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# Photonic band gaps in a two-dimensional graphite structure

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We present a design of two-dimensional periodic dielectric structures that gives rise to absolute band gaps common to $E$ and $H$ polarized waves. This structure is formed by an arrangement of parallel cylindrical rods centered at the vertices of regular hexagons. We show that two absolute band gaps exist for lattices of dielectric rods in air. Potential application of this structure at the submicrometer length scale is discussed.

It is well known that the presence of periodic potential introduces energy gaps at Bragg planes and prevents the propagation of waves with energy lying in these gaps. The properties of electronic waves in crystals have been intensively studied, and the electronic band structure expresses the relation between the energy and the wave vector of the Bloch waves. It has been proposed[1,2] that dielectric structures with periodic variation of the dielectric constant should give rise to similar phenomena for the propagation of the electromagnetic waves, so long as the wavelength is comparable to the spatial periodicity. This appealing analogy has led to numerous works[3] since the suggestion that such systems could inhibit spontaneous emission and improve the performance of optical devices. The experimental realizations of photonic band gaps (PBG's) have first been confined to the microwave region for which the wavelength is of the order of a millimeter and the existence of PBG's has been observed in three-dimensional (3D) structures. The difficulty in the fabrication of these materials at optical-length scale prevents, at the present time, the realization of such structures for submicrometer wavelength; they are particularly attractive because they present gaps in the near infrared. In this frequency range, 2D structures obtained as periodic arrangements of parallel dielectric rods have recently begun to receive some attention. For in-plane propagation, two types of electromagnetic modes can be defined according to whether the electric ($E$ polarization) or magnetic ($H$ polarization) field is parallel to the rod axis. Several structures have been found to yield PBG's for either polarization. Indeed, it is difficult to obtain structures in which the two kinds of gaps overlap, inhibiting the in-plane propagation of the light whatever the polarization. Among the various structures recently considered, the triangular lattice of air cylinders in dielectric materials was found to possess interesting PBG's for a large-volume fraction of air.[4–6] Theoretical investigations have been performed to optimize the lateral design of these lattices by reduction in the lattice symmetry and by changes in the shape of the cross section of the rods.[7] Beyond the difficulties of realizing such structures, these studies have shown that any deviation from the circular shape of the cylinders reduces the width of the gaps, and the triangular lattice of hole cylinders with a circular cross section appears as a good design to realize 2D PBG materials. To obtain a large absolute band gap, the cylinder diameter must be close to the lattice parameter. Such structures require the etching of cylinders separated by very thin semiconductor layers, which is difficult to realize. To avoid this inconvenience, another possibility of having large band-gap structures can be researched in the modification of the structure factor, which only depends on the disposition of the cylinders in the unit cell and not on the shape of their cross section. This internal structure can vary the properties of the photonic crystal without changing in the Bravais lattice, which can remain hexagonal. Taking advantage of this situation, we propose in this paper a design for 2D structures that gives rise to large absolute PBG's and avoids the fabrication of thin layers. This structure is derived from the triangular lattice by the removal of one every third cylinder, so that the 2D graphite structure is obtained with cylinders centered on the vertices of a plane lattice of hexagons. Our calculations show that two absolute band gaps are achieved in the graphite structure of GaAs rods in air when the diameter of the cylinders-to-lattice constant ratio varies in a large range, far from the close-packed condition.

To determine the photonic band gaps, we study the propagation of the electromagnetic waves from the Maxwell equations. In inhomogeneous dielectric materials, the magnetic field $\mathbf{H}(\mathbf{r})$ is

$$\nabla\times[\eta(\mathbf{r})\nabla\times\mathbf{H}(\mathbf{r})]=\frac{\omega^2}{c^2}\mathbf{H}(\mathbf{r}), \tag{1}$$

where $\eta(\mathbf{r})$ is the inverse of the dielectric constant. Because of the relation $\nabla\cdot\mathbf{H}(\mathbf{r})=0$, $\mathbf{H}(\mathbf{r})$ is transverse. For periodic systems, it can be expressed as a sum of plane waves:[8]

$$\mathbf{H}(\mathbf{r})=\sum_{\mathbf{G}}\sum_{\lambda=1}^{2} h_{\mathbf{G},\lambda}\hat{\mathbf{e}}_\lambda e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}, \tag{2}$$

