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Photonic Band Gaps in Experimentally Realizable Periodic Dielectric Structures.

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Abstract. – By solving Maxwell's equations for the propagation of electromagnetic waves in periodic dielectric structures (with dielectric constant ε_b in a uniform background ε_a), we found that several classes of periodic dielectric structures possess full photonic gaps, as in the case of dielectric spheres arranged in the diamond structure. These new structures have the additional advantage that they can be easily fabricated experimentally.

Recently, there has been growing interest in the studies of the propagation of electromagnetic (e.m.) waves in three-dimensional (3D) disordered and/or periodic, dielectric structures (photonic band structures) [1]. The reasons for this interest are both fundamental and practical. The possibility of the observation of Anderson localization of e.m. waves in disordered dielectric structures and the possible existence of photonic band gaps in 3D periodic structures have been raised. The potential applications of such photonic band gaps are very interesting. It has been suggested [2] that the inhibition of spontaneous emission in such gaps can be utilized to substantially enhance the performance of semiconductor lasers and other quantum electronic devices. It has also been speculated that the absence of e.m. modes in the photonic gap will lead to new physical phenomena in many atomic, molecular, and excitonic systems [3, 4]. In addition, John [5] has proposed that Anderson localization of light near a photonic band gap might be achieved by weak disordering of a periodic arrangement of spheres.

It is, therefore, very important to obtain structures with a frequency gap where the propagation of e.m. waves is forbidden for all wave vectors. Yablonovitch and Gmitter [6] have demonstrated the soundness of the basic idea of photonic bands in 3D periodic structures in an experiment using microwave frequencies, where the periodic structures can be fabricated by conventional machine tools. In addition, a photonic gap in a face-centered-cubic (f.c.c.) dielectric structure was reported. During the same period, theoretical studies of the propagation of e.m. waves in 3D periodic structures began. At first, the photonic band structures have been examined theoretically only in the scalar-wave approximation [5, 7-10] in which the vector nature of the e.m. field is ignored. It soon became apparent [8, 9] that this approximation gives qualitatively incorrect results for the existence of photonic gaps.

Recently by expanding the e.m. fields with a plane-wave basis set, Maxwell's equations were solved exactly, taking the vector nature of the e.m. field fully into account [11-14]. Comparison of the calculated results [11-13] of the f.c.c. structure with experiment [6] indicated that while the experimental data and theory agree very well over most of the Brillouin zone, there are two symmetry points (W and U) where the experiment indicates a gap while calculations show that propagating modes exist. It is now believed that the f.c.c. structure (a structure that transforms like the space group O_h^5) exhibits a pseudogap rather than a full photonic band gap; that is, there is a region of low density of states rather than a forbidden frequency gap.

We were the first to give a prescription for a periodic dielectric structure [13] that possesses a full photonic band gap rather than a pseudogap. This proposed structure is a periodic arrangement of dielectric spheres in a diamond lattice structure. A systematic examination [13] of the photonic band structures for dielectric spheres and air spheres on a diamond lattice as a function of refractive index contrasts and filling ratios was made. It was found that photonic band gaps exist over a wide region of filling ratios for both dielectric spheres and air spheres for refractive-index contrasts as low as 2. However, this diamond dielectric structure is not easy to fabricate, especially in the micron or submicron length scales relevant for infrared or optical devices. It is therefore important to determine new periodic dielectric structures that possess full photonic gaps but at the same time are easier to fabricate.

We believe that theoretical work will play an important role in guiding experimentalists to find the optimum dielectric structures with the desired properties. It is by now well established that the plane-wave method has been used successfully to calculate photonic band structures based on the scalar wave approximation [5-9], as well as the full vector case [9-14]. The method is straightforward [8-13] and is capable of treating any periodic arrangement of objects with arbitrary shapes and filling ratios. We find that convergence is reasonably rapid for obtaining accurate band structures for the scalar as well as the vector wave case. Most of calculations reported here involve diagonalizing real symmetric matrices of the order of 750×750, which can be done quite easily with modern computers. On the other hand, experimentally one has to adopt a tedious cut-and-try approach in which dozens of different periodic structures with different refractive index contrasts and filling ratios have to be painstakingly machined out of low-loss dielectric materials. The process is both costly and time-consuming, and an exhaustive search for optimal structures is very difficult. We therefore have the unique opportunity to use theory to design dielectric structures with desired properties.

