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PHOTONIC BAND GAPS IN THREE DIMENSIONS: NEW LAYER-BY-LAYER PERIODIC STRUCTURES

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A new three-dimensional (3D) periodic dielectric structure constructed with layers of dielectric rods of circular, elliptical, or rectangular shape is introduced. This new structure possesses a full photonic band gap of appreciable frequency width. At midgap, an attenuation of 21 dB per unit cell is obtained. This gap remains open for refractive indices $n \geq 1.9$. Furthermore, this new 3D layer structure potentially has the additional advantage that it can be easily fabricated using conventional microfabrication techniques on the scale of optical wavelengths.

It is now well accepted that the existence, in periodic dielectric structures, of a frequency gap where the propagation of electromagnetic (EM) waves is forbidden for all wave vectors, can have a profound impact on several scientific and technical disciplines[1,2] It is, therefore, very important to find 3D and 2D periodic structures that possess a full photonic band gap and can be easily fabricated experimentally. Yablonovitch and Gmitter[3] have demonstrated the soundness of the basic idea of photonic bands in 3D periodic structures in an experiment using microwave frequencies, where a pseudogap was obtained for the face-centered-cubic (fcc) structure. Theoretical calculations of Ho, Chan, and Soukoulis in 3D have shown that periodic dielectric materials with a diamond[4] or diamond-like structure[5] can indeed have photonic band gaps. One of these structures, the "3-cylinder structure" consisting of three sets of cylinders drilled into a dielectric material at 35.26 degrees off normal, has been fabricated[6] in the millimeter length scale and shown to exhibit a full photonic gap in the microwave region, in agreement with theoretical predictions.[5,6] This is a successful example where theory was used to design dielectric structures with desired properties. Narrow photonic band gaps have also been found[7] in a simple cubic geometry. For 2D systems,[8-10] theoretical studies[8-9] have shown that a triangular lattice of air columns in a dielectric background is the best overall 2D structure, which gives the largest photonic gap with the smallest index contrast. In addition, it was demonstrated[11-14] that lattice imperfections in a 2D and/or 3D periodic arrays of a dielectric material can give rise to fully localized EM wave functions. Experimental investigations of the photonic band gaps have been mostly done[6,11,13,14] at microwave frequencies because of the difficulty in fabricating ordered dielectric structures at optical length scales. In fact, the main challenge in the photonic band gap field is the discovery of a 3D dielectric structure that exhibits a photonic gap, which can be built by microfabrication techniques on the scale of optical wavelengths.

In this paper, we introduce a new 3D layer periodic structure that possesses a full photonic band gap and at the same time is easier to fabricate on the scale of optical wavelengths. The photonic band gap problem is solved with the plane-wave expansion method, and the technical details can be found elsewhere.[4] In addition, the transmission coefficient versus the incident frequency is calculated with the recently developed method of Pendry and MacKinnon.[5] The transmission studies give also the attenuation and can be directly compared with experiment.

The new structure is made of layers of dielectric rods with a stacking sequence that repeats itself every four layers with a repeat distance of c. Within each layer, the rods are arranged with their axes parallel and separated by a distance, a. The orientations of the axes are rotated by 90 degrees between adjacent layers. To obtain a periodicity of four layers in the direction of stacking, the rods of second neighbor layers are shifted by a distance of 0.5a in the direction perpendicular to the rod axes. For $\frac{c}{a} = \sqrt{2}$ the lattice can be considered as an fcc primitive unit cell with a basis of two rods, otherwise, the lattice symmetry is face centered tetragonal (fct). This layered structure can be derived from the diamond lattice by replacing the (110) chains in the diamond structure by these rods. An example of the stacking sequence is indicated in Fig. 1 for a square-rod structure. We will define the z-axis to lie along the stacking direction, and the x- and y-axes to be at 45° to the axes of the rods within the layers. Based on the above stacking sequence, this new structure can have the following variations: (i) The structure should be made out of materials having different refractive indices. We can choose to have the high dielectric materials forming the rods, or we can choose the structure to have cylindrical holes of low dielectric material in a block of high dielectric material. (ii) The ratio of the height, c, of the layer in the z-direction to the repeat distance, a, along the layer can be varied to optimize the band gap. (iii) The cross-sectional changes of the rods are not critical to the performance of the structure, in fact, circular, elliptical or rectangular cross-sections with various aspect ratios also demonstrated sizable photonic gaps. (iv) The rods between two layers can be touching each other or can overlap to a certain extent. We show in Fig. 2 our calculated photon bands for the new structure, consisting of touching dielectric rods with refractive index n=3.6 and filling ratio f = 26.6%. We find there exists a full photonic band gap in which EM waves are forbidden to propagate in any direction. The frequency at which the

