Photonic band structure of three-dimensional colloidal crystals with field-induced lattice structure transformation*

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By utilizing the electrorheological effect, three-dimensional colloidal crystals can be produced, whose lattice structure can be changed from the body-centered-tetragonal lattice to other lattices under the application of electric fields. This paper calculates photonic band structures of such crystals with lattice structure transformation, and demonstrates the existence of complete band gaps for some intermediate lattices. Thus, it becomes possible to use the electrorheological effect to achieve photonic crystals with desired photonic gap properties resulting from tunable structures.

Keywords: photonic crystals, electrorheological effects, band gaps

PACC: 4270Q, 4660H

Electrorheological (ER) fluids[1] are the suspensions in which the induced dipole moment can order the suspended polarizable particles into columns under the application of a strong electric field. The rapid field-induced aggregation and the large anisotropy of ER fluids[2−8] render this material potentially important for technological applications. As the external field exceeds a critical field, the ER fluid turns into a solid or a colloidal crystal, whose ground state is a body-centered tetragonal (bct) lattice.[9] For the colloidal crystal, R. Tao *et al.*[10] proposed that a lattice structure transformation from the bct lattice to some other lattices can appear when the particles have magnetic dipole moments and a magnetic field is simultaneously applied perpendicular to the electric field. Interestingly, this proposal was verified experimentally and a lattice structure transformation from the bct lattice to the face-centered cubic (fcc) lattice was observed as the ratio between the external magnetic and the external electric fields exceeded a minimum value.[11] It was further shown that an alternative lattice structure transformation from the bct structure to the fcc can also occur through the application of electric fields only.[12] In fact, with the ER effect, one can place uniform hollow glass beads in a host medium (e.g., a resin), and apply a strong electric field afterwards. The mismatch in the dielectric constants between the medium and the spheres will force the spheres to aggregate into a bct lattice.[13] Once the host medium hardens, the solidified piece becomes a colloidal crystal, which can serve as an inverse three-dimensional (3D) photonic crystal.[13] Similarly, its ground state is also a bct lattice.[13] The basic physics of lattice structure transformation holds as well. In fact, this method can be used to produce a general class of inverse 3D photonic crystals with the ratio of the dielectric constant of the host medium $\epsilon_{\rm m}$ to the dielectric constant of the (spherical) particles $\epsilon_{\rm p}$ being $\epsilon_{\rm m}/\epsilon_{\rm p} > 1$. Here the ratio $\epsilon_{\rm m}/\epsilon_{\rm p}$ characterizes the dielectric contrast between the two components.

Photonic crystals are man-made materials which possess unusual optical properties.[14−17] They are of particular importance in electromagnetism (especially, optics and photonics), where they are promising for a variety of optical and microwave applications, such as some types of beam steerers, modulators, bandpass filters, lenses, microwave couplers, and antenna radomes. Under favorable conditions, photonic crystals exhibit photonic band gaps. The propagation of electromagnetic waves of frequencies within the photonic band gap is forbidden, which causes a deep impact on various photonic applications.[18−21] The characteristic of photonic crystals is a periodic variation of the dielectric function with periodicities on the order of the wavelength of an incident electromagnetic

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wave. The 3D photonic crystals with the ability to control photon flow in all three spatial dimensions are of special interest. Inverse opals, an fcc air-sphere lattice in a material with high dielectric constants, are an attractive example of a 3D inverse photonic crystal,[22−25] which has been proved to be a promising structure for complete photonic band gap and practical applications. The inverse opals were suggested to consist of different materials such as metal,[26] polymer,[27] semiconductor,[28] and insulator.[29]

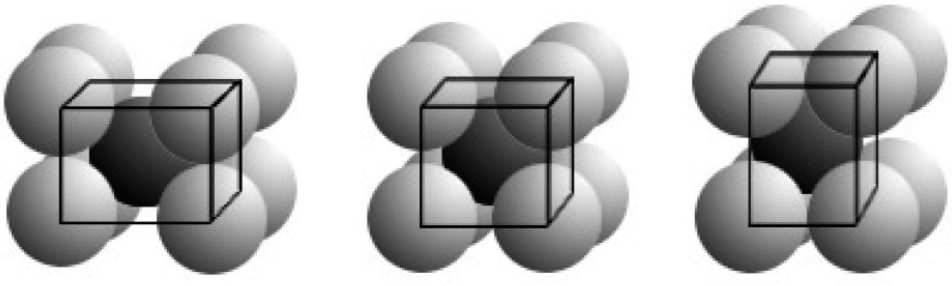
In this work, we shall investigate photonic band structures of a type of colloidal crystals, inverse 3D photonic crystals or opals, with lattice structure transformation as can be realized by using the ER effect together with an appropriate external electric field.

