Three-dimensional photonic band gaps in modified simple cubic lattices

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Complete three-dimensional photonic band gaps are found in simple cubic dielectric structures consisting of spheres or cubes on the lattice sites, interconnected with thin rods. The full higher gap, between bands 5 and 6, has a maximum value of 12% for a refractive index contrast of $n=3.6$, and is considerably larger than in the skeletal structure of simple cubic rods. This gap is about 70% of that in the widely fabricated layer-by-layer structure. In addition, there are large stop bands along the cubic axes. Such structures are candidates for recently emerging advanced semiconductor-processing methods.

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I. INTRODUCTION

Three-dimensional photonic band-gap (PBG) structures are periodic dielectric structures with a frequency region where transmission of waves is forbidden in any direction.[1–4] Recently, the fabrication of such photonic structures in the infrared and near-infrared regimes has been achieved by innovative state-of-the-art processing methods.[5,6] The fabrication of such PBG structures at optical wavelengths is a long-standing goal. Such three-dimensional PBG structures promise many novel applications[1–4] including the manipulation of light, increased laser efficiency, and controlled spontaneous emission. The bending of light around sharp corners can be achieved with photonic crystal waveguides. Photons are expected to replace electrons in future all-optical devices. To efficiently route, bend, and manipulate light on a single chip, different classes of photonic crystals are required. We propose a photonic crystal that is simple to fabricate and may be very useful to such future optical technology.

The fabrication of three-dimensional PBG structures was initiated by a three-cylinder diamondlike structure[7] (at microwave frequencies). The Iowa State University layer-by-layer structure[8] was extensively fabricated at millimeter wave frequencies by silicon micromachining[9] and at far-infrared frequencies by laser-induced chemical vapor deposition (CVD).[10] Recently, state-of-the-art silicon microfabrication methods have been utilized to fabricate the layer-by-layer structure with band-gap wavelengths in the infrared[5] (IR) (10μ) and near-IR (Ref. 6) (1.5 μ) regimes. Ultrasmall cavities were also fabricated by introducing defects with the PBG lattice. These processing techniques have made fabrication of different types of photonic lattices feasible.

Although several complex photonic lattices have been proposed,[11,12] the simple cubic is among the simplest of crystal lattices, and has only been studied briefly. Very recently, the simple cubic structure consisting of a lattice of rods has been fabricated with advanced silicon processing techniques at infrared length scales and has been found to have a complete band gap,[13] suggesting renewed interest in simple cubic photonic crystals.

Previously, a quasi-simple-cubic lattice was fabricated[14] with a lattice constant of 0.53 μ, and exhibited stop bands in the far-IR but did not have a complete gap. One advantage for experimental fabrication is that the repeat distance is two layers in the simple cubic as opposed to four layers in the layer-by-layer structure. Band calculations[15] found the simple cubic lattices of dielectric rods to have a complete three-dimensional band gap, with a magnitude of ~6% for dielectric contrasts of $n=3.6$. The band gap is fundamental, between the lowest bands (2 and 3), and is optimized for a small dielectric filling ratio of 19%. The full gap in the simple cubic structure is smaller than that in the layer-by-layer structure by a factor of ~3.

An alternative is an inverse simple cubic lattice of air spheres at lattice points enclosed by a background dielectric of $n=3.6$, and is optimized when the filling fraction of air is 81%, resulting in a sparse multiply connected network. This is analogous to the known higher gaps of fcc or hcp air cavities in a dielectric background.

II. RESULTS

We predict the fabrication of simple cubic lattices with full three-dimensional gaps using photonic band-structure calculations. The calculations are based on the well-established plane-wave technique for calculation of photonic band structure[4,16,17] that has very successfully predicted PBG crystals. Vector wave solutions of Maxwell's equations are found for plane-wave expansions of the $\mathbf{E}$ and $\mathbf{H}$ fields in a periodic dielectric structure. Using matrix diagonalization, the band frequencies $\omega(\mathbf{k})$ are calculated for each wave vector $\mathbf{k}$.

