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The history and a review of the modelling and fabrication of photonic crystals

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Abstract
An overview of the theoretical and experimental efforts in obtaining a photonic bandgap, a frequency band in three-dimensional dielectric structures in which electromagnetic (EM) waves are forbidden, is presented. Photonic crystals offer unique ways to tailor light and the propagation of EM waves.

1. Introduction

Electron waves travelling the periodic potential of a crystal are arranged into energy bands separated by gaps where propagating states are prohibited. A semiconductor has a complete bandgap between the valence and the conduction energy bands. It is now known that analogous bandgaps can exist when electromagnetic (EM) waves propagate in a macroscopic periodic dielectric structure [1–3]. EM waves with frequencies inside such a gap cannot propagate in any direction inside the material. Such dielectric crystals like lattices have been referred to as photonic crystals (PCs) or photonic band-gap (PBG) materials [4, 5]. Although the periodicity in semiconductors is predetermined, the periodicity in the PCs can be changed at will. Such structures have been built in the microwave and recently in the far-infrared regime and their potential applications continue to be examined. However, the greatest scientific challenge in the field of PCs is to fabricate composite structures possessing spectral gaps at frequencies up to the optical region.

2. Photonic crystals with the diamond lattice symmetry

Ho *et al* [6] were the first to give a prescription for a periodic dielectric structure that possesses a full PBG rather than a pseudogap. This proposed structure is a periodic arrangement of dielectric spheres in a diamond-like structure. A systematic examination [6] of the photonic band structures for dielectric spheres and air spheres on a diamond lattice, as a function of the refractive index contrasts and filling ratios, was performed. It was found that PBGs exist over a wide region of filling ratios for both dielectric spheres and air spheres for refractive-index contracts as low as 2. However, this diamond dielectric structure is not easy to fabricate, especially in the micron and submicron length scales for infrared or optical devices. However, after we communicated our findings about the diamond structure, Yablonovitch very quickly devised [7] an ingenious way of constructing a diamond lattice. He noted that the diamond lattice is a very open structure characterized by open channels along the [110] directions. Thus, by drilling cylindrical holes through a dielectric block, a structure with the symmetry of the diamond structure can be created. Since there are six sets of equivalent [110] directions in the lattice, there are six sets of holes drilled. If the crystal is oriented such that the [111] surface is exposed, then three sets of these holes will be slanted at angles of 35.26° with respect to the normal [111] direction. The remaining three sets of holes have their axes parallel to the [111] surface and are harder to construct on a thin film oriented in the [111] direction. Thus, in the end, the experimentalists decided to abandon the second three sets of holes and construct a structure with only the first three sets of holes which became the first experimental structure that demonstrates the existence of a PBG, in agreement with the predictions [8] of the theoretical calculations. This is an example where theory has been successfully used to design dielectric structures with desired properties. In figure 1, we present the historical progress of the midgap frequency of three-dimensional (3D) PCs. Notice that the first 3D PC was fabricated in 1991 by Yablonovitch [7], while he was still at Bellcore.

3. Layer-by-layer photonic bandgap structures

The main challenge in the PBG field is the discovery of a 3D dielectric structure that exhibits a PBG but, in addition, can be built by microfabrication techniques on the scale of optical wavelengths. The search for simplifying the structure and reducing the dimensionality of the structural building blocks continues. The Iowa State group has designed [9] a novel 3D

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layer-by-layer structure that has a full 3D PBG over a wide range of structural parameters. The new structure (figure 2) consists of layers of one-dimensional rods with a stacking sequence that repeats every fourth layer with a repeat distance of c. The layer-by-layer structure was first fabricated [10] in the microwave regime by stacking alumina cylinders and demonstrated to have a full 3D PBG at 12–14 GHz.

An interesting class of PCs is the A7-family of structures [11]. These structures have rhombohedral symmetry and can be generated by connecting lattice points of the A7 structure by cylinders. The A7 class of structures can be described by two structural parameters—an internal displacement u and a shear α—that can be varied to optimize the gap. For special values of the parameters the structure reduces to simple cubic, diamond, and the Yablonovitch three-cylinder structure. Gaps as large as 50% are found [11] in the A7 class of structures for well-optimized values of the structural parameters and fabrication of these structures would be most interesting. It is worth noting that the FCC structure *does* have [12, 13] a true PBG between the eighth and the ninth bands. The FCC lattice does *not* have a PBG between the lowest bands (bands two and three).