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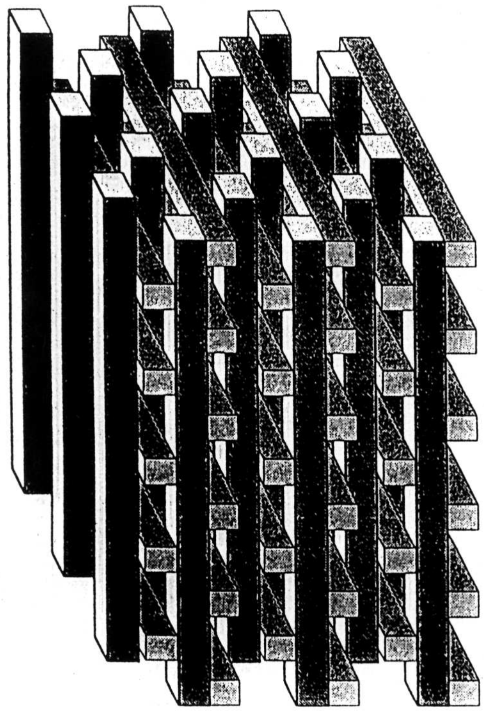

FIG. 1 This figure schematically illustrates the design of the new 3D photonic band gap crystal based on dielectric rods. The structure is built by an orderly stacking of dielectric rods (rectangular in the case shown).

lowest photon gap is centered (called the "midgap" frequency) is inversely proportional to the repeat distance a. For example, to obtain a frequency gap in optical frequencies, the repeat distance will be submicron, while for microwaves, the repeat distance will be in the millimeter range. Models of this new structure were fabricated[16] in the millimeter length scale and experimentally shown[16] to possess a full photonic band gap in the microwave region, in agreement with the predictions of our theoretical calculations. We have made a systematic examination of the photonic band gaps of the above structures. For proper choices of refractive index contrasts and volume ratios, the structures exhibit full photonic band gaps of appreciable widths.

In all the cases we examined, the distance, a, between the layers was kept constant and the width, w, of the rods was varied to change the filling ratio. We found that when we fixed the refractive index at 3.6, photonic band gaps exist over a wide region of filling for both dielectric cylinders and cylindrical holes. We plot in Fig. 3 the calculated size of the forbidden gap normalized to the midgap frequency for both cases. For cylindrical holes arranged in the way shown in Fig. 1 a maximum gap to midgap ratio $\Delta\omega/\omega_g$ of 25% is found at $f \simeq 82\%$, whereas for the case of dielectric rods $\Delta\omega/\omega_g$ can reach 18% at $f \simeq 30\%$. In both of these cases, the ratio of the repeat distance in the z-direction (c) to the repeat distance in the x-and y-directions (a) is taken to be 1.414 and the cylinders or cylindrical holes are allowed to overlap. We have also performed calculations for either cylindrical holes and dielectric cylinders, with elliptical cross sections of different aspect ratios. The results are not very sensitive to the aspect ratio, in particular for aspect ratios of to 1.25 the $\Delta\omega/\omega_g$