Since the fabrication of simple cubic lattices has recently become feasible, we investigate ways to modify the lattice and improve the size of the photonic gap. We start from the simple cubic lattice of dielectric rods that has a small but complete PBG between bands 2 and 3. We either place dielectric spheres (Fig. 1) or dielectric cubes (Fig. 2) on the lattice sites. As the size of the spheres is increased in the connected network of cylinders and spheres (Fig. 1), the lower 2-3 gap closes, and a large complete band gap opens

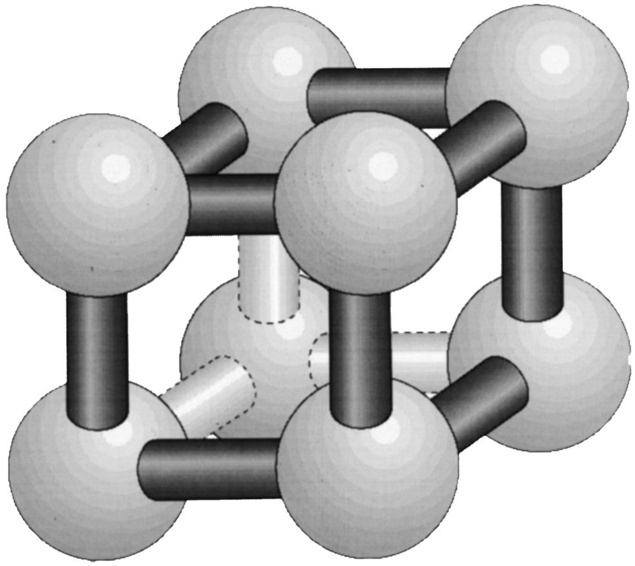

FIG. 1. Simple cubic lattice consisting of dielectric spheres on the cubic lattice sites connected by thin dielectric cylinders. This structure has a full photonic band gap between bands 5 and 6.

between the next set of higher bands 5 and 6 for a range of geometries. A similar result is found when the size of the cubes is increased. There is a small region where both the 2-3 and 5-6 gaps coexist. The optimum photonic structures have thin cylinders connecting larger spheres having a radius a factor-of-3 larger than the cylinder radius.

The maximum gap/midgap ratio of 12% is found for a filling ratio of 0.21 (Fig. 3) formed by thin cylinders (radius $0.11a$) connecting considerably larger spheres (radius $R=0.345a$) where a is the lattice constant (Fig. 4). For consistency we use refractive index contrasts of $n=3.6$, appropriate for Si or GaAs. The full gap persists at an even 40% dielectric filling ratio, an advantage for fabrication of mechanically robust structures.

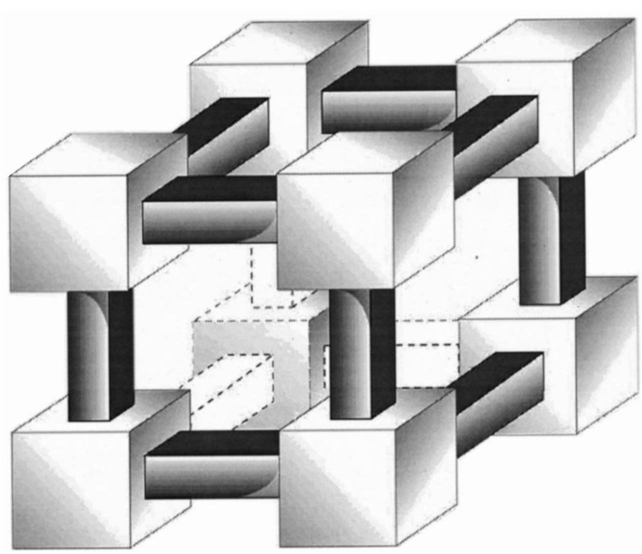

FIG. 2. Simple cubic lattice consisting of dielectric cubes on the cubic lattice sites connected by thin dielectric rods of square cross section. This structure also has a full photonic band gap between bands 5 and 6.