In this paper, we introduce new periodic dielectric structures that possess full photonic gaps and at the same time are easier to fabricate on the scale of optical wavelenghts. The photonic band structure problem is solved with the plane-wave expansion method, and technical details can be found elsewhere [13]. Here, we introduce three classes of periodic structures. The first class of structure corresponds to cylindrical rods connecting nearest-neighbor sites in a diamond lattice. The second class of structures can be created by drilling six sets of holes along the directions [1 1 0], [1 0 1], [0 1 1], [1 −1 0], [1 0 −1], [0 1 −1]. This procedure actually creates a diamondlike lattice. Examination of a ball-and-stick model of the diamond structure (fig. 1) readily reveals that one such set of holes corresponds to the open channels through the lattice. Operationally, three sets of holes can be drilled at 35.26° off the vertical into the top surface of a solid dielectric material, together with three additional sets of holes, all lying within the plane of the slab 120° apart. In addition, we have also studied a third structure which is a degradation of the second structure, retaining only the first three sets of holes ([1 1 0], [1 0 1], [0 1 1]). For each class of structure, there is always a «conjugate» structure where we interchange the role of the material and the empty space.

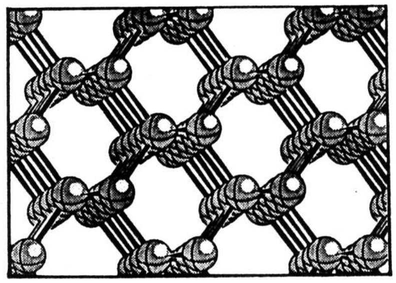

Fig. 1. – A «ball and stick» model of the diamond structure, viewed from an angle such that the channels along a [1 1 0] direction are easily observable. Drilling 6 sets of infinite cylindrical holes along [1 1 0] and equivalent directions results in a structure with full diamond symmetry. Shrinking the size of the «balls» while keeping the «sticks» result in the «rod» model discussed in the text.

We note that the first two classes of structures have the full diamond symmetry but the third class (the «3-cylinder» structure) has only the symmetry of a subgroup of the full diamond group. The «3-cylinder» structure with «air-cylinder» configuration can be fabricated by drilling or etching into a slab of materials as shown in the figure in ref. [15]. The «6-cylinder» structure can then be formed from the «3-cylinder» structure by drilling three more sets of holes in the plane of the slab and at 60° away from each other.

We have made a systematic examination of the photonic band structure for the three new periodic dielectric structures as a function of refractive index contrasts and filling ratios. We find that when we fix the refractive index at 3.6, photonic band gaps exist over a wide region of filling ratios for all three structures introduced above. In fig. 2, we plot the size of the forbidden gap normalized to the midgap frequency ($\Delta\omega/\omega_g$) *vs.* the filling ratio (f), for the first structure, *i.e.* connected rods (both «material» and «air rods») joining nearest-neighbor sites on a diamond lattice, with the refractive index contrast set at $n = 3.6$. There are a few

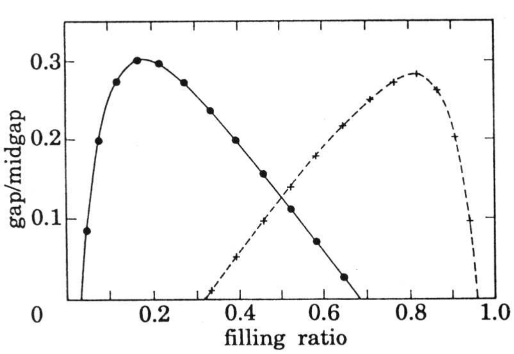

Fig. 2.

