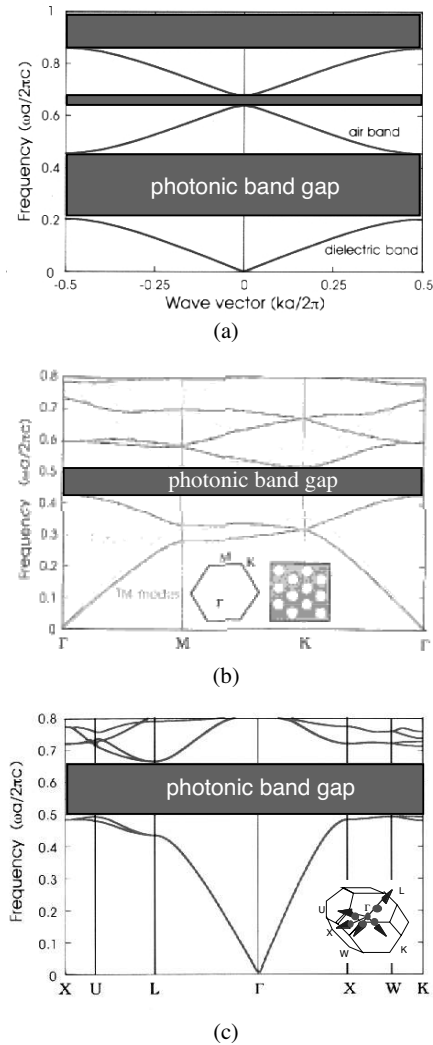
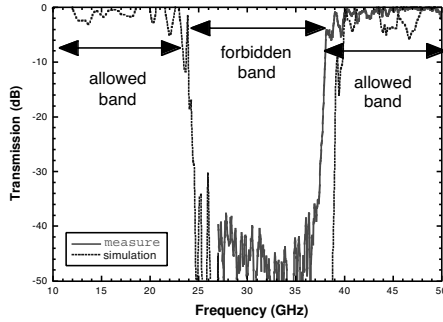
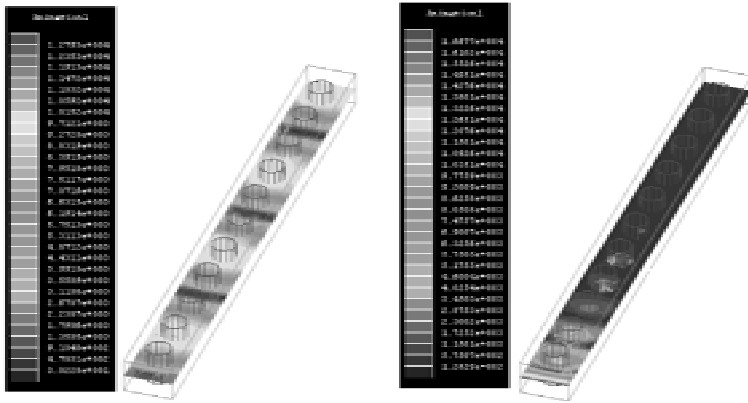


Figure 1. (a) Dispersion diagram of a one-dimensional crystal. The forbidden bands are shaded, a is the period of the lattice, c is the light velocity. (b) Dispersion diagram of a two-dimensional triangular crystal. The forbidden bands are shaded. The lattice is composed of air holes in a high permittivity dielectric ($\epsilon = 13$). (c) Dispersion diagram of a three-dimensional crystal. The forbidden bands are shaded. The lattice is composed of air spheres in a high permittivity dielectric ($\epsilon = 13$) (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).



(a)



(b)

Figure 2. (a) Calculated and measured transmission diagram of a square lattice composed from 18 rows of 11 alumina rods with a 1.5 mm diameter and a period $p = 3$ mm (transverse magnetic polarization: the electric field E is parallel to the rod axis). (b) Calculated propagation at 12 GHz (left: allowed frequency) and 30 GHz (right: forbidden frequency). The polarization of the incident wave is also transverse magnetic.

coupled cavities in the direction of the wave propagation determines the number of resonances in the allowed band. The first proposed metallo-dielectric PBG materials were simply constituted of metallic wires or rods in air arranged with a bidimensional or tridimensional periodicity. The main disadvantage of these first structures is their large size. Indeed, they can reach 1 m^3 for the 1–5 GHz frequency band. For the applications in filtering, radome or antenna substrate,