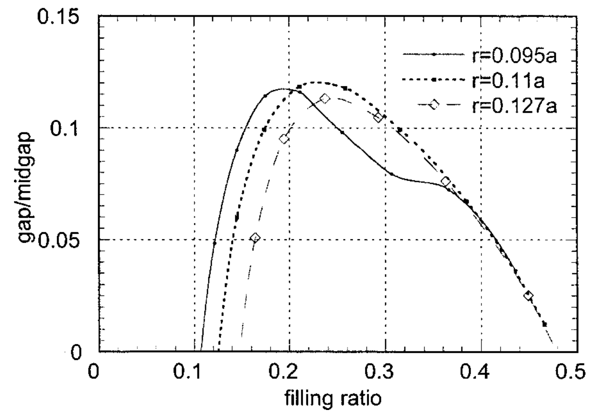

FIG. 3. The size of the full gap as a function of the filling ratio. The sphere radius is varied for each value of the cylinder radius shown in each curve. A refractive index contrast of 3.6 is used.

The calculated band structure (Fig. 5) shows that the 5-6 band gap spans relatively dispersionless higher bands, so that such stop bands would be quite insensitive to the angle of propagation of the wave in the crystal. The top of the valence

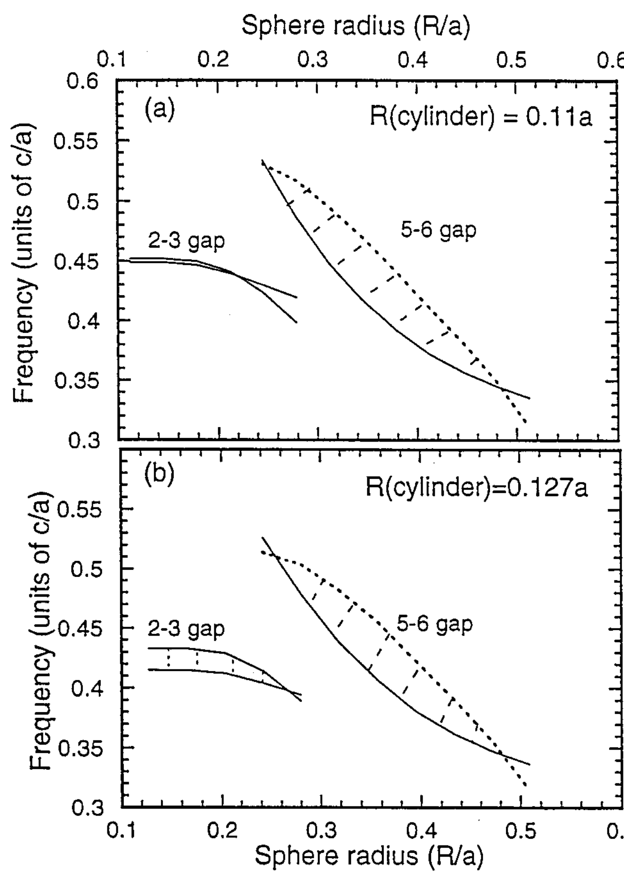

FIG. 4. The frequencies of the 2-3 and 5-6 gaps in the simple cubic structure of Fig. 1, as a function of the sphere radius (r/a). Results are shown for two radii of the dielectric cylinders in (a) and (b). The shaded regions are structural geometries with full band gaps.

