The photonic band structure of macro-‘ionic’ crystal

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Abstract

The photonic band structures depend on both the crystal symmetry and composing elements of the primary cell, the opening up of photonic gap is determined by the dielectric modulation in space. Since the high-dielectric medium acts as attractive centers while the metallic medium acts as repulsive centers for the field, the photonic crystals composed of a periodic arrangement of both high-dielectric and metallic spheres will have the highest dielectric contrast. The field distribution in such crystals is expected to resemble the electron distribution in ionic crystals, thus it should favor the formation of the absolute band gap. We show as an example that in GaAs-type photonic crystals this does prove to be the case and three large absolute gaps are found. © 2000 Elsevier Science B.V. All rights reserved.

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The presence of the absolute photonic band gap is the cornerstone for a variety of industrial application and basic physical studies [1–3] since it prevents the spontaneous emission of atoms embedded within. The major physical interests, therefore, have always concentrated on the search for the dielectric modulated structures and material components which possess a sizeable band gap. Up to now, for the 3D photonic crystals composed of purely dielectric media, an absolute band gap has been found only in the fcc structures and diamond structures. However, it is found that the photonic band gap is much more easier to form in crystals containing dispersive materials such as metals [4–6]. The existence of a photonic gap makes it possible to design various optical filters, optical polarizers, and micro-cavity lasers once defect modes are introduced into the gap [7,8], it also serves as a background to study the basic physical problems such as localization of light [9,10].

The band structures of photonic crystals depend both on the crystal symmetry as well as the materials composing the photonic crystals. The recent effort has shifted in the following two directions: (i) to further lower the point symmetry of the composite materials [11,12]; (ii) to explore other material composites [13–15]; the aim is to optimize the combination of these two factors so that the band gap/mid-gap frequency can be maximized. As is known from solid-state physics, ionic crystals made of atoms with extremely different electron negativity usually form band insulator, since atoms with small electron negativity tend to give up outer electrons, while atoms with large electron negativity tend to capture electrons when they form solids; there is very little
overlap of the outer electron wave function and thus the crystals becomes a band insulator. Since the high-dielectric medium acts as attractive centers while the metallic medium acts as repulsive centers for the field, the photonic crystals composed of a periodic arrangement of both high-dielectric and metallic spheres will have the highest dielectric contrast. The field distribution in such crystals is expected to resemble the electron distribution in ionic crystals. If the same picture also holds in the photonic crystals, one expects that photonic crystals composed of high-contrast dielectric and metal spheres are more venerable to the formation of the absolute photonic band gap [16,17].

In this Letter, we show that in photonic crystals of such macro-“ionic” atoms this does prove to be the case and that it favors the formation of sizable photonic band gap. As an example, we have calculated the photonic band structures of GaAs-type crystals with ‘Ga’ and ‘As’ standing for the dielectric and metal spheres, respectively, and three large absolute gaps are found. Because of the existence of frequency window for the expulsion of electromagnetic wave for metal spheres, it is expected that there is a sharp change of electric field at the interface of metal spheres when the frequency falls into these frequency windows. To deal with such a situation one needs a numerical method which can take the interface boundary condition accurately, instead of expanding the electromagnetic wave in reciprocal space so that the real-space boundary condition can be easily incorporated. This is the so-called multiple-scattering method which has been put into practice in the electronic band structure calculation some decades ago. Recently, the vector-wave multiple-scattering method has been also formulated for the electromagnetic wave propagating in photonic crystals [21–31]. We have also made a very efficient code and tested it for a variety of previous known results; both fast convergence and high accuracy have been proved for all cases [6]. This method is used in this Letter.

The photonic band structures of diamond crystals made of dielectric spheres have been calculated long ago by Ho et al. [19] using the vector plane-wave expansion method, which was one of the first examples of photonic crystals with an absolute photonic gap. The band structures of diamond crystals composed of perfect metal spheres have also been calculated by Fan et al. [4]; they adopted a finite-difference time-domain method in order to treat the rapid change of the electromagnetic field near the surface of the metal spheres. The method is very time consuming and has to be done on a supercomputer; again a absolute band gap was found between the 2nd and 3rd bands. The gap size in this case is a monotonic increasing function of the filling ratio of the metal spheres, it does not saturate even when the metal spheres are touching each other. Since our above mentioned macro-‘ionic’ crystals lies in between these two cases, one naturally expects that the photonic band structure should have a mixed features of both the purely dielectric and metallic crystals. Thus multiple photonic band gaps might result from such crystals.

