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The resonance-induced in-gap modes in photonic crystals composed of metal-coated dielectric spheres

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Abstract. Using the vector wave multiple-scattering method we show that a sizable photonic band gap and resonance-induced in-gap modes can be realized simultaneously in crystals composed of metal-coated dielectric spheres. The position and width of the in-gap modes can be controlled by making appropriate choices of the dielectric constant of the inner dielectric sphere and thickness of the metal-coating layer, respectively. Such properties can be very useful in making optical band filters as well as microcavity lasers if they are sustained in the presence of dissipation. The calculated transmission spectra suggest that the resonance-induced in-gap modes decrease in intensity with dissipation and exist only for good metals.

Photonic crystals are space-modulated dielectric structures having an absolute photonic gap in the energy spectrum; much experimental and theoretical work has been concentrated on this subject recently, in the search for the various lattice types and material components which favour the formation of a photonic band gap [1–6]. The existence of a photonic gap makes it impossible for an electromagnetic wave to propagate in certain frequency ranges; it also prohibits the spontaneous emission of light for atoms embedded inside crystals [7]. This feature not only can be used to study the basic physics, such as the light localization property [8] and Lamb shift [9], but also lays the foundation for its industrial application in opto-electronic devices such as perfect mirrors, optical band filters, optical polarizers, and microcavity lasers [10, 11].

To make a microcavity laser, one usually creates defect modes within the photonic gap, with the defect modes having the same frequency as the yield media; the output power depends on the number of cavities, the Q-factor of the cavity, and the coherence among the defect modes. On the one hand, coupling between the defect modes is very important for producing a coherent output; on the other hand, the coupling should be very small, otherwise strong coupling among the defect modes may cause split modes; thus one needs to have a systematic way of controlling the coupling strength so that optimum output power of the laser can be achieved. Such a technique is also crucial for designing an optical band filter with a specified centre frequency and bandwidth.

In this paper we propose theoretically to use the photonic crystals composed of metal-coated dielectric spheres to manufacture such a microcavity laser and variable-bandwidth filter. The advantage of using such a structure is that both a large photonic gap and resonance-induced in-gap modes appear simultaneously; the size of the photonic gap can be controlled by the total filling ratio of the metal-coated dielectric spheres [12] and the position of the resonance-induced in-gap modes can be adjusted by means of the choice of material for the inner dielectric

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spheres [13], while the coupling strength among the resonance modes is controlled by the metal-coating layer thickness. Therefore, there is a greater degree of freedom as regards preparing samples with desired properties. We would like to emphasize that although previous studies [14, 15] have shown the presence of a large photonic band gap in photonic crystals composed of metal spheres, the cavity modes in the gap are usually created by introducing a defect into the photonic crystals; resonance-induced in-gap modes in photonic crystals composed of metal-coated dielectric spheres, to our knowledge, have not been addressed so far.

To understand the physical origin of the resonance-induced in-gap modes, let us start with a single dielectric sphere coated with a perfect-metal layer; since the electric field vanishes at the perfect-metal surface, the available resonance modes inside the dielectric core must satisfy the boundary condition at the interface between the inner dielectric sphere and outer metal-coating layer:

$$j_l(\kappa r) + \kappa r j_l'(\kappa r) = 0.$$

Here $j_l(\kappa r)$ is the usual spherical Bessel function and $\kappa = \sqrt{\epsilon}\omega/c$. ϵ and r stand for the dielectric constant and the radius of the inner dielectric sphere, respectively. The frequencies of the first three resonance modes are $\omega_1 = 2.7437c/\sqrt{\epsilon}r$, $\omega_2 = 3.8725c/\sqrt{\epsilon}r$, and $\omega_3 = 4.9775c/\sqrt{\epsilon}r$ with the index denoting the angular momentum of the spherical wave. The resonance mode frequency, therefore, is inversely proportional to the refractive index and the radius r of the inner dielectric spheres. Since the photonic gap for crystals composed of metal-coated dielectric spheres mainly depends on the filling ratio of the metal-coated spheres [12], the resonance mode frequency can be adjusted to fall into the photonic gap by choosing an appropriate dielectric constant for the inner dielectric spheres. This estimate is obtained for a perfect-metal coating; the resonance mode frequency can have a small deviation when a realistic metal is used or when the coating layer thickness is thin enough. In that case, one has to deal with the scattering T-matrix of the composite sphere to find the resonance modes [13].

