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Effective-medium description of dielectric-chiral photonic crystals

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Abstract

Using exact results of the properties of photonic crystals consisting of chiral spheres in conjunction with an existing Maxwell–Garnett-like model for chiral composites we examine the possibility of describing such a crystal as a homogeneous chiral entity.

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Chiral media possess an intrinsic handedness that causes right and left circularly polarised waves to propagate with different phase velocities [1,2]. This circular birefringence suggests that wave interactions in periodic chiral media will induce a richness of phenomena associated with their response to different circular polarisations evidenced in the gap region of the frequency band structure, produced by the fundamental Bragg condition [3,4]. It is clear then that periodic structures with different responses to waves of opposite circular polarisations will have applications as polarisation-sensitive filters in the optical, microwave, and millimetre-wave regimes. In particular, periodic dielectric-chiral media might serve as new composite materials for engineering periodic resonant devices with index modulation and stop band features [5,6].

In this work, we examine the effective medium behaviour of dielectric-chiral composite photonic crystals in the long-wavelength limit of electromagnetic (EM) waves. For this purpose we use the results of the calculation of the EM response of photonic crystals of chiral spheres [4] in conjunction with an effective medium approach to chiral composites developed by Lakhtakia et al. [7,8]. In the case of high optical contrast, for a variety of chiral responses and volume filling fractions, we compare the effective EM response of the crystal with the exact one, and discuss the concept of homogenisation in the frequency range extending up to the first band gap of the EM spectrum.

Many effective medium descriptions of long wavelength EM waves in composite structures are based on the well-known Maxwell–Garnett (MG) theory [9–11]. The MG model was applied to the case of chiral composite materials, only recently [7,8,12–14]. Here we adopt an MG-like approach developed by Lakhtakia et al. [7,8] for composite materials consisting of chiral spheres.

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We consider a homogeneous isotropic chiral sphere obeying the Drude–Born–Fedorov constitutive equations [1,15]

$$\boldsymbol{D} = \epsilon\epsilon_0[\boldsymbol{E} + \beta\, \nabla \times \boldsymbol{E}], \tag{1}$$

$$\boldsymbol{B} = \mu\mu_0[\boldsymbol{H} + \beta\, \nabla \times \boldsymbol{H}]. \tag{2}$$

The dimensionless coefficients ϵ, μ represent the relative permittivity and relative permeability of the chiral medium and β (in units of length) is the chirality parameter. A photonic crystal formed by a periodic arrangement of chiral spheres, such as the above one, in a dielectric host defined by ϵ_h and μ_h can be described as a homogenised chiral medium possessing the following three dimensionless effective parameters [8],

$$\bar{\epsilon}(\omega) = \frac{\epsilon_h[(2\epsilon_h+\epsilon) - 2f(\epsilon_h-\epsilon)][(2\mu_h+\mu) - 2f(\mu_h-\mu)] - 4(f-1)^2\epsilon_h\mu_h\epsilon\mu\omega^2\beta^2/c^2}{[(2\epsilon_h+\epsilon) + f(\epsilon_h-\epsilon)][(2\mu_h+\mu) - 2f(\mu_h-\mu)] + 2(f-1)(f+2)\epsilon_h\mu_h\epsilon\mu\omega^2\beta^2/c^2}, \tag{3}$$

$$\bar{\mu}(\omega) = \frac{\mu_h[(2\epsilon_h+\epsilon) - 2f(\epsilon_h-\epsilon)][(2\mu_h+\mu) - 2f(\mu_h-\mu)] - 4(f-1)^2\epsilon_h\mu_h\epsilon\mu\omega^2\beta^2/c^2}{[(2\epsilon_h+\epsilon) - 2f(\epsilon_h-\epsilon)][(2\mu_h+\mu) + f(\mu_h-\mu)] + 2(f-1)(f+2)\epsilon_h\mu_h\epsilon\mu\omega^2\beta^2/c^2}, \tag{4}$$

$$\omega\bar{\beta}(\omega)/c = \frac{9f\epsilon\mu\omega\beta/c}{[(2\epsilon_h+\epsilon) - 2f(\epsilon_h-\epsilon)][(2\mu_h+\mu) - 2f(\mu_h-\mu)] - 4(f-1)^2\epsilon_h\mu_h\epsilon\mu\omega^2\beta^2/c^2}, \tag{5}$$

where f, known as the volume filling fraction, is the fraction of the total volume fraction occupied by the spheres.