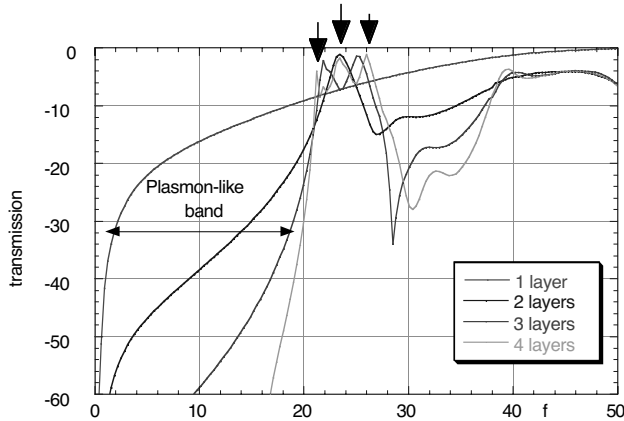


Figure 3. Calculated transmission of a square metallic lattice with 1.5 mm diameter copper rods, 6 mm spacing, for different layer numbers. With four layers the allowed band have three resonances peaks marked with arrows on the figure. The plasmon-like band is also indicated by an double arrow.

the thickness of the material is critical. For integration in microwave device and systems, the lateral sizes of the crystal may also be reduced. These considerations have led to the design of very specific metallo-dielectric PBG materials like the high impedance of Sievenpiper [22] and the compact uniplanar PBG material proposed by Itoh [23–26]. In both cases these new metallo-dielectric structures use the classical fabrication methods of the microwave devices and are designed to be integrated with active parts and devices in microwave applications. This capability of integration with electronic devices is used in the design of controllable photonic band gap materials.

Using the coupled cavities principle, other PBG structures were conceived with cells in the sequential layers having different sizes, but with close resonance frequencies to give the same results and keeps a larger allowed band [29]. Some biological structures like the scale of some butterfly's wing seem follow this strategy to obtain a diffraction effect in the visible domain [30]. Others biological PBG are purely periodic, like the feather of certain bird [31]. Mineral structures, opal for example, are also periodic.

At microwave frequencies the fabrication of dielectric, metallic and metallo-dielectric passive structures is practicable for microwave engineers due to their sizes, the same goal is more challenging in the infrared and optical domains. Materials like semiconductors, metals

or composite were used [32]. As the dimensions of these structures are micrometric or nanometric in the infrared and optical domains, they often reach the limits of the microelectronic technology [33]. Actually, similar periodic structures like Frequency Selective Surfaces (FSS) were studied many years ago [34]. The main differences between FSS and PBG materials are the third dimension used in the latter, the solid state theory formulation of photonic crystals, and the highly attractive concept of defect in PBG.

3. DOPED PHOTONIC CRYSTALS

The analogy between Electromagnetism and Solid State Physics has led to the study of band structures of periodic materials and further to the possibility of the occurrence of localized modes in the band gap when a defect is introduced in the lattice. These defect-enhanced structures are called doped photonic crystals and present resonant transmissions in the band gap corresponding to localized states appearance (Fig. 4). When the light propagates inside the periodic structure, it obeys to some selection rules. In particular, depending on the geometrical symmetries of the materials, some modes are allowed or not in the cavity created by a defect inside the photonic crystal. The defect mode can be excited by a source with an appropriate frequency and polarization. Numerical calculations have predicted modes that could really appear in the band gap [35, 36]. A single defect can produce a transmission peak (in a forbidden band) having a width depending on the quality factor associated with the defect cavity. Moreover, experiments demonstrate that the level of transmission depends on this quality factor but also on the strength of the coupling between the defect and the emitter of the incident wave. This coupling depends on the localization of the defect in the structure. If the frequency of the resonance mode of the defect corresponds to a forbidden frequency for the material, the coupling depends on the distance and the number of layers of the material between the source and the defect. To increase the coupling between the defect and the incident wave, a periodic lattice of defects has been proposed [37]. The transmitted energy was then increased. With these defects lattices we can obtain 0dB transmission and an adjustable width of the transmission peak depending on the number of defects perpendicular to the direction of the wave.

The concept of defect in the PBG materials has led to a large number of applications as for the semiconductor materials. Sharp bend waveguides, high power optical fiber, selective or wide band filters and duplexers have been proposed in optics and at microwave frequencies.

