PHYSICAL REVIEW E VOLUME 56, NUMBER 6 DECEMBER 1997

Absolute photonic band gap in a two-dimensional square lattice of square dielectric rods in air

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(Received 25 July 1997)

We show that an absolute photonic band gap exists in a two-dimensional square lattice of square dielectric rods in air. The index of refraction of the square dielectric rods must be larger than 2.65 to have the band gap. This structure is a good candidate for two-dimensional photonic crystals in the IR or the visible to near-IR wavelength range, and can be applied to high efficiency optoelectronic devices. [S1063-651X(97)50312-6]

PACS number(s): 42.70.Qs, 41.90.+e

It has been well known that periodic dielectric structures (photonic crystals) can possess a frequency region in which electromagnetic (EM) waves cannot propagate in any direction [1,2]. This frequency region is called the photonic band gap (PBG), which is analogous to the electronic band gap due to the spatial periodic electrostatic potential in natural crystals. The absence of normal modes of EM waves inside PBG can give rise to unusual physical phenomena, such as the suppressed dipole-dipole interaction between atoms [3] and the photon-atom bound states [4]. The enhancement of the density of states of EM waves near PBG edge can improve the performance of optoelectronic devices [5]. Thus, the search for photonic crystals generating PBG in two or three dimensions has attracted a lot of attention [6,7]. Photonic crystals have very useful and attractive properties which semiconductor crystals do not. Defects in photonic crystals are easily created by either adding other dielectric materials to or removing dielectric material from a chosen unit cell in the periodic lattice [8]. This defect can create a local mode of EM wave in PBG and act like a microcavity. Thus, it is possible to tune the defect modes to any frequency in PBG by designing the size, the shape, and the dielectric constant of the defect.

Two-dimensional (2D) photonic crystals can be fabricated more easily than three-dimensional ones in the infrared (IR) or the visible to near-IR wavelength ranges. For this reason, attention may have been drawn towards 2D photonic crystals. They have been mainly investigated for square and hexagonal lattices of air rods and dielectric rods with various cross sections. It was reported that square and hexagonal lattices of circular air rods can give rise to absolute PBG's [9]. A hexagonal lattice of single-circular dielectric rods in air do not give rise to absolute PBG's. On the other hand, it has been recently known that a hexagonal lattice of two- and three-basis circular dielectric rods in air can give rise to large absolute PBG's [10,11]. In a square lattice, while a symmetry breaking by changing the shape of square air rods to rectangular reduces the width of the absolute PBG's [9], a symmetry reduction by placing an air rod of smaller diameter at the center of each square unit cell enlarges it [11].

It was reported that a square lattice of square and circular dielectric rods in air do not give rise to absolute PBG's [9,12]. However, we discuss in this paper that a square lattice of square dielectric rods in air can have a sizable absolute PBG at higher frequencies of EM waves. The absolute PBG of a square lattice of square dielectric rods can occur when the index of refraction of dielectric square rods is larger than 2.65, which is smaller than those of useful semiconductors. The absolute PBG of a square lattice of square dielectric rods lies in a higher frequency region than those of both a square lattice of square (circular) air rods and a hexagonal lattice of circular air rods, and exists over a wide range of filling fractions.

We calculate the photonic band structure for the electric field (E polarization) and the magnetic field (H polarization) by the plane-wave method, where $E(H)$ polarization means the field parallel to the rod axis. The eigenvalue equations are as follows:

$$\det\left(A(\mathbf{K},\mathbf{K}')-\frac{\omega^2}{c^2}\right)=0, \tag{1}$$

where

$$A(\mathbf{K},\mathbf{K}')=|\mathbf{K}||\mathbf{K}'|\epsilon^{-1}(\mathbf{K}-\mathbf{K}') \tag{2}$$

for the E polarization, and

$$A(\mathbf{K},\mathbf{K}')=\mathbf{K}\cdot\mathbf{K}'\epsilon^{-1}(\mathbf{K}-\mathbf{K}') \tag{3}$$

for the H polarization. Here, $\mathbf{K}=\mathbf{k}+\mathbf{G}$, $\mathbf{K}'=\mathbf{k}+\mathbf{G}'$, where $\mathbf{k}$ is the wave vector in the first Brillouin zone, and $\mathbf{G},\mathbf{G}'$ the reciprocal vectors. $\epsilon^{-1}(\mathbf{K}-\mathbf{K}')$ is the Fourier transform of the inverse of dielectric constant $\epsilon(\mathbf{r})$. We use 797 plane waves in our calculations. When the number of plane waves was increased to 1297, the difference in the results was less than 0.5%. Thus, we believe that the results are well converged within at least 1% of their true value.