To treat the photonic crystals with metallic components, the most efficient numerical method is based on the vector wave multiple-scattering theory. The multiple-scattering method was originally developed for electronic band structures [16–18] where electrons are described by the scale wave function. The extension of the multiple-scattering method to the case of an electromagnetic wave was carried out independently by Ohtaka *et al* [19–23], Lamb *et al* [24], and Modinos [25]. More recently, vector wave multiple-scattering methods have also been derived and implemented by many other groups [26–30] from different points of view. We have also written a general computer code to implement the vector wave multiple-scattering method for the photonic band structure in three-dimensional photonic crystals, and the code is very efficient and much faster than the finite-difference time-domain method [12]. Using our recently developed vector wave multiple-scattering code, we have calculated the photonic band structures of face-centred cubic (FCC) and diamond-type crystals composed of metal-coated dielectric spheres. To describe the metal-coating layer, we model the metal using a plasmon-like dielectric function: $\epsilon(\omega) = 1 - \omega_p^2/\omega^2$ with ω_p denoting the plasmon frequency. As an example, we consider a sample with an aluminium-coating layer; the plasmon frequency is $\omega_p = 15.3$ eV. We take the lattice constant $a = 1.2$ μm [31]; the reduced plasmon frequency is $\omega_p a/2\pi c = 14.8$. In the following numerical computation, $l_{max} = 7$ is taken in the local expansion of the electromagnetic wave and the eigenfrequency is determined to the accuracy of the third digit.

For photonic crystals composed of metal-coated dielectric spheres, the photonic band structures depend on the metal-coating layer thickness. For a very thick metal-coating layer (e.g., 15% of the total sphere radius), the photonic bands look exactly the same as those for a

sample made of solid metal spheres; this is physically understandable since the inner resonance modes cannot leak out. As the metal-coating layer becomes thinner, the inner resonance modes can be coupled out. In fact, one finds a distinct flat band corresponding to the inner resonance frequency when the metal-coating layer is about 5% of the total sphere radius. If the metal-coating layer is even thinner, then there exists a strong coupling among these inner resonance modes if the resonance modes are within the gap or strong mixing between the inner resonance modes and bands of a connected network of voids if the inner resonance modes fall into the latter bands. Since the previous study of photonic band structures demonstrates that all of the crystal types composed of solid metal spheres favour the formation of absolute photonic gaps [12], we only have to choose the appropriate materials for the inner dielectric spheres and metal-coating layer thickness to ensure that the resonance modes fall into the photonic gap.

In figure 1 we show the photonic band structures of FCC crystals made of metal-coated dielectric spheres in air; the filling ratio of the total spheres is $f = 0.7$, which is slightly smaller than the close-packing value 0.74. The use of a smaller filling ratio is relevant in real-life applications, since separation of metal spheres can prevent the formation of long-range currents and hence minimize dissipation. The dielectric constant of the inner dielectric spheres is $\epsilon = 1.4$. Figure 1(a) displays the photonic band structures at a metal coating of 15% of the total sphere radius. There is a large indirect photonic gap between the Γ point in the valence band (the fifth band) and the X point in the conduction band (the sixth band) [12]. The gap/mid-gap frequency is 0.16, which is quite large and leaves a large margin for the gap-edge distortion due to crystal imperfection. The absence of resonance-induced in-gap modes suggests that a thick metal-coating layer effectively prevents the resonance modes from leaking out of the metal layer because the penetration depth of the field is much smaller than the metal-coating layer thickness. However, the internal resonance mode does appear upon reducing the metal-coating layer thickness to 5%; the result is illustrated in figure 1(b). The most significant change of the band structures from figure 1(a) is the appearance of three distinct modes at frequencies $\omega a/2\pi c = 1.07$, 1.49, and 1.89; these are exactly the resonance modes with angular momenta $l = 1$, 2, and 3, respectively. The degeneracy of these modes depends on l and is given by $2l + 1$; however, this degeneracy is destroyed in the presence of a crystal field [32]. The dielectric constant of the inner dielectric spheres is chosen such that the resonance mode for $l = 1$ is located more or less at the centre of the photonic gap. Due to the weak coupling among the resonance modes, the in-gap band is almost dispersionless, but its bandwidth can be enhanced when the metal-coating layer thickness is further reduced. The result for the metal-coating layer thickness 2% of the total sphere radius is displayed in figure 1(c). Note that the surface plasmons of metal-coated spheres [33] are well above the photonic band structures presented in figure 1; since the plasmon frequency is very high, they almost decouple from the resonance modes discussed here.