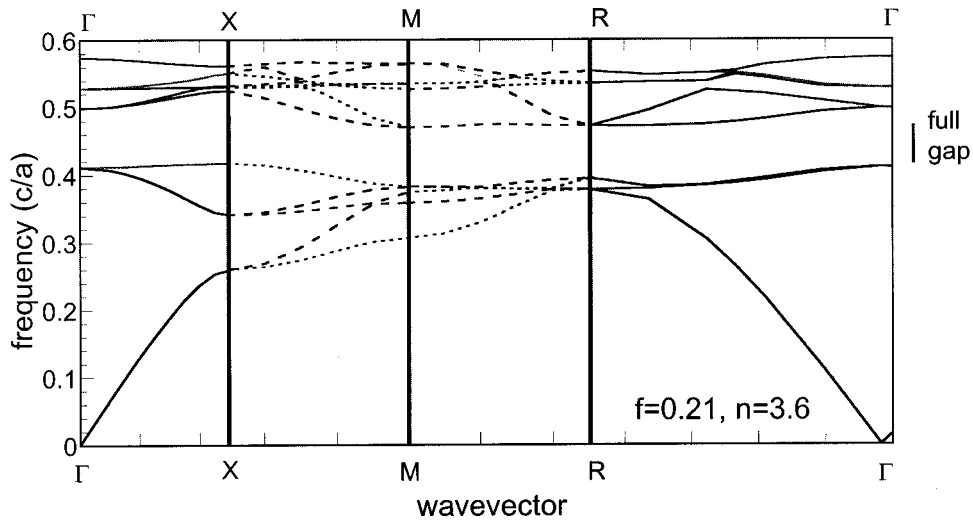

FIG. 5. Photonic band structure of the optimized simple cubic lattice of spheres and rods, displaying the wide and full photonic band gap between bands 5 and 6. The high-symmetry points follow usual conventions where $\Gamma=(0\,0\,0)$, $X=(.5\,0\,0)$, $M=(.5\,.5\,0)$, and $R=(.5\,.5\,.5)$. Dotted lines $(\cdots)$ are modes with s polarization and dashed lines $(---)$ are modes with p polarization. Modes with mixed polarization are solid lines in the highest-symmetry directions $(\Gamma X,\, R\Gamma)$. Filling fraction f is 21%. Cylinders have $r=0.11a$ and spheres have radius $R=0.345a$.

band (band 5) is at $X(.500)$ and very close to Γ since the ΓX band is flat. The bottom of the conduction band (band 6) is at $M(.5.50)$ although the M and $R(.5.5.5)$ frequencies are nearly degenerate. Some dispersion is found between X and M. Modes have been decomposed into s and p polarizations along the XM and MR directions (Fig. 5).

The simplicity of the ball and stick or cube and stick structure (Figs. 1 and 2) may facilitate experimental work since all connecting rods are at right angles to each other. In analogy with other PBG crystals with higher gaps, the minimum refractive index contrast for observing the full band gap is $n \cong 2.8$, and the size of the gap increases with the contrast.

Fabrication of the simple cubic structure may be easier with the spheres replaced by cubes and connected by rods of square cross section (Fig. 2). We have repeated our calculations for such cubes connected by square rods. We find the same qualitative results, except that the magnitude of the full gap/midgap ratio is reduced to 8% for a filling ratio of 24% (Fig. 6), somewhat smaller than the sphere/cylinder structure of Fig. 1. Here the optimum configuration consists of cubes of half width $0.28a$ connecting rods of square cross section of half width $0.11a$.

Experimental observations are frequently performed along the 100 crystal direction (ΓX). We predict from the band structure (Fig. 5) that observations should find a lower partial 2-3 gap followed by a higher full 5-6 gap along the 100 direction. We calculated the magnitude of these (100) stop bands (Fig. 7) for the cube and square rod structure. Both the 2-3 and 5-6 stop bands are very wide (30%–40% and 15%–20%, respectively) and exist over a large range of filling ratios. The 2-3 gap is the remnant of the full gap in the skeletal rod structure, and vanishes along the X to M direction.

