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A method to fabricate a diamond structure with a complete photonic bandgap in the near infrared is proposed. The procedure starts by building an opal with body-centered-cubic symmetry composed of two types (organic and inorganic) of microspheres by means of a microrobotic technique. Then, the organic particles may be selectively removed to obtain a diamond structure of inorganic particles. This method can be extended to make diamond inverse opals of silicon with full gap to midgap ratios as large as 13% for moderate filling fractions. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1406560]

One of the most important goals in photonic band gap (PBG) technology[1,2] is the search for methods to produce three-dimensional (3D) systems with reasonably large full gaps in the visible and infrared regions of the spectrum. The approach many researchers have followed is the search for appropriate assemblies that present the most spherical Brillouin zone,[3] e.g., face-centered-cubic (fcc) or diamond structures as a particular case thereof. Structures with a diamond lattice can show large gaps providing a refractive index contrast above 2 is achieved. So far there are, mainly, two approaches that allow one to obtain PBG materials with reasonably broad full gaps. One involves lithographic techniques to build up woodpile arrangements[4,5] or layered structures;[6] these methods are time consuming, technologically sophisticated, and allow stacking reduced numbers of layers. Alternatively, the opal templating route is very attractive because it is an easy and cheap method.[7,8] Inverted opals can develop full gaps when the refractive index contrast is above 2.8,[9] as has recently been reported for inverted silicon[10] and germanium.[11] However, the full gap that appears between the eighth and the ninth bands is very fragile because it is strongly influenced by the presence of defects.[12,13] This problem could be solved if avenues leading to the packing of microspheres in a diamond lattice by self-assembly techniques could be found. Unfortunately, unlike fcc arrangements, which are obtained simply by gravity deposition[14] or template directed sedimentation,[15] this structure is far from minimum free energy requirements to self-assemble.

Here we present a method based on robot-aided micromanipulation[16,17] that opens up the possibility of building 3D photonic crystals with a diamond structure (20 μm in size typically). Robot-aided manipulation of single microspheres on a template substrate allows the assembling of a body-centered-cubic (bcc) lattice, which, in fact, is a combination of two diamond structures.[18] What is crucial at this moment is designing a way in which the right atoms from the bcc structure can be removed in order that the remaining ones are arranged in the sought after diamond structure. This can be achieved if the sacrificial atoms are of a class, in some sense, that is chemically different from the other atoms thus providing a means for dissolution. This can be done with inorganic versus organic microspheres arranged in points of a bcc lattice. So our method starts with the construction of a heterogeneous structure of mixed inorganic and organic (e.g., silica or silicon and latex) spheres in a bcc lattice. This structure, composed of two kinds of spheres, we will call, from now on, mixed body-centered-cubic (mbcc). Subsequently, upon selective removal of the organic particles a diamond structure of the inorganic ones is obtained. Since adjacent spheres are in contact, the remaining diamond opal made of inorganic particles should be stable.

The construction of a mbcc lattice as an intermediate step presents some advantages over direct diamond lattice assembly. The diamond lattice has a very low filling fraction ($\sim$34%) for spheres that touch which makes it too unstable to be constructed directly. On the other hand, a mbcc lattice allows stacking spheres along at least two orientations: (001) and (111). In both cases the sphere positions are minimum energy locations once the first layer is in place. In either case the initial layer should be ordered on a template substrate.

In order to algebraically describe the lattices let us summarize by saying that two interpenetrated diamond structures form a bcc that can be represented as a fcc with a four-atom basis. This choice is based on the fact that the most convenient description of a diamond structure is as a fcc with a two-vector basis. Our mbcc will be presented too as a fcc with two two-atom bases made of different materials, e.g., inorganic (i) and organic (o). The fcc primitive vectors are[19] $\mathbf{a}_1 = a/2(1,1,0)$, $\mathbf{a}_2 = a/2(1,0,1)$, and $\mathbf{a}_3 = a/2(0,1,1)$ where a

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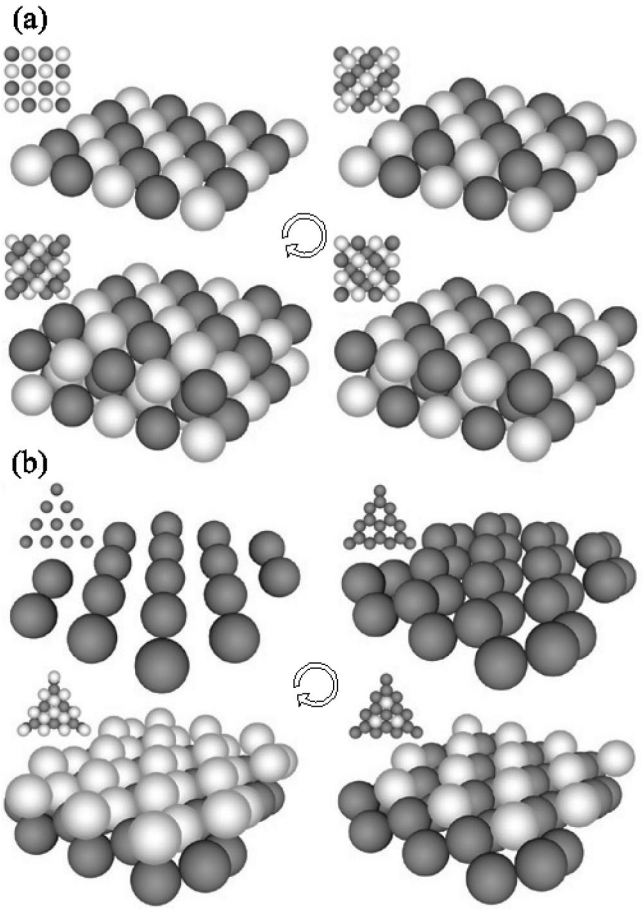