Figure 1 depicts the photonic band structure for a square lattice of square dielectric rods in air. The index of refraction of the rod is 3.5, which corresponds to that of GaAs in the IR wavelength range, and a filling fraction of the dielectric rods $f=(d/a)^2=41\%$, where d is the width of the square dielectric rods and a the lattice constant. An absolute PBG occurs where E_8 and H_6 gaps overlap, where E_i and H_i denotes the gap that occurs between the ith and $(i+1)$th bands for the corresponding polarization. The shaded area represents the absolute PBG. The midgap frequency $\omega_{\rm mid}=0.6696(2\pi c/a)$ and the gap size $\Delta\omega=0.0370(2\pi c/a)$. While the first gap of

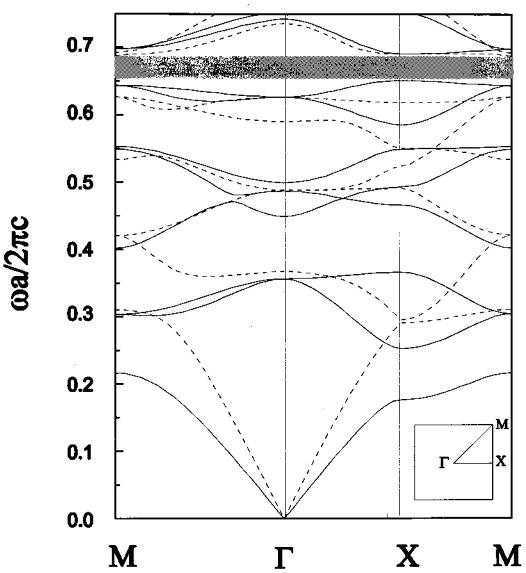

FIG. 1. Photonic band structure of a square lattice of square dielectric rods with the index of refraction 3.5 when the filling fraction of square dielectric rods is 41%. Solid line (—) and dashed line (- -) denote the E polarization and H polarization, respectively. The frequency is normalized in units of $2\pi c/a$, where a is the lattice constant and c the vacuum velocity of light, so that $\omega a/2\pi c$ is dimensionless. The absolute PBG is represented in gray. The inset shows the first Brillouin zone of a two-dimensional square lattice.

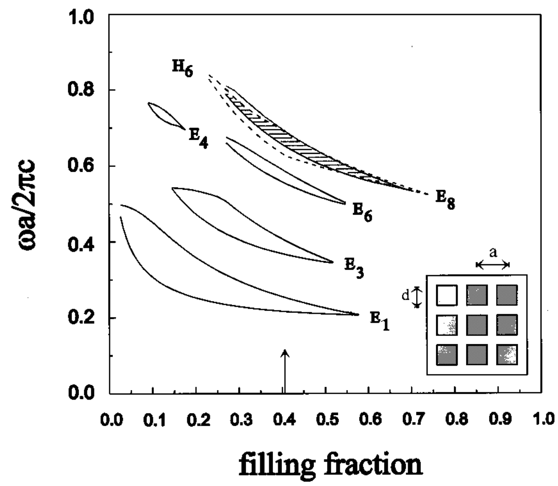

FIG. 2. The gap map for a square lattice of square dielectric rods with the index of refraction 3.5 as a function of the filling fraction of square dielectric rods $(d/a)^2$, where d is the width of square dielectric rods. E_i and H_i denotes the gap that occurs between the ith and $(i+1)$th bands for E and H polarizations, respectively. The solid line denotes E_i and the dashed line H_i. An absolute PBG results from the superposition of the E_8 and H_6 and is hatched. An arrow is drawn at $f=0.41$ where the width of the absolute PBG is maximum. The inset shows the cross section of the array of square dielectric rods at $f=0.41$. The gray squares represent square dielectric rods.