To proceed, we should first indicate the inherent differences between a fluid and an (inverse) opal. The rheological fluid is a suspension of particles in a solvent. The particles are free to respond in the solvent as a function of the applied electric field. As a consequence, the relative position of the particles can change. Nevertheless, in this work, once a certain lattice structure is reached for an ER fluid subjected to an appropriate electric field, the system may be refrigerated into a solid (where the particles are no longer free to change their relative positions), thus yielding an (inverse) opal. In other words, applying an electric field to the ER fluid can lead to a specific lattice structure for the system. After refrigeration, the system just becomes a solid (inverse) opal with this type of lattice as expected. In this sense, an (inverse) opal can also have lattice structure transformation, which enriches the realm of conventional opals with the fcc lattice structure. Or, alternatively, according to the proposal of this work, opals can have an fcc crystal structure, and also have other lattice structures like bct and bcc.

Since it has been revealed that the bct lattice is the ground state of ER fluids,[9] to investigate the role of lattice structure transformation in the band structures, let us start by considering the bct lattice to be a tetragonal lattice, plus a basis of two spherical particles, one of which is located at a corner and the other of which at the body centre of the tetragonal unit cell. The tetragonal lattice has a lattice constant $c = q\xi$ along the z axis and lattice constants $a = b = \xi q^{-1/2}$ along the x and y axes. The volume of the tetragonal unit cell remains $V_c = \xi^3$ as q varies. In this way, the degree of anisotropy of the tetragonal lattice is measured by how q is deviated from unity and the uniaxial anisotropic axis is directed along the z axis. Till now the lattice parameter q remains arbitrary. For hard spheres of our interest, however, the lattice parameter q can be determined from the relation

$$2a^2 + c^2 = 16R^2, \tag{1}$$

where R is the radius of the particles. The hard-sphere condition requires $a \geq 2R$ and $c \geq 2R$. For the bct lattice, $a = b = \sqrt{6}R$ and $c = 2R$, while for the fcc lattice, $a = b = 2R$ and $c = \sqrt{8}R$.[9] The body-centered cubic (bcc) lattice is characterized by $a = b = c = \sqrt{16/3}R$.[12] So far, according to this model,[12,30] the bct lattice is simply characterized by $q = 0.87358$, the bcc lattice by $q = 1.0$, and the fcc lattice by $q = 1.25992$. In other words, here q is the only parameter characterizing the type of specific lattices. Thus, by tuning q, it is convenient to investigate the effect of lattice structure transformation on the band structures of the 3D inverse photonic crystals with $\epsilon_{\rm m}/\epsilon_{\rm p} > 1$, as also schematically shown in Fig. 1. For obtaining such band structures, we resort to the commercial software Rsoft. Incidentally, regarding the electric field strength that would be necessary to achieve the requested q values, it depends on both the dielectric constants of the particles and host fluid and the volume fraction of the particles.[12]



(a) bct unit cell (b) bcc unit cell (c) fcc unit cell

Fig. 1. A schematic sequence of unit cells during lattice structure transformation: (a) a bct lattice ($q = 0.87358$); (b) a bcc lattice ($q = 1.0$); (c) an fcc lattice ($q = 1.25992$).

The simulation results are shown in Fig. 2 for three q's (three intermediate lattices), in which the ratio is set to be $\epsilon_{\rm m}/\epsilon_{\rm p} = 31$. It shows that the change of the band gap is quite different as the lattice structure changes gradually. For example, at $q = 1.1$ [see Fig. 2(b)], the photonic crystal has no complete photonic band gaps. At $q = 0.95$ [Fig. 2(a)], the photonic crystal has one complete band gap between the sixth and seventh bands. Interestingly, at $q = 1.1$ [Fig. 2(c)], the photonic crystal has two complete band gaps, one of which is between the second and third bands and the other of which between the eighth and ninth bands.

