Photonic band gaps from metallo-dielectric spheres


Department of Physics, Hong Kong University of Science and Technology, Clear water bay, Kowloon, Hong Kong, People’s Republic of China

Abstract

Joint theoretical and experimental efforts are launched to study the optical properties of photonic band-gap systems constructed with spheres containing a metal core or metallic coating. Using a multiple scattering method, we show that there can be photonic band gaps in different types of periodic structures as long as the sphere filling ratio exceeds a certain minimum. We have experimentally realized photonic crystals in the microwave regime, with the measured results in excellent agreement with the theoretical predictions. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Photonic band gap; Coated spheres; Multiple scattering

Photonic band-gap material is a new class of man-made material that possesses unusual optical properties [1,2]. These materials are by definition those that possess a gap in the electromagnetic wave spectrum, in which light cannot propagate in any direction. Such a gap can suppress spontaneous emission, and can be used to confine and control light propagation. Besides their intrinsic scientific interest, these materials are projected to have an impact on emerging technologies in a broad frequency range from the microwave all the way up to optical wavelengths.

However, photonic band-gap materials do not exist in nature. While it is not difficult to make these material artificially in the microwave length scale, their fabrication becomes increasingly challenging as we move up to the optical frequencies. Currently, high-frequency (micron scale) photonic crystals are made using micro-fabrication techniques (see e.g. Refs. [3,4]) or synthetic opal/ inverse-opal synthesis technologies (see e.g. Ref. [5]). These conventional photonic crystals are based on dielectric materials. Here, we propose to build photonic crystals using metallo-dielectric spheres as the fundamental building blocks. We note that metallo-dielectric photonic band gap systems have received far less attention than dielectric photonic crystals, but they have nevertheless been demonstrated to be viable in certain situations [6,7]. The spheres we have in mind have a dielectric core and a metal coating, encapsulated in another layer of dielectrics. It is the metal layer that plays the most important role. In fact, a system made up of non-touching solid metal spheres will have qualitatively similar behavior. However, it is advantageous to include an encapsulating insulating layer which ensures that the metallic components will not touch even if the spheres are in contact with each other. A desired separation between the metallic cores can always be prescribed as a certain thickness of the encapsulating dielectric layer. In addition, the multiply coated sphere configuration becomes more flexible in fabrication in smaller length scales, and the scattering properties are more tunable. We will show by theoretical calculations that such systems possess robust photonic gaps for a large variety of lattice structures. In fact, these systems possess photonic gaps for any periodic structure as long as the volume filling ratio of the spheres exceeds a certain threshold of the total volume. Glass cores are available in various sizes, from sub-micron to centimeters in diameters, and thus can cover a broad frequency range. The coating of metal layers and dielectric material can be achieved by processes such as electroless plating and sol-gel processes. For example, some of us have demonstrated that 45 μm glass spheres can be coated with multiple layers of Ni, TiO2 and PZT, and these coated spheres can self-assemble into an ordered structure under the action of an external fields [8]. In order to have a proof of principle
demonstration, we fabricated metal coated spheres in the microwave length scales, and constructed photonic crystal slabs using these spheres. The transmission through the photonic slabs is measured, and the results agree well with theory.

In order to have a systematic study of photonic band structures of our system, we need an accurate and efficient numerical method that can handle spherical scattering object with multiple coating layers, including metallic components. The multiple scattering method, which have been formulated for electromagnetic waves (see e.g. Refs. [9,10]), is probably best suited for this purpose. In particular, the scattering matrix of each sphere with concentric coatings can be handled analytically, thus the convergence can be greatly improved over methods that involve spatial discretization. We have developed a computer code to implement the multiple scattering method for the photonic band structure of three dimensional photonic crystals. The multiple scattering method amounts to solving the following secular equation:

\[
\text{Det}(\partial_{\sigma} \partial_{\sigma'} \delta_{mm'} \delta_{ss'}) - \sum_{l'm'a'} G^{s's'}_{lm; e': l'm'a'}(k) \gamma^{s's'}_{l'm'a'} = 0,
\]