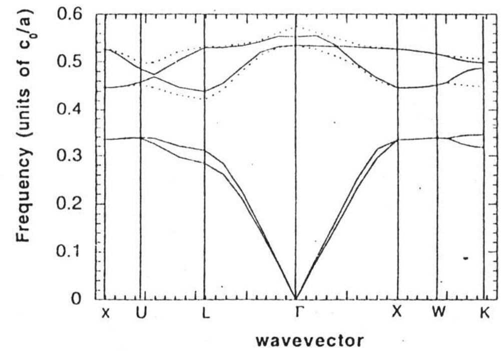

FIG. 2 Calculated photonic band gap for the new 3D layer dielectric structure (shown in Fig. 1) consisting of rectangular rods of refractive index 3.6 in an air background. The filling ratio of the dielectric material is 26.6%. The frequency is given in units of c_0/a, where c_0 is the velocity of light in vacuum and a is the distance between the rods in the x- and y- directions. In this case c/a=1.22. Bands are plotted along important symmetry lines of the Brillouin zone.

can reach 28% at $f \simeq 82\%$ for the cylindrical hole case. We have also performed calculations for dielectric cylinders with rectangular cross-section of different aspect ratios. The dependence of $\Delta\omega/\omega_g$ of touching rectangular rods with n=3.6 on the ratio c/a is shown in Fig. 4. Notice that there is an optimum value of c/a that gives the maximum $\Delta\omega/\omega_g$. As c/a increases above 1.5 or decreases below 0.8, the maximum gap to midgap ratio decreases dramatically. We found that the circular, elliptical, and rectangular dielectric rods give roughly similar results, if the filling ratio, f, the refractive index, n, and the ratio c/a are kept constant in each case indicating insensitivity of photonic band gap to structural details.

Another important fact that our theoretical calculations give for this new layer structure is the minimum refractive index contrast required for the onset of photonic band gaps. It is found that a minimum refractive index contrast around 1.9 is necessary to produce a photonic band

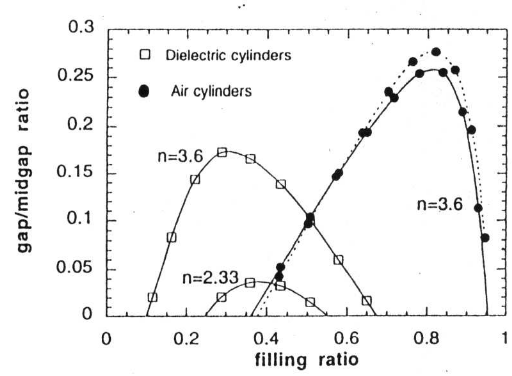

FIG. 3 Gap to midgap frequency ratio ($\Delta\omega/\omega_g$) as a function of the filling ratio for the case of dielectric rods in air and cylindrical holes in a dielectric. The refractive index of the material is chosen to be 3.6 and 2.33, and c/a=1.414. The dotted line is for cylindrical holes with elliptical cross section and aspect ratio of 1.25, for which the largest band gap was found.

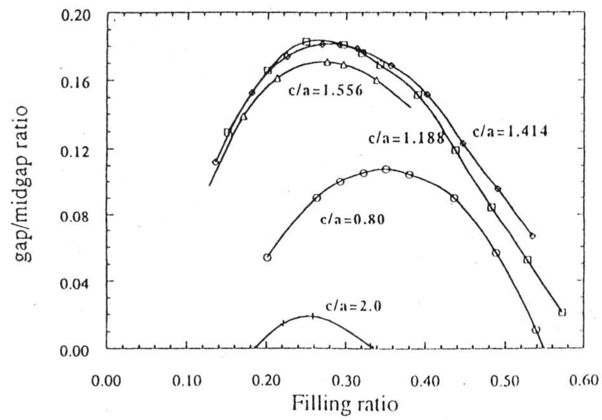

FIG. 4 Gap to midgap ratio ($\Delta\omega/\omega_g$) as a function of filling ratio for touching rectangular dielectric rod structures (shown in Fig. 1) with different c/a ratios and n=3.6. For each curve, the filling ratio was varied by changing the width of the rods and keeping c and a constant.