4. Fabrication of photonic bandgap structures

There have been intensive efforts to build and test PBG structures, dating back to the original efforts of Yablonovitch [14] shortly after his first proposal for PBG crystals. Fabrication can be either easy or extremely difficult, depending upon the desired wavelength of the bandgap and the level of dimensionality. Since the wavelength of the bandgap scales directly with the lattice constant of the PC, lower frequency structures that require larger dimensions will be easier to fabricate. At microwave frequencies, where the wavelength is of the order of 1 cm, the PCs are decidedly macroscopic, and simple machining techniques or rapid prototyping methods can be employed in building the crystals. At the other extreme, optical wavelength PBGs require crystal lattice constants <1 μm. Building PBGs in the optical regime requires methods that push current state-of-the-art micro- and nano-fabrication techniques. In a similar manner, the dimensionality of the PBG has a big impact on the ease or difficulty of fabrication. Since one-dimensional (1D) PBGs require periodic variation of the dielectric constant in only one direction, they are relatively easy to build at all length scales. 1D PBG mirrors (more commonly known as distributed Bragg reflectors) have been used in building optical and near-infrared photonic devices for many years. Two common examples of devices using 1D PBGs are distributed feedback lasers and vertical-cavity surface-emitting lasers. Two-dimensional (2D) PBGs require somewhat more fabrication, but relatively mainstream fabrication techniques can be employed to achieve such structures. There are several examples of 2D PBGs operating at mid- and near-IR wavelengths [1]. Clearly, the most challenging PBG structures are fully 3D structures with bandgaps in the IR or optical regions of the spectrum. The fabrication of 3D PBGs is complicated by the need for large dielectric contrasts between the materials that make up the PBG crystal, and the relatively low filling fractions that are required. The large dielectric contrast means that the materials must be dissimilar, and often the low-dielectric material is air with the other material being a semiconductor or a high-dielectric ceramic. The low dielectric filling fraction means that the PBG crystal must be mostly air, while the high dielectric material must be formed into a thin network or skeleton. When these difficulties are combined with the need for micron or sub-micron dimensions to reach into the optical region, the fabrication becomes very difficult indeed. This area of PBG research has been one of the most active, and perhaps most frustrating, in recent years.

As we have discussed above, the first successful PBG crystal was fabricated by Yablonovitch [7] in the millimetre-wave region of the spectrum. Since 1991, both Yablonovitch and Scherer have been working towards reducing the size of the structure of micrometer length scales [15]. However, it is very difficult to drill uniform holes of appreciable depth with micron diameters. Consequently, Scherer's efforts were partially successful in producing a PBG crystal with a gap at optical frequencies. This is the reason why it is not included in figure 1.

Another approach was undertaken by a group at the Institute of Microtechnology at Mainz, Germany, in collaboration with the Research Center of Crete and Iowa State University. They fabricated PBG structures using deep x-ray lithography [16]. PMMA resist layers with a thickness of 500 μm were irradiated to form a 'three-cylinder' structure. In figure 3 a PC with a lattice constant of 114 μm made from negative tone resist is shown. Since the dielectric constant of the PMMA is not large enough for the formation of a PBG, the holes in the PMMA structure were filled with ceramic material. After the evaporation of the solvent, the samples were heat treated at 1000 °C, and a lattice of ceramic rods corresponding to the holes in the PMMA structure remained. A few layers of this structure were fabricated with a measured bandgap centred at 2.5 THz. This frequency and the fabrication year are shown in figure 1, and labelled with the name Liga. Recent experiments have attempted to fill the PMMA holes with metal.

The layer-by-layer structure shown in figure 2 was fabricated [17] by laser rapid prototyping using laser-induced direct-write deposition from the gas phase. The PGB structure consisted of oxide rods and the measured PBG was centred at 2 THz. This frequency and the fabrication year are shown in figure 1, and labelled with the name Germany. However, our calculations were unable to confirm those measurements. More experiments in this promising direction are needed.

Very recent work at the Sandia Labs by Lin [18], as well as at Kyoto University by Noda [19], have been able to grow up to five layers, of the layer-by-layer structure of the Iowa State University shown in figure 2, at both the 10 and 1.5 μm wavelengths. This is really a spectacular achievement. The measured transmittance shows bandgaps centred at 30 and 200 THz, respectively. They were able to overcome very difficult technological challenges, in planarization, orientation and 3D growth at micrometer length scales.

Finally, colloidal suspensions have the ability to spontaneously form bulk 3D crystals with submicron lattice parameters. Also, 3D dielectric lattices have been developed from a solution of artificially grown monodisperse spherical SiO_2 particles. However, both these procedures give structures

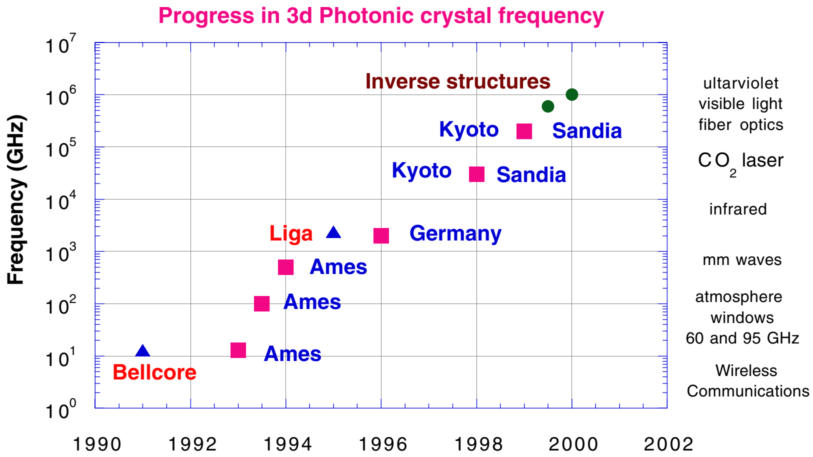

Figure 1. The frequency of the mid gap in GHz of 3D PCs versus the fabrication year. The triangular symbols denote the 'three-cylinder' suggested by Yablonovitch, the square symbols denote the layer-by-layer structure produced by the Ames Laboratory at Iowa State University and the circular symbols denote the inverse closed-packet structures.