(1)

where \((l, m)\) are the angular momentum indices, \(s\) is the index of scatterer inside the unit cell. \(G^{s's'}_{lm; e': l'm'a'}(k)\) are the Fourier transformation of the structure factors which can be expressed as

\[
G^{s's'}_{lm; e': l'm'a'}(R) = \left\{ \begin{array}{ll}
\sum_{\mu} C(l1l'; m - \mu) g_{lm-\mu,l'm'-\mu} C(\ell1\ell'; m' - \mu) & (\sigma = \sigma') \\
\sqrt{\frac{2l' + 1}{l + 1}} \sum_{\mu} C(l1l'; m - \mu) g_{lm-\mu,l'e' - 1m'-\mu} C(\ell1\ell'; m' - \mu) & (\sigma = m \text{ and } \sigma' = e), \\
- \sqrt{\frac{2l' + 1}{l + 1}} \sum_{\mu} C(l1l'; m - \mu) g_{lm-\mu,l'e' - 1m'-\mu} C(\ell1\ell'; m' - \mu) & (\sigma = e \text{ and } \sigma' = m),
\end{array} \right.
\]

(2)

where the \(C\)'s are the Clebsch–Gordon coefficients, \(g\) is the scalar structure factor given by \(g_{lm1'm'} = 4\pi \sum_{l''m''} Y_{l''m''}^* Y_{l'm'}^{*} \hat{h}_l(kR) Y_{l''m''}^* (-R)\), and the \(C_{lm1'm1'm'}\) are the Gaunt coefficients. The \(\hat{h}_l\) and \(Y_{lm}\) are Hankel function of the first kind and the Spherical Harmonics, respectively. This type of formulation can be called a vector-KKR approach. In the calculations reported below, we use angular momentum index up to \(l = 7\) for most of the calculations. Such a cut-off already provides good enough convergence for a quantitative comparison with experimental results, while the code is still fast enough to run on a PC with a single Pentium processor.

An interesting property of these photonic crystals constructed with metal coated sphere is that any periodic structure of such spheres exhibits photonic band gap as long as the filling ratio exceeds a certain threshold. This is illustrated in Figs. 1–4, where we show the calculated photonic band structure for four different structures: simple cubic (SC), face-centered cubic (FCC), body-centered cubic (BCC), and the diamond structure. These photonic crystals are constructed from spheres with a metal core, and coated with a dielectric layer with \(\varepsilon = 12\) and has thickness equal to 5% of the radius of the spheres. These spheres are positioned at the lattice points of a simple cubic lattice. The spheres are touching and have a dielectric coating (thickness equal to 5% of the radius, and dielectric constant \(\varepsilon = 12\)) encapsulating a metallic core which is modeled with \(\varepsilon = -200\). The frequencies are given in dimensionless units of \(2\pi c/a\) where \(a\) is the lattice constant.
Fig. 2. The photonic band structure for a photonic crystal where spheres (same as those in Fig. 1) are placed at the FCC lattice.

Fig. 3. The photonic band structure for a photonic crystal where spheres (same as those in Fig. 1) are placed at the BCC lattice.

Fig. 4. The photonic band structure for a photonic crystal where spheres (same as those in Fig. 1) are placed at the diamond lattice.

Fig. 5. The comparison of the calculated photonic band structure (middle) for a face centered cubic photonic crystal with the measured transmittance through a 3-layer [10 0] orientated slab (right) and a 3-layer [1 1 1] slab (left). See text for details.

all four structures (SC, FCC, BCC, diamond) we have considered possess photonic gaps, and the size of the photonic gap always increases as the spheres come closer together when the filling ratio of the spheres increases. We have also considered other structures such as hexagonal close-packed (HCP), body-centered tetragonal, hexagonal diamond, and they all have photonic gaps. We note that this behavior of exhibiting complete photonic band gaps for any periodic arrangement is an unique and potentially very useful property of these photonic crystal made up with metallo-dielectric spheres. Conventional photonic crystals, which are usually periodic structures crafted from a dielectric material, behave quite differently. For conventional dielectric photonic crystals, the opening of a complete photonic band gap depends a lot on the symmetry and the structural details, and only a handful of structures exhibit photonic gaps. In three dimension, the high dielectric component in a conventional photonic crystal usually form a percolated network of some prescribed symmetry (say diamond-like) [11], and such requirements make the fabrication of photonic crystals difficult at micron or sub-micron length scales. For example, a simple collection of dielectric spheres will not support complete photonic gaps. The metallo-dielectric spheres are much stronger scatterers, and they will support full photonic gaps as long as they are put together, essentially in whatever way one choose to.

