Robust Photonic Band Gap from Tunable Scatterers

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We show theoretically and experimentally that photonic band gaps can be realized using metal or metal-coated spheres as building blocks. Robust photonic gaps exist in any periodic structure built from such spheres when the filling ratio of the spheres exceeds a threshold. The frequency and the size of the gaps depend on the local order rather than on the symmetry or the global long range order. Good agreement between theory and experiment is obtained in the microwave regime. Calculations show that the approach can be scaled up to optical frequencies even in the presence of absorption.

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Photonic band gap (PBG) is a spectral gap in which electromagnetic waves cannot propagate in any direction [1]. Recently, two promising routes have been discovered that may lead to PBG in the IR/optical frequencies: (i) microfabrication [2] and (ii) inverse-opal and related techniques [3]. Both methods seek to create some predefined artificial structure with an interconnected array of high dielectrics. Here we propose an alternate route. Instead of emphasizing the structure, we focus on the building blocks. The building blocks we propose are spheres with a dielectric core, a metal coating, and an outer insulating layer. With multiple coatings of variable thicknesses, these coated spheres have continuously tunable scattering cross sections and resonances. In analogy with semiconductor physics, we have designable "photonic atoms" which have continuously tunable properties. Depending on how we assemble these spheres together, we can choose the crystal structure which in turn can be changed by external fields [4]. In this paper, we show by physical argument and by explicit calculation and experimentation that *any* periodic structure formed from such spheres can exhibit photonic band gaps. This contrasts with the conventional PBG systems where the global symmetry and the structure factors are equally important, which in turn lead to added difficulties in their fabrication.

In order to handle the calculation involving spherical scatterers with metallic coating, we developed a band structure code based on the multiple scattering technique (MST) [5]. We checked our results against photonic band structures calculated using the finite-difference time domain (FDTD) method, where the convergence has been carefully monitored [6]. The test case is the photonic band structure of ideal metal spheres arranged in the diamond structure with a filling ratio $f = 0.31$, embedded in a medium with $\epsilon = 2.1$. This is a demanding test case since the metal spheres touch at $f = 0.34$. With our code, we obtain a gap/midgap frequency of 0.56 (with angular momentum up to $l = 7$), which is in excellent agreement with that of FDTD [6]. Our result lies between their finest grid value of 0.53 and the extrapolated value of 0.56. The transmission spectra reported below are computed with the layer-MST formalism of Stefanou-Yannopapas-Modinos [7]. The agreement between the band structure code and the transmission code is excellent.

Since metallic elements are involved, our system should be classified as a metallodielectric photonic band gap system [8], which has been considered by a few authors although these systems have received far less attention than pure dielectric PBG systems. Brown and McMahon [9] have fabricated metallodielectric PBG material with metal spheres arranged in a fcc lattice, and observed stop bands in the microwave regime. Fan *et al.* [6] showed that the experimentally observed stop band is the result of a directional gap in the (111) direction, while a complete band gap can be realized by arranging the spheres in the diamond structure. We argue here that by using metal or metal-coated spheres as building blocks, photonic gaps are guaranteed for *any* periodic structure. For the sake of discussion, we first consider perfect metal spheres arranged in some periodic lattice with lattice constant a, and the spheres are touching. Neighboring spheres inscribe a void with a scale on the same order as a, and the fundamental resonance modes in the void should have frequencies of the order of $\omega_u = c/a$. These voids are always connected together by channels, so that the mode energy can hop, forming a pass band. The lowest frequency that can pass through this system depends on the structure dependent "hopping parameters" but the frequencies cannot be much lower than ω_u. As long as the metallic part percolates, the system behaves as a low-frequency filter [10]. Now imagine that the spheres are not touching. There exists a finite but large ϵ_{eff} in the long wavelength limit. Low frequency waves can propagate through the three-dimensional structure as an effective medium, albeit with a small group velocity. This low pass band will have zero group velocity when the wave vector approaches the zone boundary, where the wave vector $k \approx \pi/a$. Thus the highest frequency ω_l of this low frequency pass band $\approx c/(\sqrt{\epsilon_{\text{eff}}}a)$. Since ϵ_{eff} increases when the distance between the spheres decreases, it is always possible to have $\omega_l < \omega_u$ when the filling fraction of the spheres exceeds a certain minimum value. Between ω_l and ω_u, a gap should be formed. Note that this argument does not depend on the structural details. Periodicity is not crucial either. As long as the ϵ_{eff}

is large, the low frequency pass band can be made "flat" enough for the gap to appear. The argument holds equally well for solid metal spheres and metal-coated spheres [11].