H polarization is H_1 in a square lattice of square (circular) air rods, H_6 is the first gap of H polarization in a square lattice of square dielectric rods in air. It seems that 2D lattices of dielectric rods in air have a larger absolute band gap in higher frequency regions than 2D lattices of air rods [10,11].

Figure 2 shows the gap map for a square lattice of square dielectric rods with the index of refraction 3.5 as a function of the filling fraction of the square dielectric rods. The absolute PBG is hatched. We only consider the bands below the tenth band for both E and H polarizations. The absolute PBG starts near f is about $27\%(d/a=0.52)$ and ends at about $70\%(d/a=0.84)$. The gap size $\Delta\omega$ reaches the maximum value $0.0370(2\pi c/a)$ at $f=41\%$, which corresponds to $d/a=0.64$. We should note here that H_6 is the only band gap appearing below the tenth band of H polarization. Therefore, the only one absolute PBG exists due to the overlap of E_8 and H_6 gaps in this frequency region.

Figure 3 shows the gap size $\Delta\omega$ in units of $2\pi c/a$ as a function of the index of refraction of the square dielectric rods when the filling fraction of the rods is 41%. A square lattice of square dielectric rods in air requires significantly smaller index of refraction for the appearance of an absolute PBG than a square lattice of square air rods. The minimum value 2.65 of the index of refraction of square dielectric rods in air for generating an absolute PBG is smaller compared to the values, 3.51 for a square lattice of square air rods and 2.70 for a square lattice of circular air rods, but is comparable to the value 2.66 for a hexagonal lattice of circular air rods [12]. The index of refraction of useful semiconductors (GaAs, AlAs, Si) used in semiconductor optoelectronic devices is larger than 2.65 in the IR or the visible to near-IR wavelength ranges.

In the IR wavelength range, 1.5 μm is an important wavelength in optical telecommunication. ω_{mid} of the absolute PBG of the square lattice of square GaAs rods in air can be matched to $\lambda=1.5$ μm when $d=0.64$ μm, $a=1.0$ μm. A square lattice of square dielectric rods in air can be fabricated more easily than the hexagonal lattices of two- and three-basis circular dielectric rods in air in the IR or the visible to near-IR wavelength range. We suggest that a square lattice of square dielectric rods in air should be a good candidate for the fabrication of 2D photonic crystals in the IR or the vis-

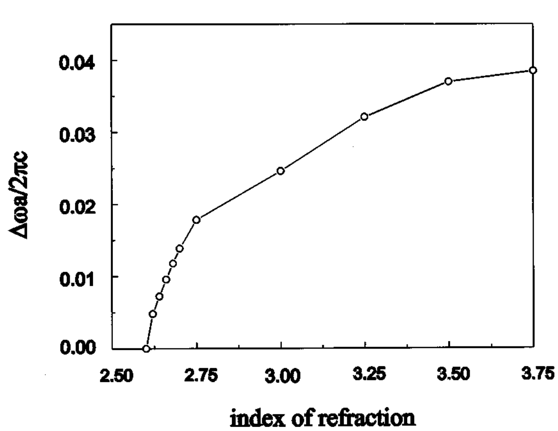

FIG. 3. The gap size for a square lattice of square dielectric rods in air as a function of the index of refraction of square dielectric rods in units of $2\pi c/a$ at the filling fraction of 41%.

ible to near-IR wavelength range.

In conclusion, we find an absolute PBG in 2D square lattice of square dielectric rods in air. The minimum value of the index of refraction of square dielectric rods to generate an absolute PBG is smaller than that of widely used semiconductors. It is easy to fabricate this structure in the IR or the visible to near-IR wavelength range by etching technology.

This work was supported in part by the Korea Science and Engineering Foundation through the Semiconductor Physics Research Center at Jeonbok National University.

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