With this motivation in our mind, we have studied the photonic band structure of the macro-‘ionic’ crystals of the ‘GaAs’ type with ‘Ga’ and ‘As’ atoms representing the dielectric and metal spheres, respectively. For the numerical computation we have chosen the dielectric constant of the dielectric to be \( \varepsilon = 12 \) and dielectric constant of metal sphere to be \( \varepsilon = -200 \). The large negative \( \varepsilon \) value of the metal spheres mimics the metal properties with large plasmon frequency and prevents the external electric field from penetrating into its interior. We have used our recently developed vector-wave multiple-scattering code to compute the photonic band structures along the high symmetry points. Their coordinates in the first Brillouin Zone are \( X(1,0,0) \); \( U(1,1/4,1/4) \); \( L(1/2,1/2,1/2) \); \( \Gamma(0,0,0) \); \( W(1,1/2,0) \); and \( K(3,4.3/4,0) \) in unit of \( 2\pi/a \), \( a \) is the lattice constant of GaAs crystal. The radii of the dielectric and metal spheres are assumed to be the same size and the sphere filling ratio, given by \( f = (32\pi/3)(R/a)^3 \), \( l_{\text{max}} = 7 \), is incorporated in the local expansion of the electromagnetic wave; the eigenfrequency is determined to the accuracy of the third digit.

In Fig. 1, the photonic band structures of macro-‘ionic’ crystal are shown for the filling ratio of \( f = 0.34 \), i.e. the maximum filling ratio of such crystal. The \( x \)-axis is the wave vector in the first Brillouin zone along the high-symmetry points and \( y \)-axis
Fig. 1. The photonic band structures of macro-ionic crystals of the GaAs type in air. The dielectric constants are $\varepsilon_s = 12$ for dielectric spheres and $\varepsilon_m = -200$ for metal spheres, the filling ratio is $f = 0.34$.

is the reduced frequency $\omega a/2\pi c$ with respect to the lattice constant $a$. In the frequency range displayed here, there exist three large photonic band gaps located at 0.545, 0.753, and 0.994. The first gap is the direct gap between the 2nd and 3rd bands at the U-point of the Brillouin zone, the second gap is an indirect gap between the fifth band at the L-point and sixth band at the U-point, and the third gap is also an indirect band gap between the 13th band at X-point and 14th band at $\Gamma$-point. The gap/mid-gap frequencies of these gaps are 0.182, 0.131, and 0.068, respectively. In view of the single gap in the

Fig. 2. The gap size as a function of filling ratio $f$ for macro-ionic crystal of the GaAs type. The dots are calculated points and lines are guide to the eyes. Three gaps are numbered in order of increasing frequency. The other parameters are the same as in Fig. 1.
situation of purely dielectric or metal spheres, the existence of multiple photonic band gaps is rather interesting and offers more freedom in designing multi-channel devices with specific requirements.

However, the scenario of multiple photonic band gaps appears only near the maximum filling ratio $f = 0.34$, two of the photonic band gaps with the lower and higher frequencies diminish rather quickly as the filling ratio decreases. The dependence of the gap size as a function of filling ratio $f$ is shown in Fig. 2. One finds that the first and third photonic gaps disappear roughly around $f = 0.27$ and $0.2$. The second gap enhances slightly first, then decreases rapidly as the filling ratio is reduced. The physical reasoning might be inferred from the photonic band structures of corresponding crystals of purely dielectric [19] and metal spheres [4]: it is known that the diamond structure of purely metal spheres favors the first band gap formation while that of purely dielectric crystal favors the second band gap. Since the gap size is a monotonic increasing function of the filling ratio for metal sphere structure and takes the maximum value at around $f = 0.2$ for the dielectric spheres, it is not surprising to see that the first gap decreases and the second gap slightly increases as the filling ratio is away from $0.34$.

As with photonic crystals with metallic components, it is important to check whether the photonic band gap remains when the metal absorption is taken into consideration. To do so, we have calculated the transmission spectra of such macro-ionic crystals of 32 double-layers along the (111) crystal plane. The transmission spectra with a normal-incident beam are presented in Fig. 3; the parameter set takes the same values as those of Fig. 1. It is seen that the transmission spectrum in the absence of absorption (Fig. 3a) is in perfect agreement with the photonic band structures (Fig. 1): there are three photonic band gaps visible around the frequencies 0.545, 0.753, and 0.994. Including the absorption coefficient into the dielectric constant does not change the spectrum significantly, but mainly broadens the spectrum slightly as can be seen in Fig. 3b. The dielectric constant of metal is taken as a complex number $\varepsilon = -200 + 50i$ to mimic the metal absorption, the imaginary part of the dielectric constant does not influence the spectrum that much, since the penetration length is so short and absorption process only takes place in a narrow outer shell of metal spheres. Thus, the photonic band gaps do survive, even in the presence of absorption.

Note that while the above calculation has been done for the ‘ionic’ crystals in air, the cases with other background dielectric media can be easily extracted from those presented above using the scaling relation.

In summary, we have studied in this Letter the photonic band structures of macro-ionic crystals made of dielectric and metal spheres, and three absolute photonic band gaps are found for large filling ratio. This is important in view of the fact that diamond crystals made of purely dielectric or metal spheres have only one absolute photonic gap. The multiple photonic gaps of this structure offer more freedom in designing the optical devices with multiple channels.
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References