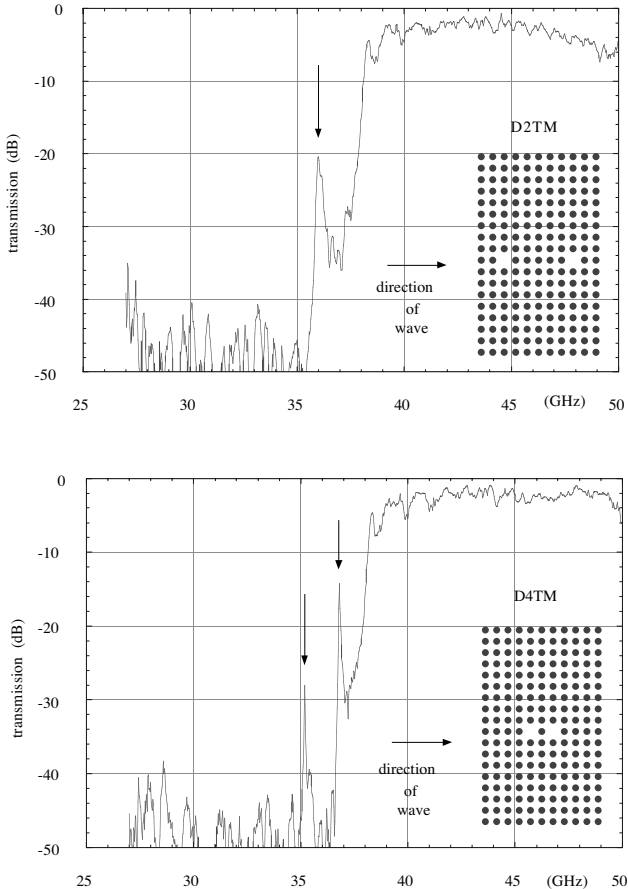


Figure 4. Measured transmission spectra of square lattices of alumina rods of 1.5 mm diameter spaced by 3 mm (transverse magnetic polarization) having two removed rods as local defects. The transmission peaks associated with these defects split when the defects are strongly coupled on the lower figure.

4. NEW PHENOMENA IN PBG MATERIALS

Recently new phenomena have been investigated and experimentally demonstrated in PBG materials. They are the super-prism [38] and super-lens [39] phenomena, the ultra-refraction [40] and negative refraction in a PBG crystal [41]. Finally, the proposition of John Pendry to realize negative permeability material [42] and its experimental demonstration in a composite material with a negative

permittivity part were a stimulating moment of the physics [43]. In this material, a lattice of metallic stripes on a dielectric substrate realizes the negative permittivity at frequencies corresponding to a forbidden band. This material is called left-hand as the electric and magnetic fields and the wave vector form a left-hand set. The capability to fabricate a material with simultaneously a negative permittivity and permeability triggered many new fascinating applications for these materials. In the past, materials with an analog but disordered structure and totally different properties have been studied. They are called chiral materials [44]. In fact, they have disordered structures and they have not shown negative permeability. Even if some of these phenomena are linked, they show that the physics of the PBG crystals is unexplored so far. Rigorous physical theory and numerical methods of simulation allow this exploration.

5. NUMERICAL METHODS OF SIMULATION OF PBG CRYSTALS

There are six main methods to study numerically photonic crystals: (1) the Plane Wave Method [45], (2) the Finite Difference Time Domain (FDTD) method [46], (3) the Finite Element method [47], (4) the so-called Transfer Matrix Method (TMM) [48], (5) a method based on a rigorous theory of scattering by a set of rods (for a two-dimensional crystal) [49] or a set of spheres (for a three-dimensional crystal) [50], and (6) the study of diffraction gratings [51]. All of these methods are very efficient and revealed results highly accurate when compared to experimental results. However depending on the problem tackled, they are not equivalent. Indeed, some of these methods like methods (1) to (4) have a high flexibility: they can simulate any doped or non-doped crystals [45–48]. Methods like method (5) are limited to certain types of PBG materials that are parallel cylinders (for 2d photonic crystals) and spheres (for 3d) [49, 50]. Some of these methods like methods (1), (4) and (6) can deal only with infinite crystals [45, 48, 51] and method (5) only with finite-sized structures [49, 50]. Finally, to study defect structures, methods (1), (4) and (6) use a super-cell. On the contrary, methods (2), (3) and (5) can deal with a finite structure having a single defect. In the following sections, we outline briefly these main numerical methods used to study doped and non-doped photonic crystal properties.

The main advantage of the Plane Wave Expansion method is that is very easy to implement and to obtain the band structure, since you specify the direction, and the codes give you all the propagating/evanescent energies for that direction. A defect in the

infinite photonic crystal will be treated using a super-cell. The interested reader can find in [45] information on the theory. Many results have been obtained with this method [52–56]. The limitation of the method is linked to the memory storage that depends on the number of plane waves used for the expansion of the field, and this number escalates when the photonic crystal diverges from a periodic structure. Sophisticated defects are then not possible.