FIG. 1. Computer design showing the layout of the first four layers in a mixed body-centered-cubic lattice where dark and light gray spheres represent organic and inorganic particles, respectively. (a) Stacking along the (001) direction; the fifth layer would be exactly as the same as first one; (b) stacked along the (111) orientation. The insets represent a top view of the layout.

is the lattice parameter. The two-vector basis for material i is (0,0,0) and $1/4(\mathbf{a}_1+\mathbf{a}_2+\mathbf{a}_3)$ while for material o the basis is $1/2(\mathbf{a}_1+\mathbf{a}_2+\mathbf{a}_3)$ and $3/4(\mathbf{a}_1+\mathbf{a}_2+\mathbf{a}_3)$. The lattice parameter may be calculated in terms of sphere diameter (d) assuming that neighboring spheres are in contact: $a=2.31d$.

Growth in the (001) orientation consists of stacking layers of mixed $i-o$ spheres in a square lattice configuration where the nearest neighbors are of opposite character, leading to diagonals of like character, reminding one of a checkerboard. The cyclic arrangement of subsequent layers is shown in Fig. 1(a). Each layer is shifted with respect to the layer underneath by half the pitch (both along the x and y directions). The pitch is $1.15d$ (where d stands for the sphere diameter) and the distance between successive layers results in $\phi_{100}=0.58d$.

The stacking procedure along the (111) direction is shown in Fig. 1(b). Here each layer presents a triangular lattice configuration and, as opposed to the (001) case, the layers are homogeneous in composition (completely organic or inorganic). The layering sequence is reminiscent of that of a fcc lattice ($ABC,\ldots$) but, in this case, two layers of each material are laid successively. For example, $A_iB_oC_o-A_iB_iC_o-A_oB_iC_i,\ldots$, where the subindices indicate inorganic or organic particles. The in-plane distance between neighboring spheres is $1.63d$ and the interlayer distance is $\phi_{111}=d/3$.

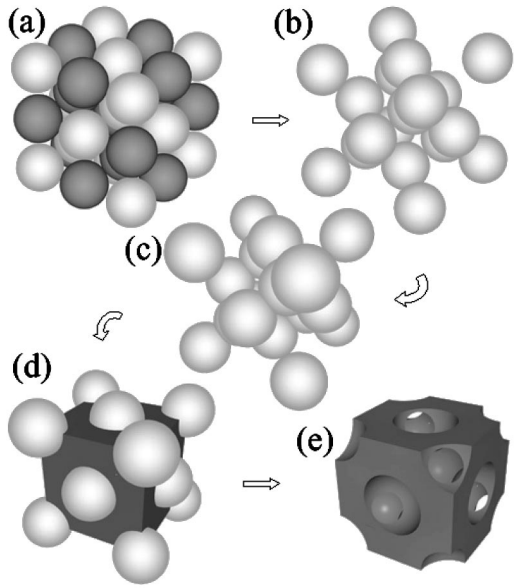

FIG. 2. Computer simulation showing, in five steps, the fabrication of an inverse diamond structure with a full photonic band gap. First a (a) mixed body-centered-cubic lattice is assembled (b) after which latex sublattice is removed; (c) then the structure is sintered to a filling fraction of ~50%; after that (d) silicon or germanium infiltration takes place and finally (e) silica elimination.

Once the mbcc is constructed along either the (001) or (111) orientation, organic particles are selectively removed, leaving a diamond structure of inorganic particles [see step (b) in Fig. 2]. At this point two different, avenues can be pursued depending on the refractive index contrast of the structure. If the spheres used have a refractive index above 2.0, an opal with an omnidirectional gap results.[3] The gap width may be fine tuned through a sintering process similar to that reported for templating silica opals[20] [step (c) in Fig. 2]. A method has recently been proposed[21] to produce monodisperse spheres from several oxides with high refractive indices that could serve this purpose. Photonic band gap calculations predict full gap widths as large as 13% for a diamond lattice of high refractive index spheres, e.g., silicon ($\varepsilon=12$) in an air background when the filling fraction is 43%.