All full PBG's (for both wave polarizations) are formed in interconnected dielectric structures. The lower-frequency valence band is a wave propagating in the dielectric, whereas the higher-frequency conduction-band wave propagates primarily in the air region. The frequency difference between these two modes generates the band gap. Since a dielectric mode can have large amplitude at the vertices of the simple cubic lattice, introducing extra dielectric spheres or cubes at these vertices can lower the frequency of the dielectric mode and open up a band gap, as we find in the calculations. When extra spheres/cubes are instead placed at the midpoints of the cylinders, the gaps vanish, since the dielectric modes have nodes at the midpoints (i.e., vanishing amplitude)—supporting this qualitative argument. When the structure becomes disconnected, by introducing spheres at body-centered points, the band gaps disappear. Although the higher gaps are more susceptible to disorder and absorption, state-of-the-art

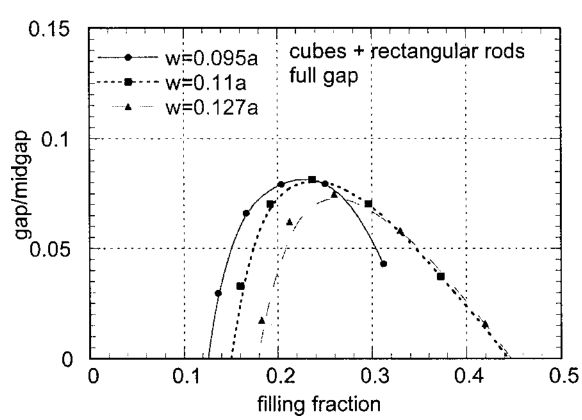

FIG. 6. The size of the full gap as a function of the filling ratio for the structure of cubes connected by square cylinders. The half widths of the rods are shown. The rod widths are kept constant and the cube size is varied for each curve.

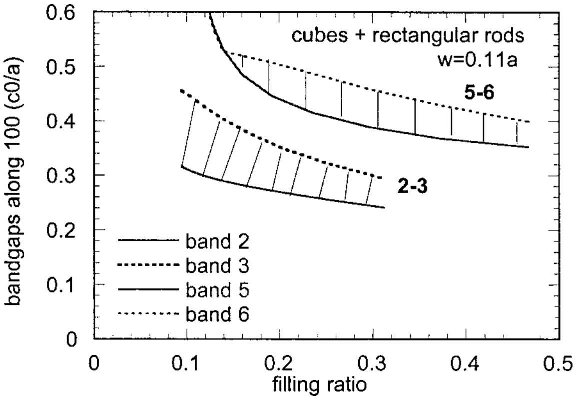

FIG. 7. The band gaps or stop bands along the 100 direction for the structure with cubes and square rods as a function of the filling ratio. The rod width is kept fixed.

fabrication methods have achieved very highly ordered photonic lattices. We have also found such full higher gaps in interconnected fcc lattices of dielectric spheres.

A very promising alternative technique for fabrication of photonic crystals is the recently developed laser-induced CVD technique[10] that has generated three-dimensional (3D) wire-cage structures with complex connectivity, by scanning a laser through a gas mixture of alumina vapor. The angle between dielectric rods can also be varied in this process. The simple cubic structure studied here is reminiscent of molecular modeling kits, and may be an appealing structure for this fabrication method.

In addition, the rapidly developing advanced silicon processing methods have already been able to fabricate simple cubic lattices. This technique is currently being used to fabricate the simple cubic lattice with cubes and rods (Fig. 2). To further simplify fabrication, the cubes can be shifted to be aligned with the edges of the rods with comparable performance. This structure can be broken down into a four-level mask, three levels to describe the portions with the cube and one level to describe the vertical connector. This scheme is feasible for fabrication.

III. COMPARISON WITH SIMPLE CUBIC ROD STRUCTURE

There are very interesting comparisons of our ball and stick structures with the simple cubic structure of rods. The photonic band structure of rods in the simple cubic structure shows a fundamental band gap between bands 2 and 3 [Fig. 8(a)]. The top of the valence band is at $R(111)$, the largest wave vector in the Brillouin zone, and the bottom of the conduction band is at $X(100)$, the smallest wave vector in the Brillouin zone, as expected from the theory of plane-wave propagation. When the spheres are introduced the gap at R closes first (Fig. 5) although the ΓX gap is still present, and the gap between the next-higher 5 and 6 bands opens.