The FDTD method analyses the Maxwell equations in time domain. Many works on photonic crystals have been done using this method. Some works comparing FDTD results with experimental measurements can be found in [57–63]. As for the Finite Element method, electromagnetic modes of a defect can be calculated as the transmission ratio of the material. To obtain the transmission spectrum of the crystal, an electromagnetic pulse is sent on the material and the output signal recorded. A fast Fourier transform is applied to both incident and transmitted signals and the transmission spectrum calculated. The FDTD method allows the simulation of finite or infinite crystals with inner or outer electromagnetic sources. In some cases, this method permits the simulation of an entire experimental set-up with a PBG crystal. Results of this experiment are then analyzed. The FDTD method is the most commonly technique to simulate a PBG crystal. The only limits of this method are the size of the memory to calculate a large crystal and the lack of an accurate electromagnetic model for some particular objects like thin wires for example. Another advantage of this method is the attractive capability to simulate non-linear materials [46, 61].

The Finite Element method, well established in electromagnetism, has the great advantage to be implemented in very efficient commercial software: MAFIA, HFSS, etc. This method can simulate infinite and finite doped or non-doped crystals with inner or outer source [43].

The Transfer Matrix Method (TMM) is well described in [48]. The method consists on writing the Maxwell's equations in the k -space and rewriting them on a mesh. This is essentially a layer-by-layer calculation. The TMM is capable of handling PBG materials of finite thickness. Structures with defects can be dealt only by considering a super-cell. An implementation of this method can be found on Internet [64]. The method permits to obtain band structures and provides the reflectivity and transmission coefficients. Many works have used this method [65–69]. It has also proved particularly useful, and accurate, when comparisons with experimental structures are undertaken [67, 69]. Recently, a new version of this method has been developed to describe the emission properties of infinitely long cavity structures sandwiched between two photonic crystals [70]. The

limitations of the TMM method are the memory storage but also, although sophisticated versions of the method, it is difficult to deal with a geometry different from the cubic geometry.

Many groups have implemented numerical methods based on the rigorous scattering of light by a set of cylinders/spheres [49, 50]. The theory is very well explained in [49]. The photonic crystals are finite-sized. The main advantage of this method is that cylinders/spheres can be located anywhere in space. Accordingly, a periodic arrangement is just a particular case and it is possible to deal with a single defect without the need of a super-cell. In the same manner, it is very simple to change the geometry of the structure. Although limitations are linked to the size of the memory, a large number of cylinders has been implemented (about one hundred). As the dimension increases, the number of spheres must be smaller.

The use of diffraction gratings theory [51] allows the calculation of reflection and transmission coefficients of a PBG structure constituted of a stack of a finite number of infinite grating layers. The method can deal only with an infinitely long cavity as a defect for the structure. Moreover, to the best of our knowledge, this method can not simulate new PBG materials that are sophisticated doped and active structures.

Others methods of simulation are less often used: the oscillating dipole method [71–73], the real space green function method [74], the eigenmode expansion method [75], and the array scanning method [76].

6. MANUFACTURE OF PBGS

Several problems arise in manufacturing these structures. Of course, the difficulties encountered depend on the frequency domain wished. For the microwave domain, the typical size of the elementary cell constituting the PBG material is of the order of the centimeter or millimeter, and therefore can not generate any problem, generally speaking. For the optical domain, difficulties are highly significant. It is then necessary to evaluate tolerances of such materials [77–79]. The next section is devoted to a brief description of a few techniques used to build photonic crystals in the optical domain.

Many processes have been used to build photonic crystals. The most common successful processes are based on classic microelectronic fabrication. One of these techniques is the electron beam lithography and dry etching which provide three dimensions photonic crystals working in the optical domain [80]. In addition the layer-by-layer fabrication of diamond-like structure was successfully achieved in high refractive index semiconductors by using the wafer fusion technique in III-V [81]. Recently, Kawakami had the idea to fabricate 3D periodic