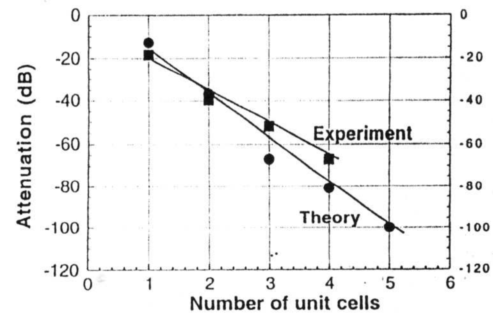

FIG. 5 Log of the attenuation coefficient at midgap versus the number of unit cells for the layer structure shown in Fig. 1. The refractive index of the cylindrical alumina rods is 3.1, their diameter is 0.318cm and the distance a between the rods in a plane is 1.123cm. The solid circles present the theoretical results, while the solid squares are the experimental results.

gap in these structures. This is very important, because in the optical region there are many transparent optical materials available with a refractive index above 1.9.

All the results presented above were obtained with the plane-wave expansion technique, which gives accurate band structures for EM waves propagating in either 2D or 3D periodic dielectric structures. The plane-wave expansion technique for EM waves is now well developed. However, most of the theoretical techniques concentrate on the calculation of the dispersion of the photon bands in the infinite periodic structure, while experimental investigations focus mainly on the transmission of EM waves through a finite slab of the photonic band gap patterned in the required periodic structure. Even with the knowledge of the photon band structure, it is still a non-trivial task to obtain the transmission coefficient for comparison with experiment. Another quality important for the design of photonic band gap experiments and devices is the attenuation length for incident EM waves inside the photonic band gap. Another topic of interest is the behavior of impurity modes associated with the introduction of defects into the photonic band gap structure. While this problem can be tackled within a plane wave approach using the supercell method[11,12] where a single defect is placed within each supercell of an artificially periodic system, the calculations require prohibitive amounts of computer time and memory. Recently, Pendry and MacKinnon[15] introduced a complimentary technique for studying photonic band gap structures. Their method has the advantage that the transmission coefficients and attenuation coefficients for incident EM waves of various frequencies can be obtained directly from the calculations. We have also calculated the transmission coefficient for the new structure introduced here and fabricated and measured in the microwave regime by Ref. 16. The theoretical results agree reasonably well with the experiment. To support this statement, we present in Fig. 5 the experimentally measured and the theoretically calculated attenuation at the midgap versus the number of unit cells. At midgap we theoretically find an attenuation of 21 dB per unit cell, while the experiment gives a value of 17 dB per unit cell. This information is very important, since it clearly states that the photonic band gap crystal need not be many layers thick to expel the EM wave effectively. Our theoretical calculations suggest that even a two conventional unit cell structure (for a total of 8 stacked layers) will give a photonic band gap with 42 dB attenuation, which is large enough for many applications. We also want to stress that the transmission coefficient method can be efficiently used even in cases where the dielectric constant, ε, is frequency dependent or when ε has large imaginary values.

In conclusion, we have introduced a new and very practical 3D periodic dielectric structure constructed out of layers of dielectric rods. This new structure possesses a full photonic gap, for refractive index contrasts as low as 1.9. Furthermore, this new 3D layer structure is amenable to fabrication at a submicrometer scale by conventional epitaxial methods, and, therefore, one avoids the problems associated with drilling holes by reactive ion etching. Finally, our band structure results for this new structure are complemented by studies of the transmission coefficient versus frequency, which directly compare with experiments. At midgap an attenuation of 21 dB per unit cell is obtained, which suggests that only a few layers are needed to produce photonic band gap materials with appreciable attenuation (more than 50 dB). This new structure has the potential to solve the only outstanding problem in the photonic band gap field, that is the microfabrication of a photonic structure at optical wavelengths.

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