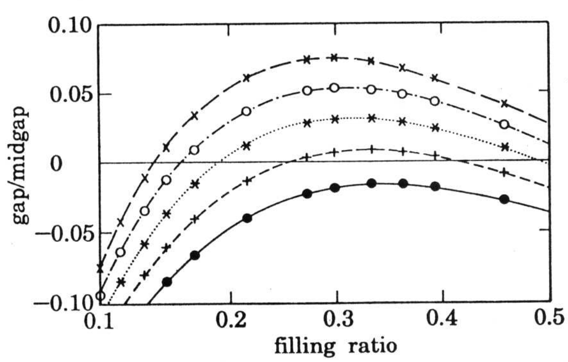

Fig. 3.

Fig. 2. – Gap-to-midgap frequency ratio ($\Delta\omega/\omega_g$) as a function of filling ratio for «material» rods (solid circles) and «air» rods (crosses) joining nearest-neighbors sites in a diamond lattice.

Fig. 3. – The search for the minimum refractive index contrast required for the onset of photonic gaps for the case of «material rods» connecting nearest-neighbor sites in a diamond lattice. The gap is defined as the bottom of the «conduction band» (3rd band) minus the top of the «valence band» (2nd band). The lines serve as a guide to the eye only. Negative gaps exhibited in the figure have no physical meaning other than highlighting the onset of the photonic gap as the refractive index contrast increases and the filling ratio changes. –●– $n = 1.8$, – – + – – $n = 1.9$, · · · ∗ · · · $n = 2.0$, – · –○– · – $n = 2.1$, – ∗ – $n = 2.2$.

points worth noting. First, the largest relative gap size $\Delta\omega/\omega_g$ occurs in the «material» rod configuration, achieving a maximum $\Delta\omega/\omega_g$ of over 30% at $f \sim 19\%$, whereas for the case of «air» rods, $\Delta\omega/\omega_g$ can reach 28% at $f \sim 80\%$. This structure by far has the largest $\Delta\omega/\omega_g$ in all the structures we have considered. Second, this structure also has the smallest refractive index contrast (slightly less than 1.9) required for the onset of the photonic gap (see fig. 3), which can be achieved with a material rod configuration with $f \sim 33\%$. Together with the fact that a material rod configuration is a self-supporting structure even for very low filling ratios, this structure deserves attention in future applications.

We plot in fig. 4 the calculed size of the forbidden gap normalized to the midgap frequency for the «6-cylinder» and «3-cylinder» structures discussed above with refractive index contrast fixed at $n = 3.6$. We note that appreciable photonic gaps exist in both classes of arrangements, and in both cases larger $\Delta\omega/\omega_g$ can be obtained with «air-cylinders» (corresponding to hole drilling) than «material-cylinders» (corresponding to building up structures with long solid cylinders pointing in 6 or 3 directions). In both classes of structures at refractive index contrast 3.6, maximum $\Delta\omega/\omega_g$ is reached for the case «air-cylinders» at $f \sim 80\%$, while for «material-cylinders» maximum $\Delta\omega/\omega_g$ occurs at a filling ratio of slightly above 20%. The maximum $\Delta\omega/\omega_g$ achievable and the corresponding filling ratio depend on the refractive index contrast, although the general shape is essentially the same as depicted in fig. 4 (where $n = 3.6$). The «6-cylinder» arrangement always has a larger gap than the «3-cylinder» arrangement, and the maximum gap achievable decreases monotonically with decreasing refractive index contrast. At lower contrasts, the peaks in $\Delta\omega/\omega_g$ as a function of the filling ratio for «air-cylinder» and «material-cylinder» configurations move towards each other. Although the «3-cylinder» arrangement has a smaller gap, the maximum $\Delta\omega/\omega_g$ achievable with $n = 3.6$ is still appreciable (over 19% with an «air-cylinder» configuration at a filling ratio of 79%), and this structure is easier to fabricate than the «6-cylinder» arrangement. The «3-cylinder» arrangement has been successfully fabricated and the existence of photonic gaps has been verified [15]. We also investigated the minimum refractive index required to obtain a true photonic gap for the «3-cylinder» arrangement (see fig. 5), and we found that the smallest contrast required is $n \sim 2.1$, and can be achieved with an «air-cylinder» configuration at a filling ratio of about 70%.