We consider in particular an fcc crystal, of lattice constant a, consisting of non-overlapping chiral spheres (ϵ, μ and β) in a dielectric host medium (ϵ_h, μ_h). Assuming a sphere of radius S per lattice cite, the crystal will have a volume filling fraction $f = 16\pi(S/a)^3/3$. We view the crystal as a sequence of (001) planes. The physical solutions of Maxwell's equations (normal modes) for the infinite crystal of given ω may be written as propagating Bloch waves of $\boldsymbol{k} = (\boldsymbol{k}_{\parallel}, k_{z;\mathrm{L,R}}(\omega))$. We shall consider normal incidence in which case, $\boldsymbol{k}_{\parallel} = \boldsymbol{0}$; $k_{z;\mathrm{L,R}}(\omega)$ characterise the circularly polarised propagating modes of the EM field of left (L) and right (R) handedness respectively for the given ω. As functions of ω, $k_{z;\mathrm{L,R}}(\omega)$ define the corresponding frequency bands which are similarly distinguished as L- and R-bands [4]. At this stage, it should be mentioned that the calculation in Ref. [4] of the frequency band structure of the infinite crystal, as well as the transmittance of light through a finite slab of the crystal, is based on an exact method that takes fully into account multiple scattering by the spheres [16,17]. In the case of photonic crystals of chiral spheres the exact results are obtained using a modified version of the program in Ref. [17].

The dispersion curves of the corresponding homogenised effective chiral crystal, the effective-medium frequency bands, are given by [1,2]

$$\bar{k}_{z;\mathrm{L,R}}(\omega) = \frac{\bar{n}\,\omega/c}{1 \pm \bar{n}\bar{\beta}\,\omega/c}, \tag{6}$$

where $\bar{n} = \sqrt{\bar{\mu}\,\bar{\epsilon}}$ is the effective index of refraction for the crystal while the other effective parameters are those defined in Eqs. (3)–(5).

We shall test an effective-medium description of the crystal for frequencies below the lower frequency edge ω_g of the first Bragg gap. We note that formation of the well-known Bragg gaps in photonic crystals is due to destructive wave interference, an effect which cannot be accounted for by an effective-medium theory. An in-depth investigation of the effective parameters given in Eqs. (3)–(5), in the above frequency range ($\omega a/c < 2$), shows that the zeroth order terms of their Taylor expansion with respect to $\omega a/c$ and up to order f can adequately describe the situation within a relative error of a fraction of a percent. We then replace the effective parameters with their ultra-low-*ka* approximations, which are explicitly given in Ref. [8], as follows,

$$\bar{\epsilon}(\omega) \simeq \bar{\epsilon}_0 = \epsilon_h\left[1 - \frac{3f(\epsilon_h-\epsilon)}{2\epsilon_h+\epsilon}\right], \tag{7}$$

$$\bar{\mu}(\omega) \simeq \bar{\mu}_0 = \mu_h\left[1 - \frac{3f(\mu_h-\mu)}{2\mu_h+\mu}\right], \tag{8}$$

$$\bar{\beta}(\omega) \simeq \bar{\beta}_0 = \frac{9f\epsilon\mu\beta}{(2\epsilon_h+\epsilon)(2\mu_h+\mu)}. \tag{9}$$

The above clearly implies the validity of the Clausius–Mossotti equation for the effective permittivity and effective permeability of the composite system under study.

Therefore, by substituting Eqs. (7)–(9) into Eq. (6) we can compare the effective band structure of the crystal with the exact one. This is shown in Fig. 1. We can safely say that the ultra-low-*ka* MG approximation, for the chiral composite employed here, describes adequately the properties of the crystal in the long-wavelength limit. Our choice of rather large β is meant to demonstrate that the above model will be valid in those cases also. Finally, from the same figure it is evident that the effective chiral medium description begins to diverge in the vicinity of the gap.

We have also tested the accuracy of the effective-medium model with respect to the specific rotatory power of a finite slab of the crystal of thickness d. This is done, for normal incidence, by calculating the angle of rotation from the explicit form of the transmitted fields as compared to the incident. In the case of the effective crystal, this is done in a straightforward manner as for a chiral slab with chiral properties as the ones given by Eqs. (7)–(9). The explicit formulas, as well as their approximate versions, for optical rotation in the MG formalism are given in Ref. [8]. The result is shown in Fig. 2 and it is clear that the effective-medium description of the crystal can predict accurately its chiral behaviour at long wavelengths. The exact result was obtained as in Ref. [4].

In order to have an overall picture of the error introduced in the present analysis with respect to the exact crystal behaviour we define a relative error factor Q^{err} as follows,

$$Q^{\mathrm{err}} = \frac{\langle k_{z;\mathrm{L,R}}(\omega)\rangle_\omega - \langle \bar{k}_{z;\mathrm{L,R}}(\omega)\rangle_\omega}{\langle k_{z;\mathrm{L,R}}(\omega)\rangle_\omega}. \tag{10}$$

The mean values appearing in Eq. (10) with respect to the frequency are defined as

$$\langle k_{z;\mathrm{L,R}}(\omega)\rangle_\omega = \frac{1}{\omega_g}\int_0^{\omega_g} k_{z;\mathrm{L,R}}(\omega)\,\mathrm{d}\omega. \tag{11}$$

We calculated Q^{err} for different filling fractions of the fcc crystal and different chirality parameters of the spheres; the results are presented in Fig. 3. A maximum relative error of $\sim 20\%$, indicates that the MG approximation employed here describes the crystal in the long-wavelength region, reasonably well. We note, however, that L-bands are given with lesser accuracy. This is due to the fact that the L and R modes propagate with an effectively lower and higher refractive index,

