Photonic properties of an inverted face centered cubic opal under stretch and shear

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We present the results of numerical calculations of the dispersion relations for an inverted fcc opal structure subjected to a stretch and shear. We find that shearing of the crystal only lowers the gap width and slightly changes the midgap frequency. Interestingly, that in a large range of stretch amplitudes (up to 10%) the gap width is preserved and even slightly enhanced. The midgap frequency depends almost linearly on the stretch amplitude allowing for tuning an inverted fcc opal structure to a desired operational frequency. This last property may be important for the manufacturing process. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1558898]

To date, the route towards fabricating materials exhibiting a complete photonic band gap (PBG) through a self-assembly process has been aggregation of spherical colloidal particles.[1] In such experiments it is the fcc lattice which is most easily obtained. Many theoretical calculations[2,3] and experiments[1] confirmed that an inverted closed packed fcc crystal displays a complete PBG. It has been suggested[4] that the band gap width can be enhanced by introducing non-spherical particles and breaking some of the symmetries possessed by the fcc lattice composed of spherical atoms. Some experimental efforts to explore this possibility have already been made. Thus, in Ref. 5 silica spheres have been subjected to the plastic deformations by exposing them to the high-energy irradiation. Another and probably the easiest way to break the original symmetries is through the mechanical deformations of the original PBG material.[6–8] Unfortunately titania, which is often used in photonic crystals designed for the visible region of the spectrum, is perhaps too fragile to allow significant macroscopic deformation. Recently, however, a process of emulsion templating has been used for the preparation of the inverted structure. It involves easily deformable oil droplets stabilized by surfactants in the immisible liquid—titania sol.[9] First the droplets are ordered, next the gel is formed, oil droplets are removed, gel is aged, dried in air, and calcinated to transform the matrix into the rutile phase. During the process template remains flexible till the last stage. Thus, inverted fcc opal can be prepared in the deformed state. Moreover flexibility avoids large stresses and therefore the breakage of the material during the preparation. Another way to implement macroscopically deformable inverted fcc opal is to use a matrix with rubber properties.[10]

Despite the fact that recent years brought a surge of interest of experimentalists in the deformations of photonic crystals[11] there is a clear lack of theoretical papers concerning the subject. Our paper is intended to fill this gap.

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In this letter we address the following two issues.

(i) How sensitive are the photonic gaps widths to stretching or shearing of an inverted fcc lattice?
(ii) Is it possible to tune the operational frequency preserving the original gap width?

Photonic crystal is a periodic arrangement of regions with different dielectric constants ϵ. The laws governing the propagation of electromagnetic waves in such a medium are given by the Maxwell's equations (ME). Ignoring the nonlinear effects, possible solutions of ME can be expressed as a superposition of the time-harmonic modes. The frequencies of these modes are eigenvalues of a linear Hermitian operator[12] forming discrete sequence of bands ("dispersion relations") $\omega_n(\mathbf{k})$ as a functions of the "wave vector" $\mathbf{k}$. The solutions of the eigen-problem are fully scalable,[12] i.e., for the isotropic stretching $\mathbf{r}\rightarrow\mathbf{r}'=\alpha\mathbf{r}$ of the original material with known spectra $\omega_n(\mathbf{k})$ frequencies are given by $\omega_n'(\mathbf{k})=\omega_n(\mathbf{k})/\alpha$. However, the interesting and experimentally accessible deformations include anisotropic stretching and shearing of the material. Unfortunately these do not have the elegant property of simple scaling. In order to check how the photonic properties respond to a deformation of an inverted opal fcc lattice we had to perform numerical calculations.

The inverted opal closed packed fcc lattice consists of air spheres ($r/a=\sqrt{2}/4$ where a is the lattice constant of the cubic supercell) of a dielectric constant (DC) $\epsilon_{\mathrm{air}}=1$ immersed in a dielectric matrix (ϵ_m). We have set the matrix DC to $\epsilon_m=13$. Such materials (e.g., GaAs matrix) have already been synthesized.[1] In such experiments one usually obtains a slab of the material with the (111) crystalline plane parallel to the substrate. In order to simulate the experimental conditions we have chosen an orthogonal basis with the z axis pointing in the [111] direction of the lattice. The x and y axes have been set to lie in the substrate plane ([1 1 −2] and [1 −1 0] crystalline directions, respectively).