For the skeletal structure of rods the optimum gap is at a filling fraction of 19% [Fig. 8(b)]. Although the full gap/midgap ratio is about 6%, a very large stop band of 35% is expected in the 100 direction and is a signature for experimental studies.[13,14] This stop band is somewhat larger than that in the structure with cubes/spheres (Fig. 7). As evident from the band structure [Fig. 8(a)], the lower edge of the 100 stop band should move to higher frequencies as the transmission direction changes from 100 to 110 or 111.

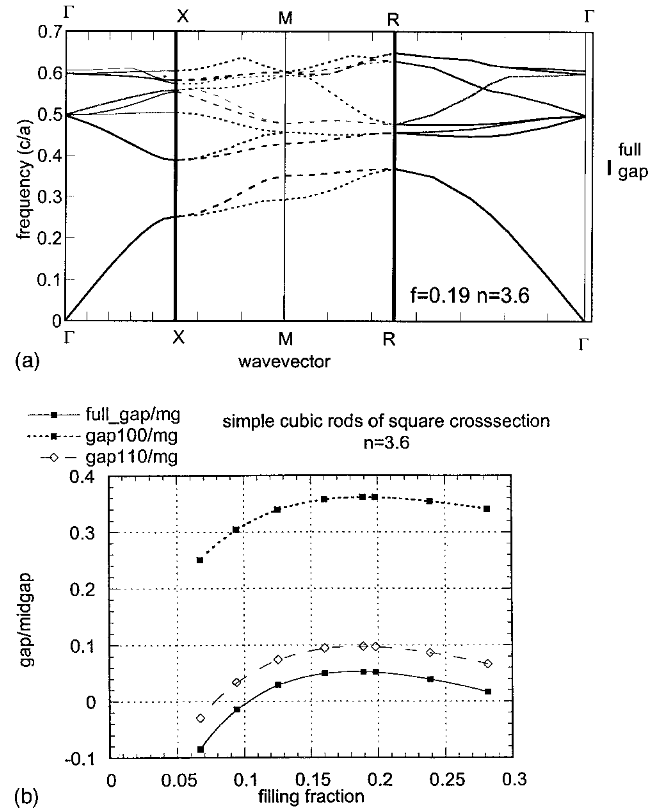

FIG. 8. (a) Photonic band structure of the simple cubic structure connected with dielectric rods ($n=3.6$) and a filling ratio of 19%. (b) The gap to midgap ratios for the full gap, the 100 gap, and the 110 gap as a function of the filling ratio, for the simple cubic structure with rods. Dotted lines are modes with s polarization and dashed lines indicate modes with p polarization. Modes with mixed polarization are solid lines in the highest-symmetry directions (ΓX, $R\Gamma$).

IV. CONCLUSIONS

We have found classes of periodic cubic dielectric lattices, consisting of spheres or cubes at lattice sites connected by cylinders, where large full gaps are present for all directions of wave propagation. Structures proposed here are an alternative to the three-hole structure[7] or to the layer-by-layer structure.[8,9,18] Such photonic lattices may lead to fundamental comparisons between theory and experiment, and different physics for controlling spontaneous emission. The incorporation of light sources inside photonic crystals, such as fluorescent dyes inside the photonic structure, provide characterization of the emission process[19] as the wavelength of the fluorescent source varies through the band gap. They provide fundamental tests of using higher band gaps, a feature that has only recently been possible in 3D PBG crystals.[20]

These PBG structures can be suitable for applications such as waveguides and microcavities, since sizable gaps in three dimensions enhance confinement of light within the waveguide. Waveguides can be more easily fabricated in the simple cubic geometry than in other existing three-dimensional photonic crystals. Such optical waveguides are expected to replace electrons as the carriers of information in future all-optical circuits. Switching, routing, and bending of light on a chip may be possible with the structures proposed here.

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