We have constructed photonic crystal slabs and measured the transmittance. Results for the FCC structure are presented in Fig. 5. The spheres used in the experiment have a glass core with diameters of 19.7 mm. A copper layer of approximately 40 μm was coated on the glass core by the conventional electroless plating technique. Using a small amount of epoxy, these spheres are glued together to construct slabs of FCC symmetry orientated in the FCC(1 1 1) and FCC(1 0 0) directions. These slabs...
are three layers thick and the transmission of microwave from 1 to 18 GHz was measured through these slabs. The volume filling ratio of the spheres are approximately 64%, in the sense the volume of the sphere is 64% of that of the primitive FCC unit cell. We first look at the middle panel, which is the calculated photonic band structure of this model system, where the glass core is taken to have \( \varepsilon = 2.5 \), and the metallic layer is modeled by \( \varepsilon = -10^4 \) (i.e. basically a perfect metal). We see an absolute gap from about 12–14 GHz, and directional gaps along the high symmetry lines. These gaps are indeed observed experimentally in the microwave transmittance experiment. The left panel displays transmission through the (111) orientated slab. We see two wide stop bands at about 6 and 13 GHz. When we compare the transmission data with the calculated photonic dispersion, we see that the lower stop band corresponds to the directional gap along \( \Gamma L \), while the upper stop band is due to the absolute gap. The depletion of transmission at 16 GHz can be traced to a directional gap along \( \Gamma L \), just above the absolute gap. We note that a maximum rejection of about 30 dB is achieved near the center of the directional gap at 6 GHz, while a maximum of about 40 dB rejection is achieved for the absolute gap. The right panel shows the measured transmission along (100) along. The lower-frequency stop band centered at 7 GHz is derived from the directional gap along \( \Gamma X \). Note that this (100) stop band at 7 GHz happens to overlap with the stop band along (111). From the measured transmission spectrum, we see that the (100) gap near 7 GHz is narrower than that along (111). These features are in good accord with the calculated band structure results. From the middle panel, we see that the directional gap along \( \Gamma L \) is clearly wider than that along \( \Gamma X \). The higher stop band along the (100) direction centered at about 13 GHz is derived from the absolute gap.

In Fig. 6, we compare the calculated photonic band gap for a simple cubic structure photonic crystal with the measured transmission spectra through a three-layer slab orientated in the (100) direction. The panel on the right-hand side is the photonic band structure for metal spheres placed at a simple cubic lattice. The spheres have diameters of 12.7 mm, and the simple cubic lattice constant is 13.4 mm, corresponding to a filling ratio of about 45%. An absolute gap exists at about 13 GHz. The left panel shows the measured transmission spectra. We have constructed two samples. One is made with solid metal spheres, and its transmission spectra is given by the dotted line. The other one contains coated metal spheres, with plastic cores coated with a copper layer approximately 40 \( \mu m \) in thickness. The solid metal and the coated metal spheres give almost the same transmission spectra, suggesting that a very thin layer of metal will do the job. We reached the same conclusion from our calculations. For transmission along (100), we should consider the \( \Gamma X \) direction, where we observe a large directional gap from about 6–15 GHz. This agree well with the transmission spectra, which shows a wide stop band centered at about 10 GHz, showing a maximum rejection of over 30 dB. Due to the geometry of the Brillouin zone, the gaps in the \( \Gamma M \) and \( \Gamma R \) directions are smaller, and so the absolute gap is smaller than the directional gap along \( \Gamma X \).

In short, we propose to use multiply coated spheres consisting of an inner metal layer as the building block for photonic crystals. We developed a multiple-scattering code for this purpose. We show by explicit calculations that just about any periodic structure assembled with these balls will have complete photonic band gaps. The theoretical predictions are verified by experimental measurements in the microwave regime.

Acknowledgements

We thank Dr. Z.Y. Liu, Dr. Z.F. Lin and Dr. Z.Q. Zhang for many helpful discussions. This work is supported by RGC Hong Kong through HKUST6136/97P (theory) and by HKUST6142/97P (experiment).

References


