Design of three-dimensional photonic crystals at submicron lengthscales

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We present a new class of periodic dielectric structures designed specifically to be amenable for fabrication at submicron lengthscales. The structures give rise to a sizable 3D photonic band gap and can be fabricated with materials widely used today in optoelectronic devices. They are made of three materials and consist essentially of a layered structure in which a series of cylindrical air holes are etched at normal incidence through the top surface of the structure. Our results demonstrate the existence of a gap as large as 14% of the midgap frequency using Si, SiO_2, and air; and 23% using Si and air.

Periodic dielectric structures—also known as *photonic crystals*—have the ability of affecting the density of electromagnetic states within their boundaries and even suppressing all modes for a range of frequencies. They can greatly affect the radiative dynamics within the structures and lead to significant changes in the properties of optical devices. This has opened a new and fascinating area for potential applications in optoelectronic devices[1,2] and has prompted research to find structures that would generate large photonic band gaps. Several structures have been found to yield full 3D band gaps[3–7] but their fabrication at submicron lengthscales appears to be a difficult endeavor. Indeed, to our knowledge, the only successful microfabrication of a photonic crystal has been reported by Wendt *et al.*[8] and consists of a triangular lattice of cylindrical holes; however, this structure was designed to give rise only to a 2D band gap. The main problem with the microfabrication of a 3D photonic crystal comes from the rather sophisticated geometry and intricate arrangement of the holes or rods needed to open a gap. These complex structures do not easily lend themselves to fabrication at submicron lengthscales. Furthermore, most applications for photonic crystals require band gaps larger than 10% which in turn requires the use of materials with large index contrasts. In this letter, we present a structure which solves all of the above problems: (i) it gives rise to large 3D gaps, (ii) its construction has an inherent simplicity, and (iii) it can be made with materials widely used today in optoelectronic devices. Moreover, our calculations show that the band gaps are not very sensitive to the parameters of the structure; therefore, deviations arising in the fabrication process should not significantly affect the results.

Our objective was to find a simple layered structure with a large index contrast that would require the etching of only one series of holes at normal incidence through the top surface of the structure. We also wanted the etching process to be done at the end of the growth procedure in order to simplify its fabrication. The structure is shown in Fig. 1. It is essentially a layered structure made of two materials (e.g., Si and SiO_2) in which a series of air columns is drilled into the top surface. The use of the cylindrical air columns is important in providing a large index contrast between the different materials. This structure can be microfabricated by growing it layer by layer using conventional lithographic techniques. We expect that ten layers should be sufficient although some applications may require a smaller or larger number of layers. A generic fabrication process of this structure is described below and is illustrated in Fig. 2. The sequence of "growth" steps in Fig. 2 is presented only to help the reader visualize the basic elements that make up the structure and does not have the pretension of describing the exact building process.

We begin by depositing a layer of Si of thickness d on a substrate of choice and by etching grooves into the Si layer as shown in Fig. 2(a). The grooves are parallel to the x-axis and are separated by a distance a; they have a depth d and width w. The grooves are then filled with SiO_2. The next step consists in growing another Si layer of height h on top of the previous layer, as shown in Fig. 2(b), and etching long grooves of depth d and width w into this layer, as shown in Fig. 2(c). We note that these grooves actually extend into the first layer and are translated by a distance $a/2$ with respect to the first layer. After filling the grooves with SiO_2, another Si layer of height h is deposited on the top surface and long parallel grooves are etched. The grooves are translated again by a distance $a/2$ with respect to the previous layer, as shown in Fig. 2(d). From this point on, the structure repeats itself every two layers. Once this process is completed, an array of long cylindrical holes is etched into the top surface

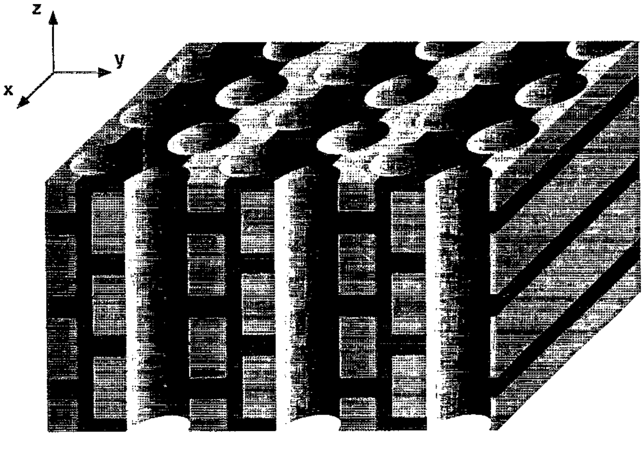

FIG. 1. 3D photonic crystal fabricatable at submicron lengthscales.The dark gray and light gray regions correspond to materials with a high and low dielectric constant, respectively. The long cylindrical columns along the z-axis are filled with air.