Although defects and metal-coated dielectric spheres both lead to in-gap states, the phase relationships among the localized modes can be quite different. Unlike the case for in-gap modes of multiple defects with random distribution in space and thus no phase coherence, the 'cavities' (spheres) in our case are fixed in their spatial periodic positions; thus the relative phases among all the 'cavities' are fixed. This makes the resonance modes of all spheres coherent and in phase; thus the output power can be greatly enhanced in a certain direction. The merit of variable bandwidth and adjustable centre frequency for the in-gap states also makes for an ideal choice for designing an optical band filter with a desired specification.

To see whether such ideas can be realized experimentally, one needs to study the transmission spectra of photonic crystals of finite layers—in particular, to investigate the absorption effect of metal spheres. The complex dielectric constant of metal becomes

$$\epsilon(\omega) = 1 - \omega_p^2/\omega(\omega + \mathrm{i}\gamma)$$

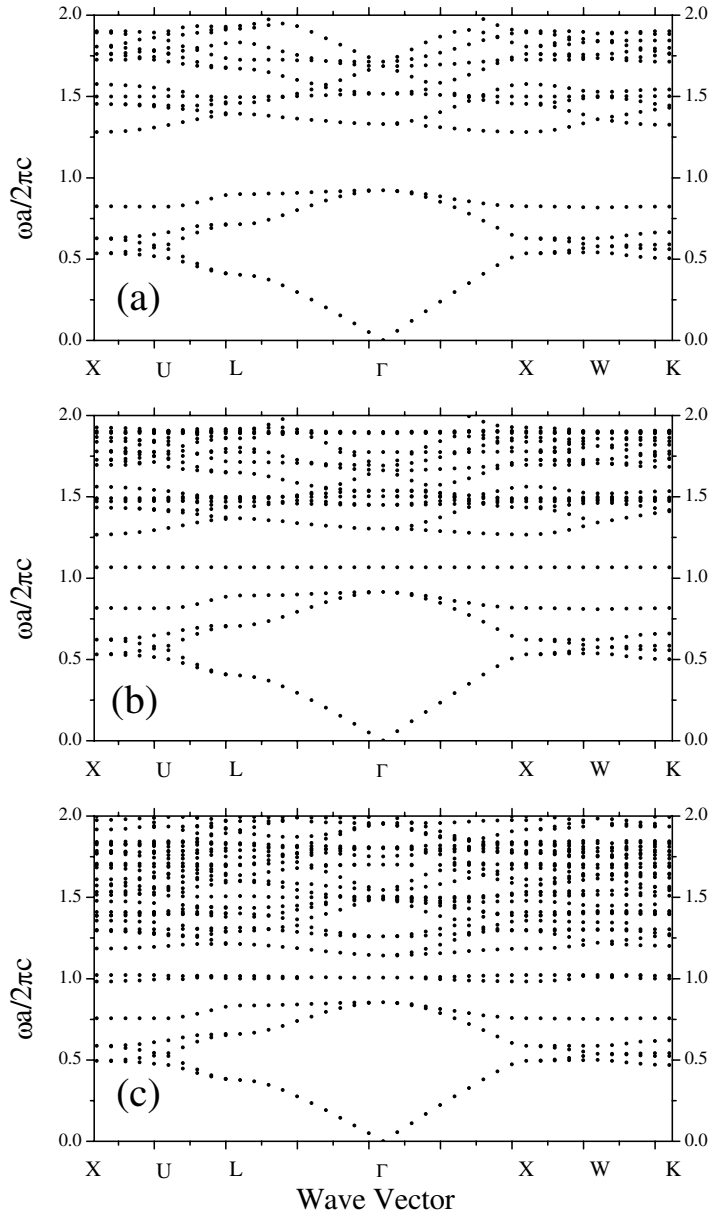

Figure 1. The photonic band structures of FCC crystals composed of metal-coated dielectric spheres in air; $\epsilon = 1.4$ for the inner dielectric spheres; $\omega_p a/2\pi c = 14.8$ for the metal-coating layer; the filling ratio of whole spheres is $f = 0.7$. The metal-coating layer thickness is: (a) 15% of the total sphere radius; (b) 5% of the total sphere radius; (c) 2% of the total sphere radius.