where $\mathbf{k}$ is the wave vector in the first Brillouin zone and $\mathbf{G}$ are reciprocal lattice vectors. $\hat{\mathbf{e}}_\lambda$ denotes two unit vectors perpendicular to $\mathbf{k}+\mathbf{G}$. So, the problem is reduced to an eigenvalue equation solved by numerical techniques. In the following, we investigate the in-plane propagation of electromagnetic waves in 2D lattices of cylinders perpendicular to the $x,y$ plane of the lattice. Two different polarizations $E$ ($H$) have to be studied according to whether the electric (magnetic) field is parallel to the cylinders. The eigenvalue equation can be separated into two equations:

$$\det\left(\mathscr{H}-\frac{\omega^2}{c^2}\right)=0, \tag{3}$$

where

 

$$\mathscr{H}(\mathbf{G},\mathbf{G}') = |\mathbf{k}+\mathbf{G}||\mathbf{k}+\mathbf{G}'|\,\eta(\mathbf{G}-\mathbf{G}') \tag{4}$$

for the $E$ polarization, and

$$\mathscr{H}(\mathbf{G},\mathbf{G}') = (\mathbf{k}+\mathbf{G})\cdot(\mathbf{k}+\mathbf{G}')\,\eta(\mathbf{G}-\mathbf{G}') \tag{5}$$

for the $H$ polarization.

Here, $\eta(\mathbf{G})$ is the Fourier transform of the inverse of $\varepsilon(\mathbf{r})$. The difference between the two polarizations lies in the fact that $\mathscr{H}(\mathbf{G},\mathbf{G}')$ depends on the scalar product of the two vectors for the $E$ polarization and on the product of their modulus in the $H$ polarization. The summation on the reciprocal lattice only depends on the Bravais lattice, whereas for the same Bravais lattices $\eta(\mathbf{G})$ varies with the exact symmetry of the configuration. Consider a lattice with a unit cell formed by $N_c$ identical cylinders of material characterized by the dielectric constant $\varepsilon_a$, centered on $\mathbf{u}_j$ positions and embedded in a background of dielectric constant $\varepsilon_b$. $\eta(\mathbf{G})$ is given by

$$\eta(\mathbf{G}) = \varepsilon_b^{-1}\delta_{\mathbf{G}0} + S(\mathbf{G})\,\eta_c(\mathbf{G}), \tag{6}$$

where $S(\mathbf{G})$ is the structure factor

$$S(\mathbf{G}) = \sum_{j=1}^{N_c} e^{-i\mathbf{G}\cdot\mathbf{u}_j} \tag{7}$$

and $\eta_c(\mathbf{G})$ corresponds to the Fourier transform for a cylinder centered at the origin. For cylinders with circular section, the Fourier transform $\eta_c(\mathbf{G})$ only depends on the modulus $G$. Some other shapes of the cylinder section have been considered in order to optimize the photonic band gaps.[7] However, any deviation from the circular form reduces the width of the superposition of the $E$ and $H$ band gaps. The various arrangements of the cylinders in the unit cell correspond to different structure factors and give an additional parameter to modify the Fourier transforms for the same Bravais lattice. This provides a potential for tailoring PBG materials while conserving the lattice symmetry, which is important to obtain large gaps.

The 2D periodic structure shown in Fig. 1 allows us to describe the configuration studied in this work. By analogy with the crystal structure of the graphite, we call graphite structure this two-dimensional arrangement of hexagons. There are two cylinders of radius $R_c$ per unit cell at the positions $\mathbf{u}_1$ and $\mathbf{u}_2$. If we only consider nonoverlapping cylinders, the maximum filling factor $\beta = 60\%$ is reached when the cylinder diameter is equal to the distance $a$ between the centers of two nearest-neighbor cylinders. We examine the two following configurations. The first one consists of hole cylinders ($\varepsilon_a = 1$) in a material of dielectric constant $\varepsilon_b = 13.6$, which corresponds to GaAs. The second one is formed by cylinders of the same material in air. We have chosen GaAs because this material presents interesting optical properties in the infrared domain and is representative of many semiconductors. This limitation is not essential and calculations on other systems of the same nature give similar results. We use 475 plane waves in the calculation, which ensures sufficient convergence for the frequencies of interest for studied structures. Hereafter, we denote by $E_i$ ($H_i$) the gap that occurs between the $i$th and $(i+1)$th bands for $E$ ($H$) polarization.