The frequency gap sizes quoted in this paper are all normalized to the midgap frequency

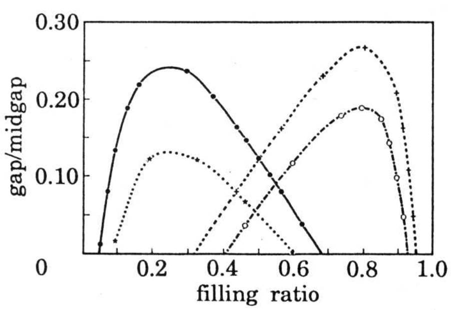

Fig. 4.

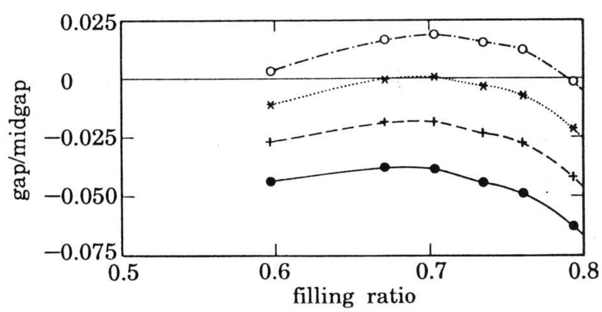

Fig. 5.

Fig. 4. – Gap-to-midgap frequency ratios for the cases of 6- and 3-cylinder arrangements. Solid circles and stars are for 6 sets and 3 sets of «material» cylinders, respectively, while crosses and empty circles are for 6 and 3 sets of «air» (empty) cylinders, respectively. The refractive index is fixed at $n = 3.6$.

Fig. 5. – The search for the minimum refractive index contrast required for the onset of photonic gaps for the «3-air-cylinder» arrangement. The lines serve as a guide to the eye only. See also the remarks in the caption for fig. 3. –●– $n = 1.9$, –+– $n = 2.0$, ···∗··· $n = 2.1$, –·○·– $n = 2.2$.

ω_g, which for a given structural arrangement is given by $\omega_g = \xi(1/\langle n \rangle)(c/a)$ where c is the speed of light, a is the cubic «lattice constant» (repeat distance) of the periodic structure, and $\langle n \rangle$ is the square root of the volume-averaged dielectric constant of the material. The proportionality constant ξ is governed by the dielectric constant constrast ratio and the geometrical structure of the periodic material, and can be determined numerically from calculation. For a material with $n = 3.6$, the maximum photonic gap for a «6-cylinder» arrangement centered at a wavelength of 0.5 μm ($\omega_g = 6 \times 10^{14}$ Hz) can be obtained by drilling empty cylinders of radius at about 0.063 μm to form a periodic structure with a lattice constant of 0.283 μm, while the maximum gap for a «3-cylinder» arrangement can be obtained by drilling cylinders of radius 0.066 microns to form a periodic lattice with lattice constant 0.278 μm. Both the «6-» and «3-cylinder» configuration would then have an «air» filling ratio close to 80%, and the maximum gap sizes are 1.62 and 1.14×10^{14} Hz, respectively. We also note that the «rod» structure and the «6-cylinder» structure discussed here can be classified as diamond structures, in the sense that they transform like the space group O_h^7 and thus have the same symmetry properties as a diamond lattice. The «3-cylinder» structure is basically a structural arrangement that strikes a compromise between structural perfection («6-cylinders» would be better) and the ease of fabrication (but 3 cylinders are easier to drill). It is gratifying that the minimum refractive index contrast required to open up photonic gaps for these structural arrangements is around 2, which suggests that it will be possible to fabricate materials with photonic gaps in the visible, since there are many optical materials available with a refractive index above 2.1.

In summary, we have demonstrated that a systematic search for the structures that possess optimal photonic gaps can be conducted via theoretical calculations. Practical three-dimensional periodic arrangements of dielectric structures are proposed. These new dielectric structures possess a full photonic gap, with refractive-index contrasts as low as 1.9, and should be much easier to fabricate than dielectric spheres arranged in the diamond lattice. We hope that these findings can be verified in future experimental measurements, and therefore the applications of photonic gaps in different areas of physics and engineering may become possible.

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