and γ is the absorption coefficient. The transmission spectra along the (111) planes are shown in figure 2; the parameters take the same values as those used in figure 1(b) but with different absorption coefficients. The incident beam is normal to the plane; the sample consists of 32 layers. The transmission spectrum for $\gamma = 0$ is illustrated in figure 2(a); the position and size of the gap are in perfect agreement with those for the band structures of figure 1(b). The

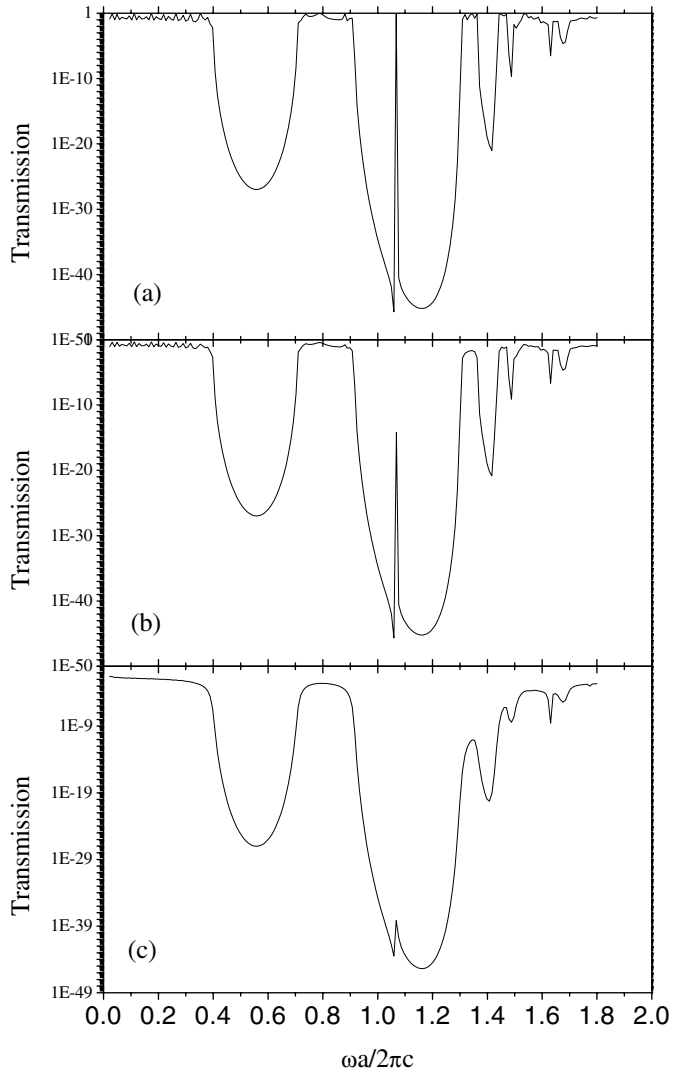

Figure 2. The transmission spectra along the (111) plane of FCC crystals having 32 layers; the parameters are the same as for figure 1(b) but with different absorption coefficients. (a) $\gamma a/2\pi c = 0.0$; (b) $\gamma a/2\pi c = 0.01$; (c) $\gamma a/2\pi c = 0.1$.

spectrum shows a large directional gap around reduced frequency 0.55 and a large full gap around 1.1; the resonance-induced in-gap modes found in the band structures are also clearly seen. However, the absorption of metal has a strong impact on the transmission spectra: while the resonance-induced in-gap states are sustained for the weak absorption, as shown in figure 2(b) for $\gamma a/2\pi c = 0.01$, they disappear almost completely at $\gamma a/2\pi c = 0.1$ (see figure 2(c)), although the overall gap structure remains. Thus, the resonance-induced in-gap states can exist only in good metals like silver and only in certain frequency windows where the absorption is small [15].