We have focused our attention on shearing in substrate plane ($x\rightarrow x+z\sin(\theta)$, $y\rightarrow y+z\sin(\phi)$, $z\rightarrow z$) and stretching

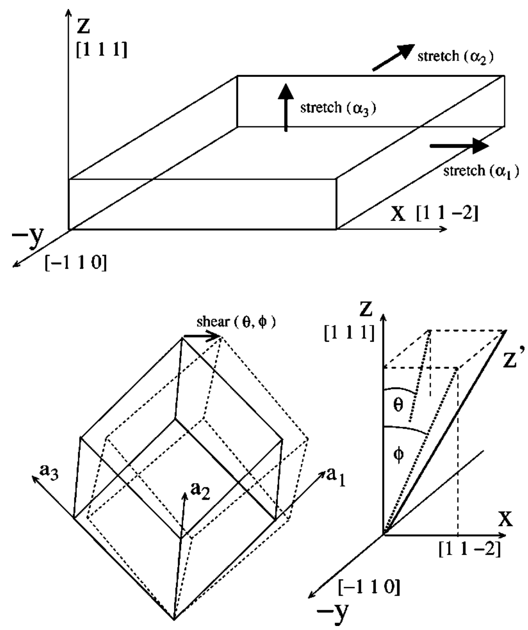

FIG. 1. The orientation of the laboratory orthogonal basis with respect to the crystal planes. The 111 plane is parallel to the substrate. The stretch amplitudes α_1, α_2, and α_3 are applied to the x (1, 1, −2), y (1, −1, 0), and z (1, 1, 1) directions, respectively. The shear amplitudes have been measured in the angles by which the original 111 direction has been shifted: θ is the angle between the original and sheared diagonal and ϕ is the angle between it's projection and the original x axis. The a_1, a_2, and a_3 directions form the basis of an undistorted cubic superlattice.

the material along the z direction ($z \rightarrow \alpha_3 z$). In the latter case we have taken into account three different scenarios in the xy plane ($x \rightarrow \alpha_1 x$, $y \rightarrow \alpha_2 y$): (i) preservation of volume by a homogeneus spreading ($\alpha_1 = \alpha_2 = \sqrt{1/\alpha_3}$), (ii) spreading only in the x direction ($\alpha_1 = 1/\alpha_3$ and $\alpha_2 = 1$), and (iii) ($\alpha_1 = \alpha_2 = 1$) which results in compression or expansion of the material. The laboratory and crystalline coordinate systems together with the shear and stretch directions are sketched in Fig. 1.

Fully-vectorial eigenmodes of Maxwell's equations with periodic boundary conditions were computed by preconditioned conjugate-gradient minimization of the block Rayleigh quotient in a planewave basis, using a freely available software package MPB.[13,14] The MPB uses smoothed effective dielectric tensor,[15] which brings convergence proportional to the square of spatial resolution even for sharply discontinuous dielectric structures. The accuracy in frequencies for the lower laying bands ($n_{\mathrm{band}} < 11$) has been checked to be better than 1%.

We have used deformed (by transformation induced by stretch or shear) standard fcc Brillouin zone (BZ). The small deformations have not changed the nearest neighbors on the fcc lattice even though the air domains are no longer spherical. For an undeformed fcc lattice the irreducible part is a 1/32 of the first BZ. When a stretch is applied and the threefold rotational symmetries are lifted the irreducible part is bigger. Thanks to the preservation of the mirror plane symmetries it is enough to compute the band frequencies within 1/8 of the first BZ. When a combination of shears is applied the preservation of the inversion symmetry guarantees that a half of the BZ is representative for all incident directions of the wave vector **k**. The (undeformed) BZ and the high symmetry points are sketched in Fig. 2 together with the path along which we have sampled reciprocal space of the sheared crystal. Upon deformation the reciprocal basis is transformed and the positions of the high symmetry points shifted. The shape of the BZ, however, is best visualized when it is undeformed (Fig. 2).