(This figure is in colour only in the electronic version)

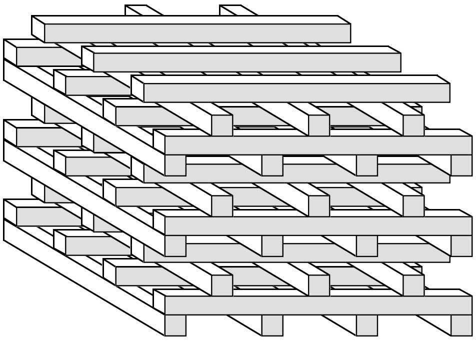

Figure 2. The layer-by-layer structure introduced by the Iowa State University group in 1993.

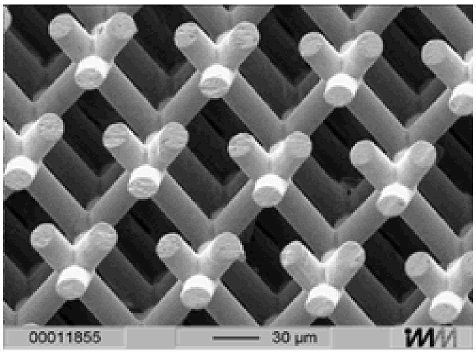

Figure 3. The 'three-cylinder' PC made from negative tone resist (from [16]).

with a quite small dielectric contrast ratio (<2), which is not enough to give a full bandgap. A lot of effort is being devoted to finding new methods in increasing the dielectric contrast ratio [20–27]. Several groups are trying to produce ordered macroporous materials from titania, silica, and zirconia by using the emulsion droplets as templates around which material is deposited through a sol-gel process. Subsequent drying and heat treatment yields solid materials with spherical pores left behind the emulsion droplets. Another very promising technique in fabricating PCs at optical wavelengths is 3D holographic lithography [28].

5. Photonic crystal waveguides and bends

One of the essential building blocks towards miniature PC-based photonic integrated circuits is a sharp bend. Light in PC waveguides is confined to, and guided along, the one-dimensional channel because the 3D PC prevents light from escaping in the bulk crystal. This property allows light to bend through sharp corners. However, it is still difficult to fabricate 3D structures at optical wavelengths. Recently, full confinement of EM waves has been experimentally demonstrated by utilizing the layer-by-layer structure [29]. Although Noda *et al* [19] have fabricated a 3D sharp bend waveguide in the layer-by-layer structure at optical wavelengths, no measurements have been reported yet.

Since the fabrication of 3D PCs at optical wavelengths is still a difficult process, an alternative method has been proposed. A three-layered dielectric structure is created in the vertical direction, with the central layer having a higher dielectric constant than the upper and lower dielectric layers. In such a structure, light is confined in the vertical direction by traditional waveguiding with dielectric index mismatch, and in the lateral direction by the presence of a 2D PC [30, 31]. There are two routes that have been followed, one where the upper and lower dielectric layers are air and the other where the upper and lower dielectric layers have dielectric constants smaller than the central layer by a value much higher than one. The first structure is called a self-supported membrane [32], while the second is referred to as a regular waveguide [33]. It is not yet resolved which structure has lower losses [32–36]. It is clear, however, that for optoelectronic applications the membrane-based PCs might not be easy to use. It is therefore of considerable importance to find out what type of structure has the lowest losses and the best efficiency of bends.

6. Conclusions

In summary, we have reviewed the efforts in obtaining 3D structures that possess a full PBG. The plane-wave results of Ho *et al* suggested the first structure to exhibit a true PBG, and the Yablonovitch 'three-cylinder' structure of diamond symmetry was the first experimental structure with a PBG. The layer-by-layer structure introduced by the Iowa State group has been proven to be the structure for the extension of photonic band crystals into the infrared and optical regimes; an area that will surely lead to new areas in basic physics together with novel applications. Both the Sandia Labs and Kyoto University groups have been able to fabricate PCs at 1.5 μm, which is the wavelength that most telecommunications take place. Another direction that is under intense study are 2D PC slabs [33, 36]. These structures exhibit a bandgap for propagation of radiation in the plane, and use total internal reflection for confinement in the third dimension. The key motivation for these studies is ease for fabrication. Clearly, the fabrication of 3D PC structures that does not require 3D periodicity is a very attractive suggestion, especially at micron and submicron length scales. Finally, PC fibres [37] might play an important role in optical applications.

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