To substantiate our physical argument, we have constructed photonic crystal slabs and measured the transmittance in the microwave regime. Simple cubic slabs are constructed by gluing together spheres 12.7 mm in diameter (lattice constant $a = 13.4$ mm, filling ratio ≈45%) using a small amount of epoxy. In Fig. 1, we compare the calculated photonic band gap for the simple cubic photonic crystal with the transmission spectra through finite-sized slabs in two different directions. The middle panel is the photonic band structure, with metal spheres modeled by $\epsilon = -10^4$. The experiment was carried out using a HP8150C network analyzer with a HP8517B S-parameter test set. The sample was placed half way between the transmitting and the detecting horns mounted vertically at 50 cm apart. A metal plate with a 10.5 cm × 7.3 cm opening at the center was placed just beneath the sample to allow radiation to go through the sample and at the same time block stray signals. In some runs a larger opening was used to increase sensitivity. The scanning range was from 45 MHz to 18 GHz. To reduce noise, 20 scans were averaged for one run. The final results were normalized to the background without the sample. In the microwave regime, the metal should have a large imaginary part in ϵ. However, as the wave cannot penetrate the metal anyway, modeling with a large and negative real ϵ give band structure results that agree well with experimental measurements. An absolute gap is observed between 11 and 15 GHz. In the left and right panels, we compare the experimental and calculated transmission spectra. The two experimental spectra in the left panel correspond to the transmission through a three-layer slab in the (001) direction of two types of spheres: (i) solid metal spheres and (ii) metal-coated spheres that have plastic cores coated with a 40 μm copper coating. We notice that the coated spheres and solid metal spheres give very similar transmission spectra, so that a very thin metal layer will do the job. The calculated transmission, which agrees well with the measured spectra, corresponds to transmission through solid metal spheres modeled with $\epsilon = (-10^4 + 10^4 i)$. We have also calculated the transmission for metal-coated spheres, and the results are very similar to those for solid metal spheres and hence not shown separately. We note from the band structure that there is a directional gap along the ΓX direction from about 6 to 15 GHz. This corresponds well with the calculated and measured transmission spectra, which shows a wide stop band at the same frequency range. The right panel compares the calculated and measured transmission through the (111) direction of a five-layer slab of the simple cubic structure. There is again good agreement between theory and experiment. The stop band at 14 GHz (skewed towards higher frequencies) is derived from the absolute gap. Even a very thin slab is noted to give a maximum rejection of over 30 dB at the center of the stop bands. We remark that we cannot expect perfect agreement among band structure calculations, transmission calculations, and transmission measurement since they correspond to a 3D infinite crystal, a 2D periodic slab of finite thickness, and a small crystal finite in all three directions, respectively.

We have also constructed fcc photonic crystal slabs, and results are presented in Fig. 2. The spheres used in the experiment have a glass core with diameters of 19.7 mm and a Cu coating of approximately 40 μm. We constructed three-layer-thick slabs of fcc crystal (filling ratio ≈64%) orientated in the fcc(111) and fcc(100) directions. The

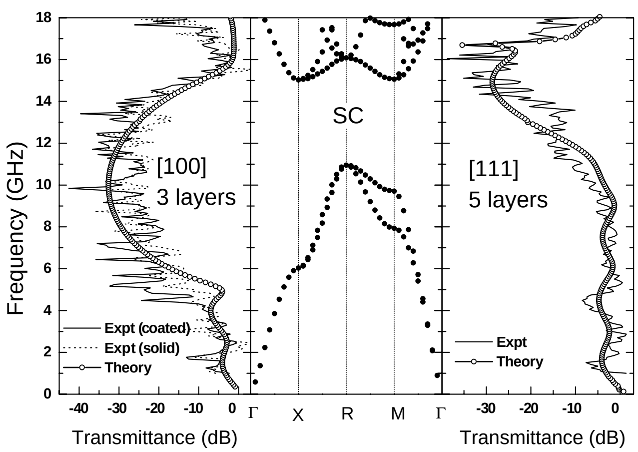

FIG. 1. Comparison of the calculated photonic band structure (middle panel) for a simple cubic photonic crystal with measured and calculated transmittance through a three-layer (100) orientated slab (left panel) and a five-layer (111) slab (right panel). The solid lines in the left and right panels are the transmittance for metal-coated spheres, while the dotted lines are for solid metal spheres. All measured spectra correspond to a single measurement. Calculated transmittances are given as open circles. See text for details.