In the case of stretching we have studied three aspects of the photonic properties of a deformed fcc lattice: (i) the complete band gap width, (ii) the gap in the direction parallel to the substrate and, finally, (iii) the 111 direction gap (L_{111} point). The complete gap width have been established by comparing the frequencies in all of the high symmetry points on the first BZ as well as along the path shown in Fig. 2(right). The gap width for light propagating in the substrate plane has been extracted by comparison of the frequencies at the K_{ij} and P_{ijk} points which correspond to the nearest neighbor and second nearest neighbor directions, respectively. The relevant K and P points are shown in the right panel of Fig. 2. Results of computations are gathered in Fig. 3. On the right mid gap frequencies ω_0 are shown as functions of a stretch strength α_3. Gaps width $100\Delta\omega/\omega_0$ dependencies on α_3 are plotted on the left. Different line styles correspond to the different stretching scenarios discussed earlier. Interestingly, full PBG width (top part of the Fig. 3)

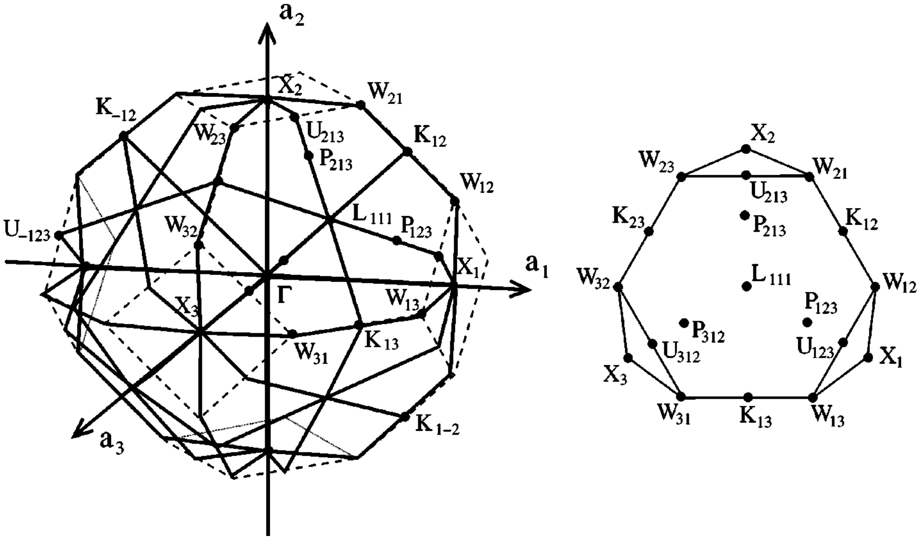

FIG. 2. Left: one half of the undeformed first BZ with some of the high symmetry points marked. The path through the relevant points taken into account in the computations of sheared samples are given by solid line. Right: projection of one eighth of the undeformed first BZ on the 111 plane. The P_{312} point corresponds to the light propagating in the x (1 1 −2), K_{12} to the y (1 −1 0) and L_{111} to the z (1 1 1) direction.