Figure 2 shows the gap variation up to the close-packed

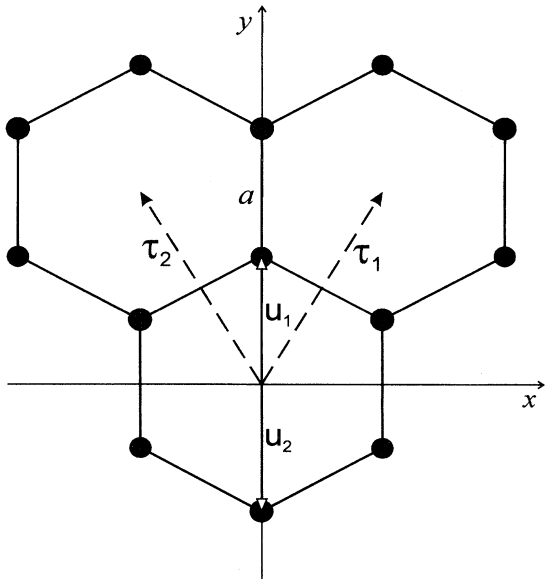


FIG. 1. Two-dimensional graphite structure. $\tau_1$ and $\tau_2$ are the primitive lattice vectors.

configuration of the cylinders. The first gap only appears for $R_c = 0.2a$ whereas most of the other gaps open for $R_c = 0.3a$. The gaps occurring for the $E$ polarization get broader with increasing values of $R_c$, the maximum value being obtained for close-packed cylinders. Two gaps $H_3$ and $H_5$ exist in $H$ polarization in the same frequency range. The $H_5$ gap lies to higher energy and its maximum relative width of 15% is reached for $0.46a$. These gaps close for small and high $R_c$ values. No absolute PBG resulting from the super-

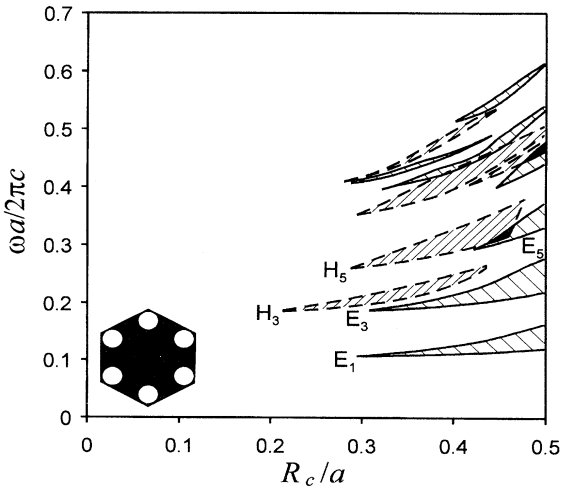


FIG. 2. Photonic band gaps for $E$ polarization (solid line) and $H$ polarization (dashed line) of a graphite structure of air cylinders in GaAs as functions of the ratio $R_c/a$. The absolute band gaps are represented in black.

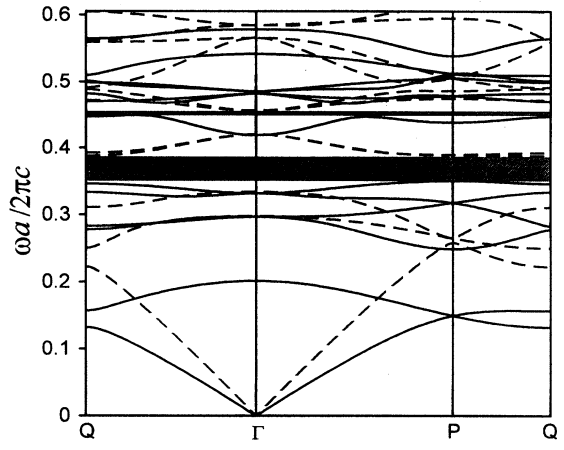


FIG. 3. Photonic band structure for $E$ polarization (solid line) and $H$ polarization (dashed line) of a graphite structure of GaAs cylinders in air for $\beta=30\%$. The symmetry points are labeled using the Lommer notations (Ref. 9) $\mathbf{k}_P=(2\pi/a\sqrt{3})(\frac{2}{3},0)$, $\mathbf{k}_Q=(2\pi/a\sqrt{3})(\frac{1}{2},1/2\sqrt{3})$.