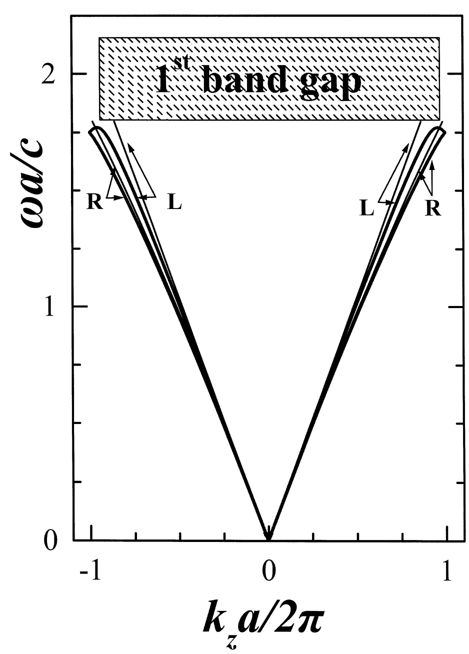

Fig. 1. Frequency band structure of the EM field along the normal to the (001) surface of an fcc crystal consisting of chiral spheres ($\epsilon = 1.1$, $\mu = 1$, $\beta = 0.3a$) in a dielectric host medium ($\epsilon_h = 12.96$, $\mu_h = 1$), with a volume filling fraction $f = 20\%$. The effective medium bands are denoted by the thinner lines.

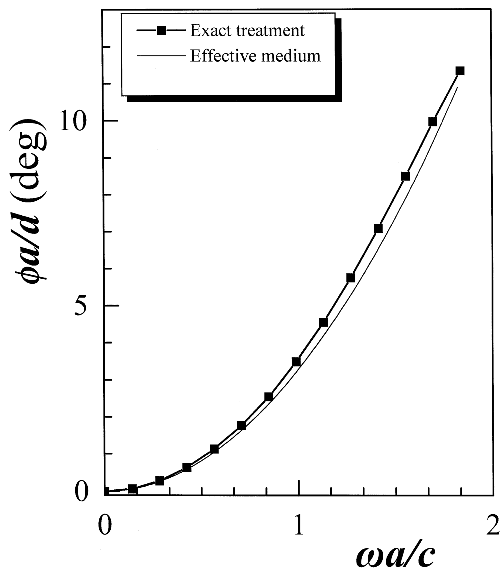

Fig. 2. Specific rotatory power of a (001) slab of an fcc crystal consisting of 32 layers of chiral spheres ($\epsilon = 1.1$, $\mu = 1$, $\beta = 0.3a$, $f = 20\%$) in a dielectric host ($\epsilon_h = 12.96$, $\mu_h = 1$) versus frequency, at normal incidence. The thicker line is an exact result; the thin line is the effective-medium result.

respectively [1]. The optical contrast between the low index modes (L) and the host medium is higher than that between the latter and the high index modes (R). And we know that a higher optical contrast implies a less accurate effective medium approximation [10].

More involved studies on the homogenisation of chiral composites of randomly distributed chiral inclusions [12,18] have set limitations on the size of the inclusions and the concentration of the composite, as far as the validity of the MG model is

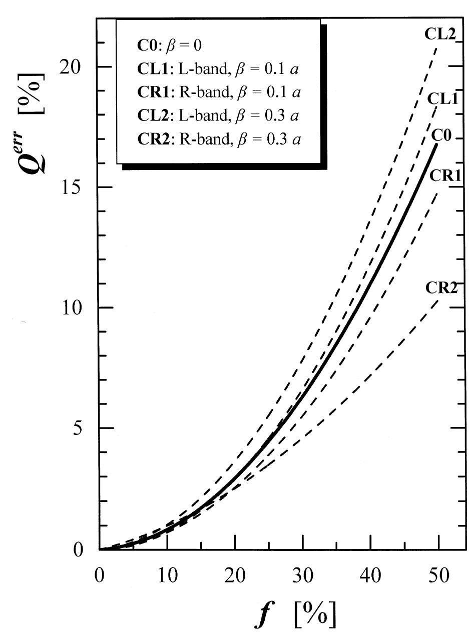

Fig. 3. Variation of the relative error factor Q^{err} with the filling fraction f of an fcc crystal of chiral spheres ($\epsilon = 1.1$, $\mu = 1$) in a dielectric host ($\epsilon_h = 12.96$, $\mu_h = 1$). The various curves correspond to different values of the chirality parameter β.

concerned. In our case the symmetry of the crystal gave more room to stretch those limitations a bit more. Although the ‘‘exact’’ MG formalism, as well as the extended MG model [12] and the Bruggeman model [18] are expected to give more accurate estimates, this is beyond the scope of the present work, since exact calculations have been carried out for the sake of a simpler description, such as the ultra-low-*ka* MG approximation.

We hope that the conclusions drawn by this study will simplify the aspects and problems associated with engineering of such composite materials of chiral behaviour.

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