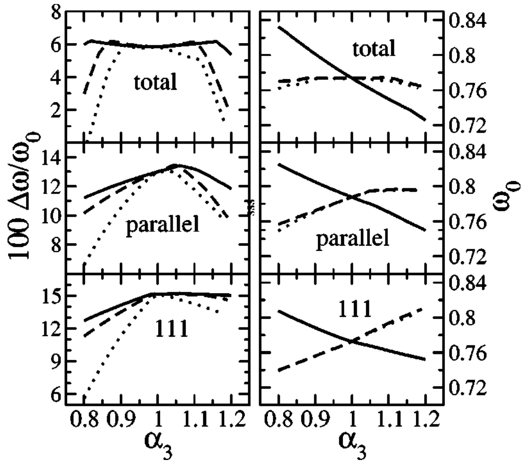

FIG. 3. The results of the numerical calculations for the stretched fcc lattice. On the left the gap width between bands 8 and 9 is shown. On the right the midgap frequencies are given. The information corresponding to the complete, parallel to the substrate and 111 (L point) gaps are given in the top, middle and bottom panels, respectively. The dashed and dotted lines correspond to preserved volume cases ($\alpha_1=\alpha_2=\sqrt{1/\alpha_3}$ and $\alpha_1=1/\alpha_3$, $\alpha_2=1$, respectively.) The solid line corresponds to the unpreserved volume case ($\alpha_1=\alpha_2=1$).

remains practically unchanged over significant range of stretch amplitudes. In the case of the stretch without volume preservation, midgap frequency changes quite notably. These two features together open a way to tune gap properties via mechanical deformation of the crystal sample. Properties of the "partial" band gaps are given in two bottom parts of Fig. 3. The gap in the substrate plane approaches $\approx 13\%$ at slight elongation of the 111 direction ($\alpha_3 \approx 1.05$). The normal direction gap is even wider ($\approx 15\%$ at $1 \leqslant \alpha_3 \leqslant 1.2$). In both cases the midgap frequencies can be tuned over a quite wide range ($\approx 10\%$)—see Fig. 3.

Results concerning full PBG properties changes under the shear applied in (111) plane are presented in Fig. 4. Here there are two parameters (angles θ and ϕ described earlier) that control the shear amplitude. In Fig. 4 iso-lines (i.e., lines in $\theta\phi$ plane, corresponding to the constant values of ω_0 and $100\Delta\omega/\omega_0$, respectively) are plotted. We have found that midgap frequency is well preserved under quite substantial shear amplitude. The gap width, however, decreases with the shear magnitude. The rate of the gap width decrease reflects the three fold symmetry in the 111 plane (see Fig. 4).

At the end let us summarize briefly the results that may be important for technological applications.

(i) Full PBG, displayed by inverted fcc opal of spheres, survives under small stretching (up to $\approx 10\%$) and shearing, i.e., they are not very sensitive to small deformations.

(ii) Midgap frequencies of the partial PBGs can be influenced via stretching the crystal along (111) direction.

(iii) Midgap frequency of the full PBG can be tuned as well if the volume of the unit cell is not preserved under the stretch.

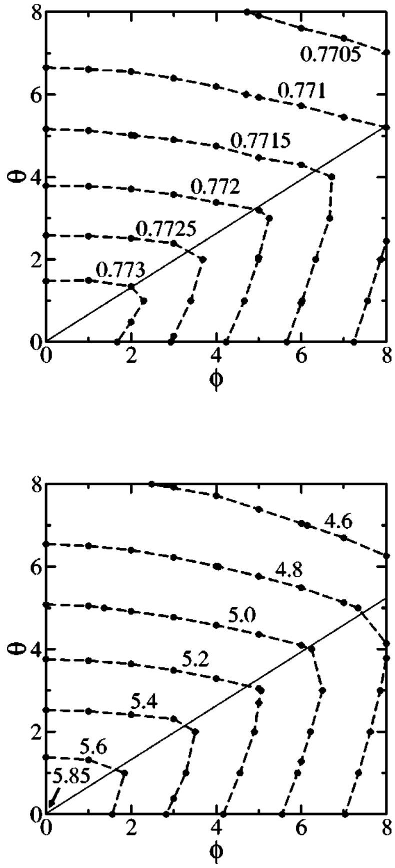

FIG. 4. The results of the numerical calculations for the sheared fcc lattice of spheres. On the top iso-lines of the midgap frequency ω_0 in the $\theta\phi$ plane are shown. In the bottom panel iso-lines of the gap width $100\Delta\omega/\omega_0$ are given. The dots are the points for which we performed numerical computations and dashed line is to guide the eye only.

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