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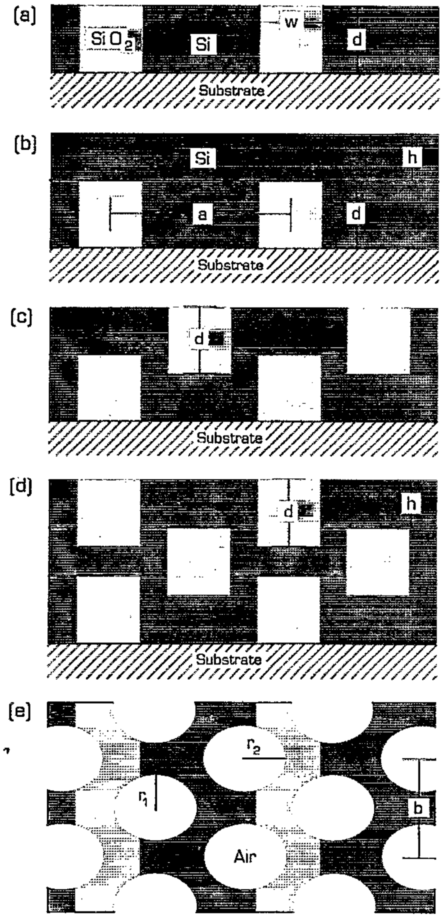

FIG. 2. (a)–(d) Cross-sectional view in the yz-plane of the photonic crystal shown in Fig. 1. (e) Plan view in the xy-plane of the photonic crystal. The cross section of the air columns can be circular or elliptical.

of the structure, at normal incidence. In general, the cross section of the holes can be either circular or elliptical with parameters r_1 and r_2, as shown in Fig. 2(e). The holes form a centered rectangular lattice on the top surface; they are separated by a distance b along the x-axis and a along the y-axis. The center of each hole is aligned in the structure as shown in Fig. 2(e). The overall structure is body centered orthorhombic with lattice constants b, a, and $2h$ along the x- y-, and z-axes, respectively. It has a point group which includes three 180° rotation operators about the x-, y-, and z-axes. In the special case where $a = \sqrt{2}b = 2\sqrt{2}h$, the lattice becomes face-centered cubic.

The design of this structure has many degrees of freedom which can be used to optimize the size of the gap, depending on the materials used in the fabrication. Although Si and SiO$_2$ were used in the above example, they can be replaced by other materials with a large index contrast. The parameters of the structure are shown in Fig. 2. It is convenient to choose one of the lattice constants as the unit length scale; we choose a and define every other parameter with respect to it. The size of the structure can then be scaled to any wavelength simply by scaling a.

In the specific case where Si and SiO$_2$ are used in the fabrication process, we found the gap to be 13.9% of the midgap frequency when the width and depth of the SiO$_2$-filled grooves were $0.40a$ and $0.49a$, respectively. Furthermore, the cross section of the air columns was chosen to be circular with a radius of $0.21a$. The other parameters used to optimize the gap were $b=0.71a$ and $h=0.35a$. We show in Fig. 3 the band diagram as computed with the method of Ref. 9 along various directions in the irreducible Brillouin zone. Without any loss in generality, we have chosen, for simplicity, a Brillouin zone associated with a *simple* orthorhombic lattice.[10] The bands were obtained by computing the six lowest eigenvalues at 121 k-points. The occasional sharp kinks in the bands are an artifact of the interpolation scheme used in joining the eigenvalues. We used a dielectric constant of 12.096 for Si at $\lambda=1.53$ μm[11] and 2.084 for amorphous SiO$_2$ also at 1.53 μm.[11] This wavelength is roughly equal to the one used in many optical devices today. In the case where the gap is centered at 1.53 μm ($f=196$ THz), a is equal to 0.79 μm and the gap extends from $\lambda=1.43$ μm to $\lambda=1.64$ μm ($f=182$ to $f=210$ THz).