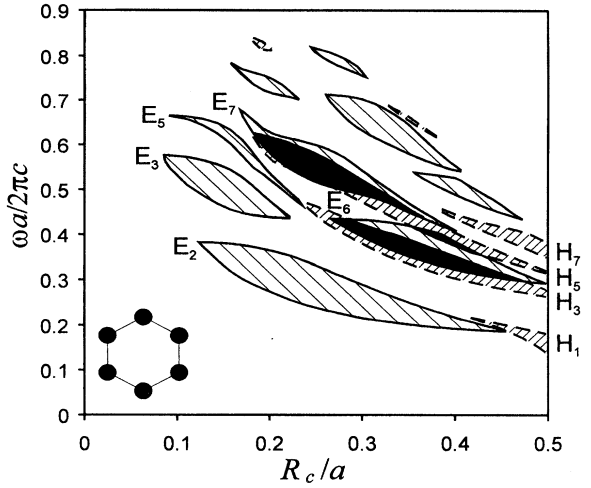


FIG. 4. Photonic band gaps for $E$ polarization (solid line) and $H$ polarization (dashed line) of a graphite structure of GaAs cylinders in air as functions of the ratio $R_c/a$. The absolute band gaps are represented in black.

position of the $E$ and $H$ gaps exists apart from a weak overlap of $E_5$ and $H_5$ lying in a very small range around $R_c=0.45a$. The photonic band structures for lattices of air cylinder in dielectric material present some similarities with the band structure of triangular lattices of dielectric cylinders in air. Results for $E$ polarization have the same features as those obtained for triangular lattices.[7] In particular, the sequence of the states and the opening of the gaps are the same. This resemblance can be easily understood from the geometric disposition of the cylinders in the graphite structure. For a close-packed arrangement, this configuration is equivalent to a triangular lattice with lattice constant $a\sqrt{3}$, formed by dielectric rods with a noncircular section.

We have also examined the case of a graphite structure formed of cylindrical GaAs rods in air. In Fig. 3, we display the photonic band structure of such a lattice for filling factor $\beta=30\%$. Three gaps $E_2$, $E_6$, and $E_7$ are present in the energy range considered. The $E_2$ and $E_6$ gaps result from the lifting of the degeneracy of the same free-photon state at $\Gamma$ point. The photonic band structure calculated for $H$ polarization shows two gaps $H_3$ and $H_5$ larger than for a lattice of hole cylinders with the same filling factor. The variation of these gaps as functions of the radius of the dielectric rods is represented in Fig. 4. The most important result is the appearance of absolute band gaps, unlike the triangular structure, which exhibits no absolute PBG for GaAs rods.[7] They exist in a limited frequency range and their widths present maxima which can be large. The lowest gap resulting from the overlap of $E_6$ and $H_3$ gaps is centered near $\omega a/2\pi c=0.37$ for $R_c=0.35a$ ($\beta=30\%$) with a 10% relative width. A second absolute band gap of the same width is obtained for $\omega a/2\pi c=0.55$ for $R_c=0.25a$ ($\beta=15\%$) by the superposition of $E_7$ and $H_5$ gaps. Finally, a smaller gap due to $E_6$ and $H_5$ gaps lies in the neighborhood of the latter one. The appearance of these gaps is essential and shows that the graphite structure of dielectric rods is a good candidate for the realization of the PBG materials. These values can be compared to the results obtained for the triangular structure of hole cylinders in GaAs.[7] The PBG is centered for this structure near $\omega a/2\pi c\approx 0.40$ for a filling factor $\beta\approx 76\%$, which corresponds to $R_c=0.45a$. As $\beta$ is the fraction of the total volume of the structure occupied by the rods in lattices of hole cylinders, the relative part occupied by the dielectric material is $1-\beta=24\%$. This proportion of material is close to the value obtained for the center of the $E_6$-$H_3$ absolute band gap in the graphite structure of dielectric cylinders; as a consequence, the mean dielectric constant is the same in the two structures. In the submicrometer range, it is possible to center the $E_7$-$H_5$ absolute band gap in the near infrared at $\lambda=0.9$ $\mu$m by realizing the graphite structure of GaAs rods of $R_c=0.12$ $\mu$m distant by $a=0.50$ $\mu$m. The same analysis for the $E_6$-$H_3$ absolute band gaps gives $a=0.34$ $\mu$m and $R_c=0.12$ $\mu$m. In these two structures, the diameter of the rods equal to 0.24 $\mu$m is large and does not require etching of thin dielectric layers.

We have presented a design of a 2D PBG crystal. This structure is formed by an arrangement of parallel dielectric rods of circular cross section, the centers of which are at the vertices of regular hexagons. Two absolute band gaps resulting from the overlap of $E$ and $H$ polarization band gaps are obtained for the rod diameter, which avoids the tricky achievement of thin dielectric layers. The existence of two photonic band gaps gives a further flexibility to optimize the dimension of the lattice parameter for a given value of the wavelength, or, inversely, to have two forbidden energy ranges when the geometry of the structure is fixed. These gaps fall into the infrared domain for reasonable values of the rod diameter. It is hoped that the fabrication and the experimental studies of such photonic crystals will be realized to compare with the theoretical results of this study.

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