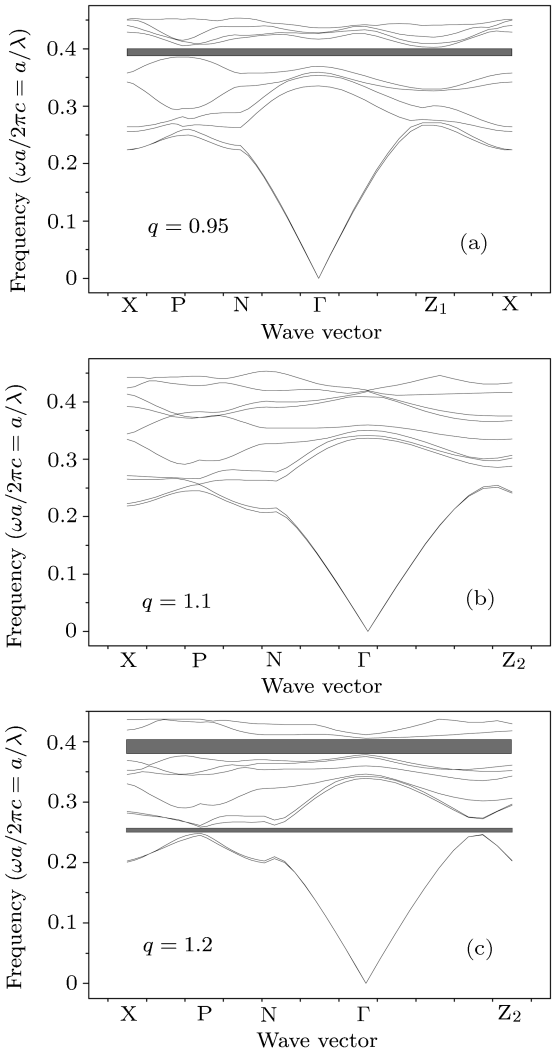


Fig. 2. Band structure (reduced frequency is denoted by $\omega a/2\pi c = a/\lambda$. ω or λ: angular frequency or wavelength of incident electromagnetic waves, respectively; C: speed of electromagnetic waves in free space) for three intermediate lattices at $q =$ (a) 0.95, (b) 1.1, and (c) 1.2, which can come to appear during lattice structure transformation: figure 2(a) contains one complete band gap between the sixth and seventh bands; figure 2(b) has no complete band gaps, and figure 2(c) displays two complete band gaps, one of which is between the second and third bands and the other of which between the eighth and ninth bands. The complete band gap regions have been shaded in both (a) and (c). Parameter(s): $\epsilon_{\rm m}/\epsilon_{\rm p} = 31$.

Figure 3 shows the complete band gap of inverse dielectric photonic crystals as the lattice structure changes. Here we choose a high dielectric constant of the medium $\epsilon_{\rm m}/\epsilon_{\rm p} = 31$. The shady part of Fig. 3 displays the areas with complete band gaps in which the propagation of electromagnetic waves is forbidden. The results are interesting: the number of complete band gaps can be zero, one, or two, depending on different values of q. In other words, this figure also shows that the complete band gaps are sensitive to the change of the lattice structure.

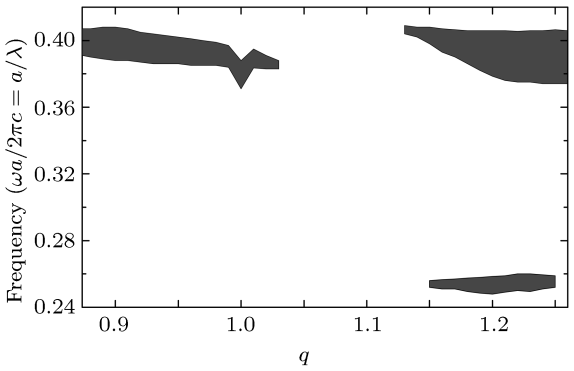


Fig. 3. Distribution of complete band gaps as a function of reduced frequency ($\omega a/2\pi c$ or a/λ) and q. The shady parts indicate the areas with complete band gaps in which the propagation of electromagnetic waves is forbidden. Parameter(s): $\epsilon_{\rm m}/\epsilon_{\rm p} = 31$.

To investigate the dependence of band gaps on the lattice structure, we also need to study the role of material properties, namely, the dielectric constant of the media. Figure 4 is the same as Fig. 3, but for a different dielectric ratio $\epsilon_{\rm m}/\epsilon_{\rm p} = 10$. Similarly, it is shown that the number of complete band gaps can also be zero, one, or two, which are related to different values of q. However, comparing with Fig. 3, evidently we find that the regions for the appearance of complete band gaps have been shrunken significantly in Fig. 4. In other words, increasing $\epsilon_{\rm m}/\epsilon_{\rm p}$ is beneficial to achieve complete band gaps. Thus, in reality, one had better set $\epsilon_{\rm m}/\epsilon_{\rm p}$ high enough, in order to obtain suitable inverse photonic crystals in which the propagation of electromagnetic waves is forbidden. So far, we may also conclude that material properties play an important role in the appearance of complete band gaps.

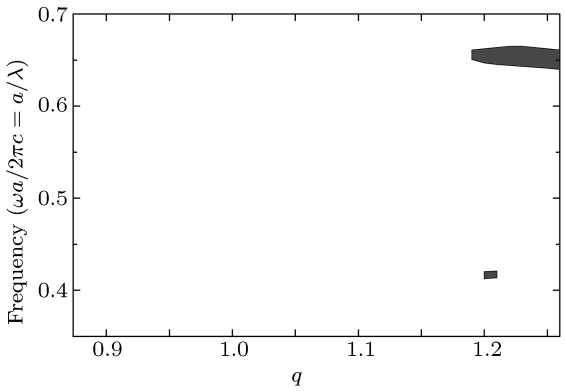


Fig. 4. Same as Fig. 3, but for $\epsilon_{\rm m}/\epsilon_{\rm p} = 10$. The regions for complete band gaps have been shrunken remarkably in comparison with Fig. 3.

In summary, we have calculated photonic band structures of ER effect-based 3D colloidal crystals with lattice structure transformation, and demonstrated the existence of complete band gaps for intermediate lattices. Thus, it seems possible to use the ER effect to achieve photonic crystals with desired photonic gap properties originating from adjustable structures.

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