When the refractive index of inorganic particles is not above the threshold for full gap openings one should proceed with the inverse diamond structure depicted in steps (d) and (e) of Fig. 2. This may hold when silica is used as the inorganic material; for instance, in the case of silica–latex particles the following procedure would be performed: First, the mbcc structure should be arranged on a patterned substrate with the aid of the microrobot technique. Next, latex spheres are selectively removed by a calcination process. The remaining diamond crystal is then infiltrated by a high dielectric constant material like silicon or germanium, and, finally, the removal of the silica spheres produces the inverse opal. Since our ultimate goal is to obtain an inverse structure with a complete PGB, one should take into account that air cavities that touch (filling ratio ~34%) in a dielectric medium provide a very narrow gap unless the air filling ratio is increased.[3] A sintering process, depicted in Fig. 2(c), per-

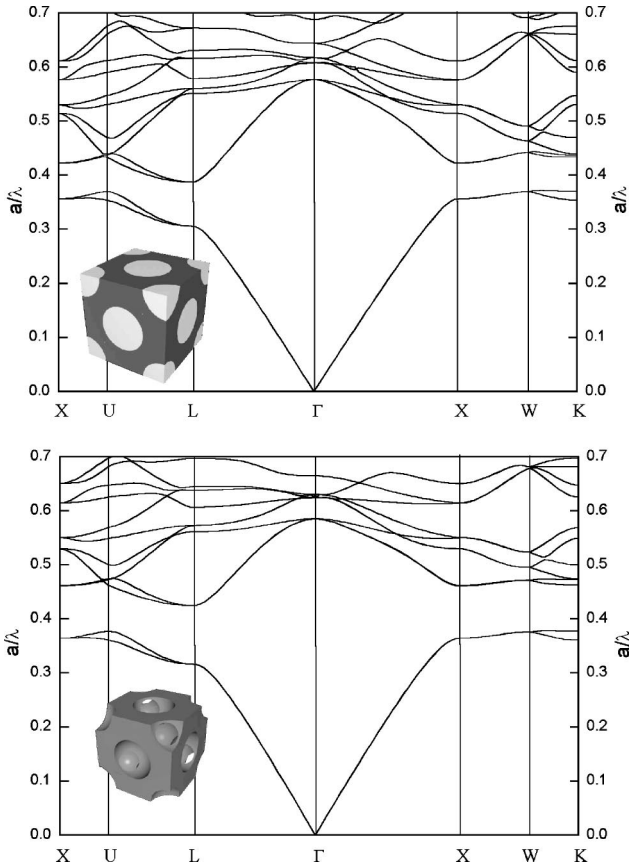

FIG. 3. Photonic band diagrams of (upper panel) a silicon/silica composite diamond opal and (lower panel) that made of air spheres in silicon resulting from the removal of the silica spheres from the former. The filling fraction for silicon is 50%. The inset shows the corresponding real space structures.

formed prior to infiltration, provides the necessary tool with which to obtain an inverse structure with a tailored full gap. Figure 3 shows the photonic band structure calculations[22] for a silicon infiltrated diamond opal of silica spheres along with that of the inverse structure resulting from silica etching. The filling fraction of the silica diamond opal is taken to be 50% (a reasonable value for a sintering process) which determines the air filling fraction of the inverse silicon structure. Maximum values of the gap width are obtained for air sphere filling fractions of 78%, however, such a high value can be unrealistic from a practical point of view.

Other possibilities can be considered when device design is envisaged. Imperfections or uncontrolled defects in the structure are more critical in photonic crystals with larger refractive index contrast. Therefore, one should also consider diamond opals with smaller dielectric contrast (like silicon/silica composites) providing they have a full gap. Table I shows the parameters involved in the fabrication of several silicon diamond lattices with different dielectric contrasts.

It can be seen that even for small dielectric contrasts (like a silica diamond lattice infiltrated by silicon) one can obtain reasonable gaps of 4%. It corresponds to a band width value of about 7 THz in the 1.5μm region, and it corresponds to a diamond lattice parameter of 0.6 μm. This figure is quite reasonable for many applications as dense wavelength division multiplexing (DWDM) devices.[23]

The procedure proposed here opens up a wide range of possibilities for engineering new structures and, in particular, allows control of structural defects (like point and line lattice defects) for direct and inverse diamond structures. Single inorganic spheres or rows of them can be replaced by their organic counterparts in the mbcc to produce point or line defects (air cavities and waveguides) after the etching.

TABLE I. Values of the full gap width ($\Delta\omega/\omega$) and midgap position (a/λ, where a is the lattice parameter) for different configurations in which the material and filling fraction (ff) percentages were varied.

Sphere	Background	$\varepsilon_1:\varepsilon_2$	ff (%)	$\Delta\omega/\omega$ (%)	a/λ
Si	Air	12:1	43	13	0.45
Si	Silica	12:2.1	42	5	0.41
Air	Si	1:12	50	12	0.40
Silica	Si	2.1:12	50	4	0.38

In summary, we have shown a method by which to construct opal-like materials with diamond symmetry by robot-aided micromanipulation, which leads to three-dimensional photonic crystal structures able to sustain robust full gaps. The position of the complete gap and its width may be controlled by varying the particles diameter and the filling fraction.

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