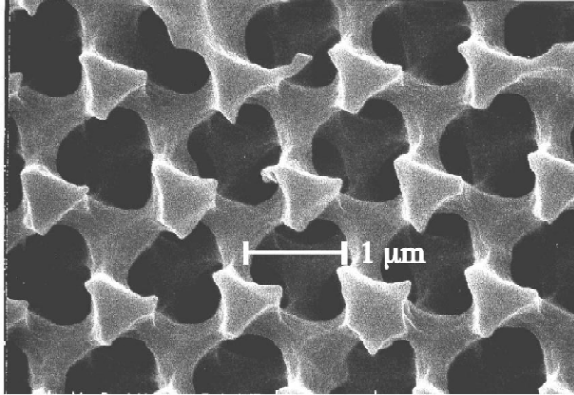


Figure 5. SEM photo of a 6.2-mm-thick PMMA Yablonovite template fabricated with a mask of $1.3\ \mu\text{m}$ period. Sample top view showing a (111) crystal plane (from Cuisin, C., A. Chelnokov, J.-M. Lourtioz, D. Decanini, and Y. Chen, *Appl. Phys. Lett.*, Vol. 77, No. 6, 770, 2000, reprinted by permission of the American Institute of Physics).

structures with a large number of periods using a thin film technology [82]. This method is based on an etching /sputtering growth technique. As a result, a three-dimensional photonic crystal with a hexagonal geometry is obtained with a lattice period inferior to $0.5\ \mu\text{m}$ and a very high accuracy. An advantage is the high flexibility to accommodate wave-guides, circuits and devices in general. A limitation is that it can not deal with all geometries. Finally, large-area face-centered cubic photonic crystals are fabricated by the two-dimensional shear-alignment of stabilized $720\ \text{nm}$ diameter PMMA spheres dispersed in an epoxy resin [83]. The resulting crystal is made permanent by exposure to UV light, thus solidifying the epoxy resin. The technique is rapid and produces high quality large-area crystals. An alternative approach consists in realizing porous templates for transferring the face-centered-cubic to high refractive index dielectrics or metals. Porous silica opal crystals and polymer photoresists can be patterned by holographic lithography. However this method cannot produce a photonic crystal with a local defect. [84, 85]. The templates may be also obtained using X-ray lithography of a poly-methyl-metacrylate (PMMA) resist. Three consecutive exposures to an X-ray beam produce a triangular lattice of holes. The different beam propagation directions correspond to the three different axes of a diamond-like structure [33]. In this reference the authors obtain 6 layers of a Yablonovite crystal in a $6.3\ \mu\text{m}$ thickness resin (Fig. 5).

7. APPLICATIONS

The following section will address the foreseen applications of the PBG materials. If in the optical domain these applications are still limited, they are already in practical development in microwave domain. In optical domain we could then consider new highly efficient opto-electronic devices such as very efficient laser diodes [86], micro-scale light circuits [58], multiplexers or demultiplexers [39] based on inhibition of spontaneous emission [87], photoluminescence [56–57, 74], wave-guiding, super-prism phenomenon [38, 39]. Studies of plasmon frequencies occurring for metal photonic crystals have also been led showing that the plasmon frequency can be controlled and could appear in the microwave region [28].

In the microwave domain the first applications appear. Many developments concern the direct control of the electromagnetic energy and its transmission: mirrors, electromagnetic windows, active radomes, radiation pattern control [87–90]. We find also the high impedance material of Sievenpiper [22] and the compact uniplanar PBG material proposed by Itoh [23–26]. Sievenpiper has proposed his structure as perfect magnetic wall to reduce the leaky waves in antenna array. The material developed by Itoh and co-workers allows the realization of magnetic wall for waveguides, low loss coplanar lines and compact integrated filter. Others applications include duplexers [91] and controllable PBG materials. Due to a certain easiness of fabrication in this frequency domain, the challenge of the electronically controlled photonic crystals has a significant interest. Recent works have demonstrated the capability to fabricate and to experimentally test these materials [5]. Industrial applications of these crystals are under development and concern mainly aerospace and telecom domains.

8. CONCLUSION

The principle of PBG materials and their very peculiar properties have been described in this paper. The properties of doped crystals are very similar to their semiconductor analogues. We have also reviewed the main numerical methods used to study PBG materials. All these methods are attractive and have proved their efficiency by comparison with experiments or others numerical calculations. Alternatively, despite significant progresses, it is still a real challenge to build a perfect photonic crystal in the optical domain. At microwave wavelength, the fabrication is easier and allows the insertion of electronic devices in the crystal. Analyzing the tolerances of such a material then becomes

necessary from an industrial point of view. At microwave frequencies, future studies should focus on telecom applications of passive and controllable PBG materials for which band gap frequency ranges and resonant peaks can be electronically controlled, and then should trigger very large potential of applications. This concept of controllability may be applied to doped crystal where only defects are active. Indeed, the entire structure of the crystal should be also controllable, including its dielectric or metallic properties. At optical frequencies the goal seems to be the fabrication of the crystal and the insertion of light sources (laser, quantum boxes, polymers) in this structure.

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