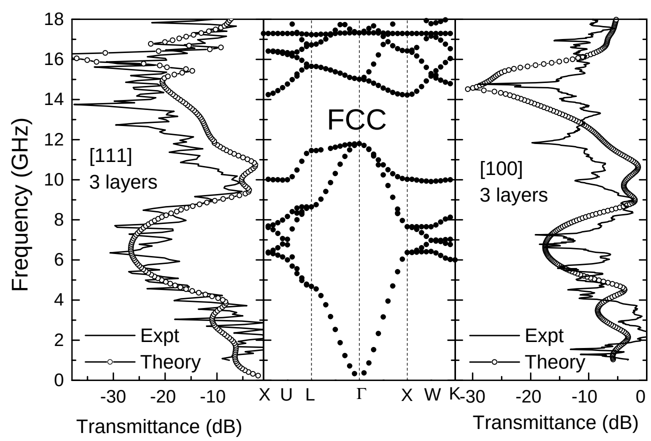

FIG. 2. Comparison of the calculated photonic band structure (middle panel) for a fcc photonic crystal with the transmittance through a three-layer (100) orientated slab (right panel) [12] and a three-layer (111) slab (left panel). Calculated transmittances are given as open circles. See text for details.

middle panel shows the calculated photonic band structure, where the glass core is taken to have $\epsilon = 2.5$, and the metallic layer is modeled by $\epsilon = -10^4$. We see an absolute gap from about 12 to 14 GHz, and directional gaps along the high symmetry lines. The left panel compares the measured and calculated transmission through the (111) orientated slab. We see two wide stop bands at about 6 and 13 GHz. The lower stop band corresponds to the directional gap along ΓL, 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 ΓL, just above the absolute gap. The right panel compares the measured and calculated transmission along (100). The lower frequency stop band centered at 7 GHz is derived from the directional gap along ΓX. 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 and transmission results. From the middle panel, we see that the directional gap along ΓL is clearly wider than that along ΓX. The higher stop band along the (100) direction centered at about 13 GHz is derived from the absolute gap.

We show by explicit calculation that essentially *any* periodic structure built from these spheres possesses PBG. Consider a generic system where the building blocks are touching metallodielectric spheres. The spheres have metallic cores coated with a dielectric coating ($\epsilon = 12$ and thickness $\approx$5% of the radius). The coating layer serves as a spacer to ensure that the metal cores are not touching. The metal is modeled by a $\epsilon = -200$ medium. In Fig. 3, we show that essentially any periodic structure constructed from these spheres has photonic band gaps. We mark in the figure the frequency (marked by the squares) and the size (marked by the bars) of the photonic gaps for a variety of structures. The angular frequency (ω) in the figure is scaled by $2\pi c/d$ where d is the diameter of the spheres. The frequency of the gap can be tuned to a certain extent by changing the dielectric constant of the outer coating.

We plot in the inset of Fig. 3 the gap/midgap frequency for a fcc arrangement of metal spheres with no coating layer, as a function of the filling ratio. An absolute gap emerges when the volume filling ratio of the metallic spheres exceeds $\approx$53%, and increases monotonically as a function of the filling ratio. Such behavior holds for all the structures we have considered, in agreement with the physical picture we have described above. Also, structures with higher packing ratios tend to have the photonic gap at higher frequencies, since the inscribed voids have smaller volumes and hence higher ω_u.

A potentially useful property of the present system is that the size and frequency of the photonic gap depend on the filling ratio and the short-range order rather than on symmetry and long-range order. This can be deduced from Fig. 3. Note that both the diamond and hexagonal diamond structure have the same fourfold coordination and local order, but different symmetries and hence different Brillouin zones. The photonic gap has almost the same size and frequency. It should be noted that the data are shifted slightly to avoid overlapping. The same is true for the fcc and hcp structures, which have the same local coordination but a different stacking sequence of close-packed planes. Even an ABCB stacking has essentially the same absolute gap.