The gap is not very sensitive to the cross-sectional dimensions of the grooves nor of the air columns. By changing

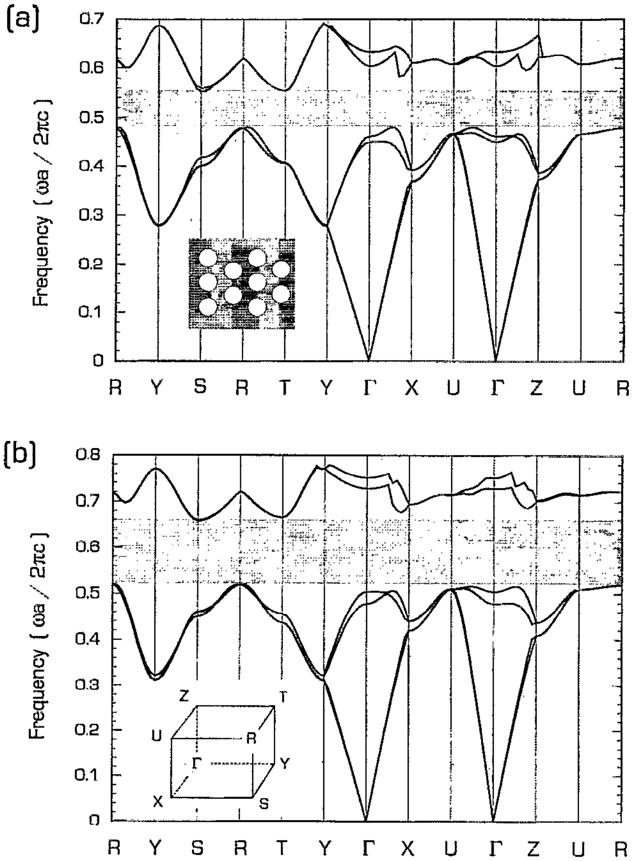

FIG. 3. (a) Band diagram of the Si/SiO$_2$/air structure with $w=0.40a$, $d=0.49a$, $r_1=r_2=0.21a$, $b=0.71a$, and $h=0.35a$. The inset shows the plan view of the dielectric structure in the xy-plane. (b) Band diagram of the Si/air structure with $w=0.36a$, $d=0.51a$, $r_1=r_2=0.24a$, $b=0.71a$, and $h=0.35a$. For simplicity, the bands are plotted along various directions of the irreducible Brillouin zone of a *simple* orthorhombic lattice, as shown in the inset. The directions Γ-X, Γ-Y, and Γ-Z correspond, respectively, to the $\hat{x}$, $\hat{y}$ and $\hat{z}$ directions of the real space lattice shown in Fig. 1.

both the width and depth of the SiO_2-filled grooves, the gap remains larger than 13% for values of w between $0.35a$ and $0.40a$ and d between $0.45a$ and $0.51a$. On the other hand, the cross section of the airholes could be made elliptical with the major axis aligned either along the x- or y-axis without affecting the gap significantly. For example, the gap would remain larger than 13% if r_1 was between $0.21a$ and $0.25a$ and r_2 between $0.19a$ and $0.23a$. Actually, our numerical calculations have shown a very small increase of the gap to 14.0% when the cross section of the air columns was elliptical (as opposed to circular) with $r_1=0.21a$ and $r_2=0.23a$.

A very significant improvement could be made to the size of the gap simply by removing the oxide in the structure. The removal of the oxide would increase the dielectric contrast between the silicon and the other materials in the structure, and would leave long holes with rectangular cross-section filled with air along the x axis. The removal of the oxide could be done, for example, with selective chemical etching. More specifically, if the oxide was removed from the structure presented in Fig. 3(a), the gap would increase to 17%. The gap could be further increased by optimizing the parameters; we have found a gap of 23% in the Si/air structure with $w=0.36a$, $d=0.51a$, and $r_1=r_2=0.24a$. The corresponding band diagram is shown in Fig. 3(b). Again, the gap remains very large even if all four parameters are changed slightly; the gap remains larger than 20% for values of w between $0.35a$ and $0.38a$, d between $0.47a$ and $0.51a$, r_1 between $0.23a$ and $0.25a$, and r_2 between $0.21a$ and $0.25a$.

Finally, we note that the structure could be fabricated with any high-index material as long as the material in the grooves could be removed at the end of the fabrication process. For example, GaAs and AlGaAs could be used since AlGaAs could be removed by wet etching. The resulting gap would be close to 22%.

We have presented in this letter a new class of photonic crystals designed specifically for fabrication at submicron wavelengths. These crystals give rise to 3D gaps as large as 23%. The viability of fabrication of these structures could solve the most important problem hindering the use of photonic crystals in the optoelectronic industry today.

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