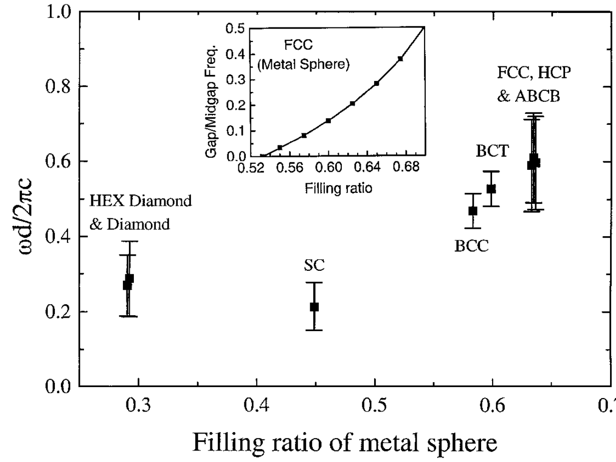

FIG. 3. The photonic band gaps for different crystal structures. All structures are made of touching metallodielectric spheres with a 5%-radius dielectric coating ($\epsilon = 12$). The filling ratio is that of the metallic core. HEX diamond, BCT, and ABCB refer to hexagonal diamond, body centered tetragonal, and a close-packing polytype of planes stacked in a repeated ABCB sequence, respectively. Other symbols such as FCC have their usual meaning. d denotes the diameter of sphere. The inset gives the dependence of gap/midgap frequency on the filling ratio in a fcc photonic crystal of metal spheres (no encapsulating layer).

An important question is whether the present approach can be scaled from the microwave frequencies up to the IR and optical frequencies. This is not obvious since metals are highly dispersive and can be strongly absorbing at optical frequencies. The choice of the coating material thus becomes an issue. We found it desirable to choose a metal such that the real part of ϵ is large and negative, while the imaginary part is relatively small at optical and IR frequencies. Silver satisfies these conditions. In Fig. 4, we compare the calculated transmission and reflection through three layers of (100) orientated simple cubic photonic crystal made up of silver coated spheres at four different length scales so that the stop band operates at four frequency ranges: (i) microwave, (ii) IR, (iii) $\lambda_{\rm gap} \approx 1.5\ \mu$m, and (iv) optical. Measured frequency dependent dielectric constant [13] is used for the Ag coating layer. The dimension of the spheres and coating thickness are given in the caption. The overall behavior is largely scale invariant. In particular, the absorption is small from 0.6 to 1.2 ω_g. Thus with dispersion and absorption taken into account, there is a good possibility of achieving photonic gaps at IR or optical frequencies with microspheres having tunable scattering properties.

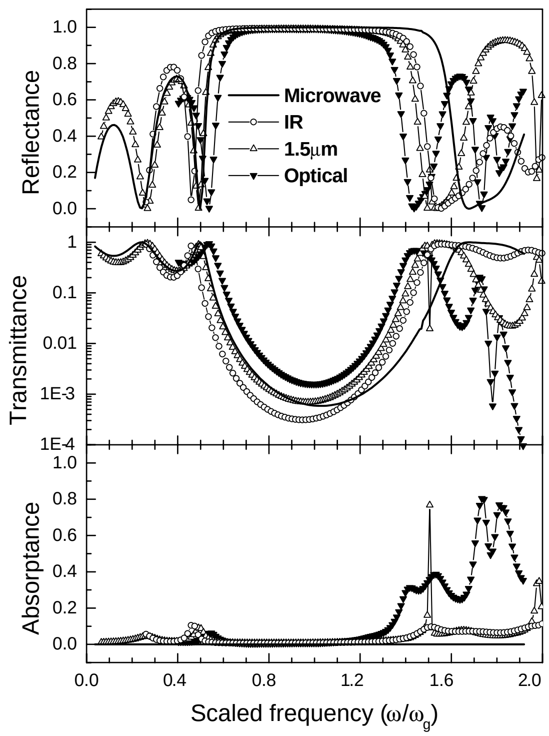

FIG. 4. Calculated transmittance, reflectance, and absorption through three layers of a (100) orientated simple cubic photonic crystal slab of Ag coated spheres at four different length scales. The core radius of the spheres (r), Ag layer thickness (t), filling ratio (f), and midgap frequency (ω_g) in (001) are given as (i) microwave: $r = 6.35$ mm, $t = 40$ μm, $f = 0.448$, $\omega_g = 9.65$ GHz; (ii) IR: $r = 1.2$ μm, $t = 0.15$ μm, $f = 0.47$, $\omega_g = 0.164$ μm^{-1}; (iii) $\lambda \approx 1.5$ μm: $r = 250$ nm, $t = 50$ nm, $f = 0.45$, $\omega_g = 0.65$ μm^{-1} (iv) Optical: $r = 80$ nm, $t = 50$ nm, $f = 0.42$, $\omega_g = 1.31$ μm^{-1}. All frequencies are given in dimensionless units of ω/ω_g. The core is assumed to have $\epsilon = 2.5$. Measured ϵ is used for Ag in (ii), (iii), and (iv).

In summary, we propose to build photonic crystals with multiply coated spheres containing a layer of metal. The resulting system has the unique property that photonic band gaps can be realized for essentially any periodic arrangement of such spheres. The consistency among band structure calculations, transmittance calculations, and measurement for two different directions and two different structures establishes the existence of photonic gaps in these systems.

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