The resonance-induced in-gap states are almost dispersionless and a dispersionless state usually indicates a localized state. So we compute the field intensity for all three degenerate

in-gap states: the field intensities are found to be very similar and strongly localized near the metallic shell; they only have tangential components with respect to the spheres. The typical field intensity for the in-gap states is shown in figure 3; the electric field concentrates in the narrow region outside of the metal shell and vanishes completely inside the metal shell. Thus, the in-gap states being dispersionless does imply a localized nature of these states.

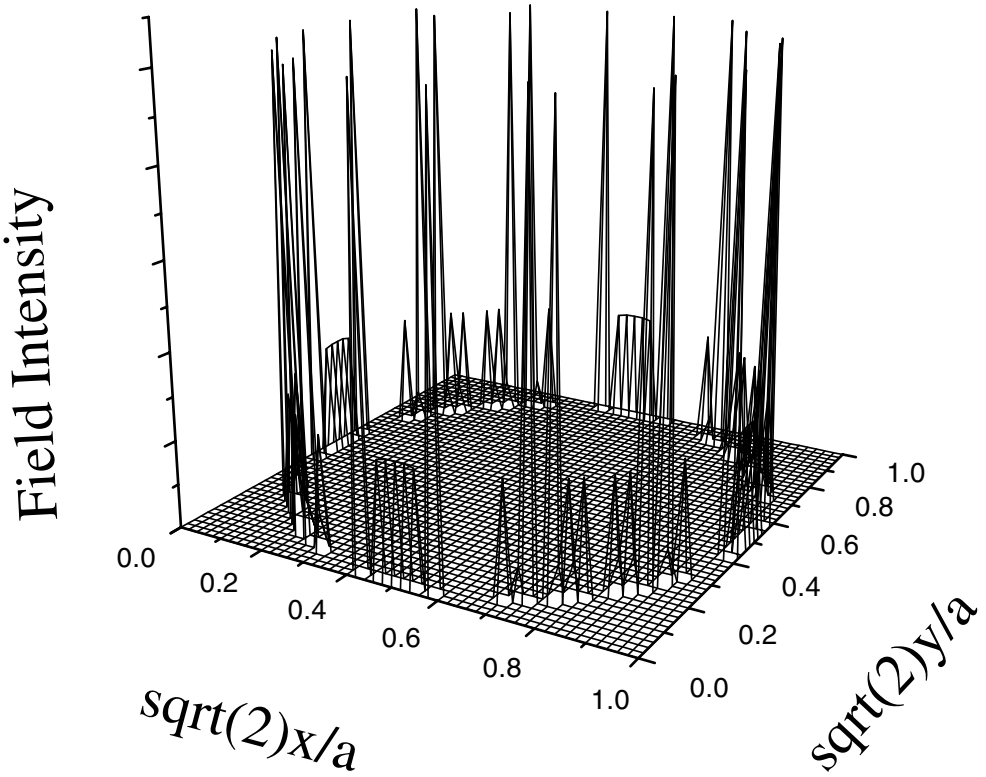

Figure 3. The field intensity of resonance-induced in-gap states in the (001) plane of FCC crystals; the x- and y-axes point to the nearest-neighbour spheres in the plane. The parameters are the same as for figure 1(b).

The novel feature of photonic crystals with both the large photonic gap and resonance-induced in-gap states is not unique to the simple FCC crystal; they occur quite generally for other crystals as well. In figure 4 we present the photonic band structures for diamond-type crystals; the filling ratio is set as $f = 0.3$—which is smaller than the maximum packing of $f = 0.34$—to prevent the contact of spheres; the dielectric constant of the inner dielectric sphere is $\epsilon = 8$. Figure 4(a) shows a large photonic band gap, as predicted by Fan *et al* [14], at the metal-coating layer thickness 15% of the total sphere radius; a huge photonic gap appears between the valence band (second band) and the conduction band (third band): it is a direct gap at the X point of the Brillouin zone. The gap/mid-gap frequency is 0.245, which is even larger than the value for FCC crystals. Although the technical data are even better, sampling the diamond-type photonic crystal is more difficult experimentally. We would like to mention here that the bands of diamond crystal composed of perfect-metal spheres were calculated before, using the finite-difference time-domain method, by Fan *et al* [14] and our result is in excellent agreement with theirs in that case. After reducing the metal-coating layer to 5%,

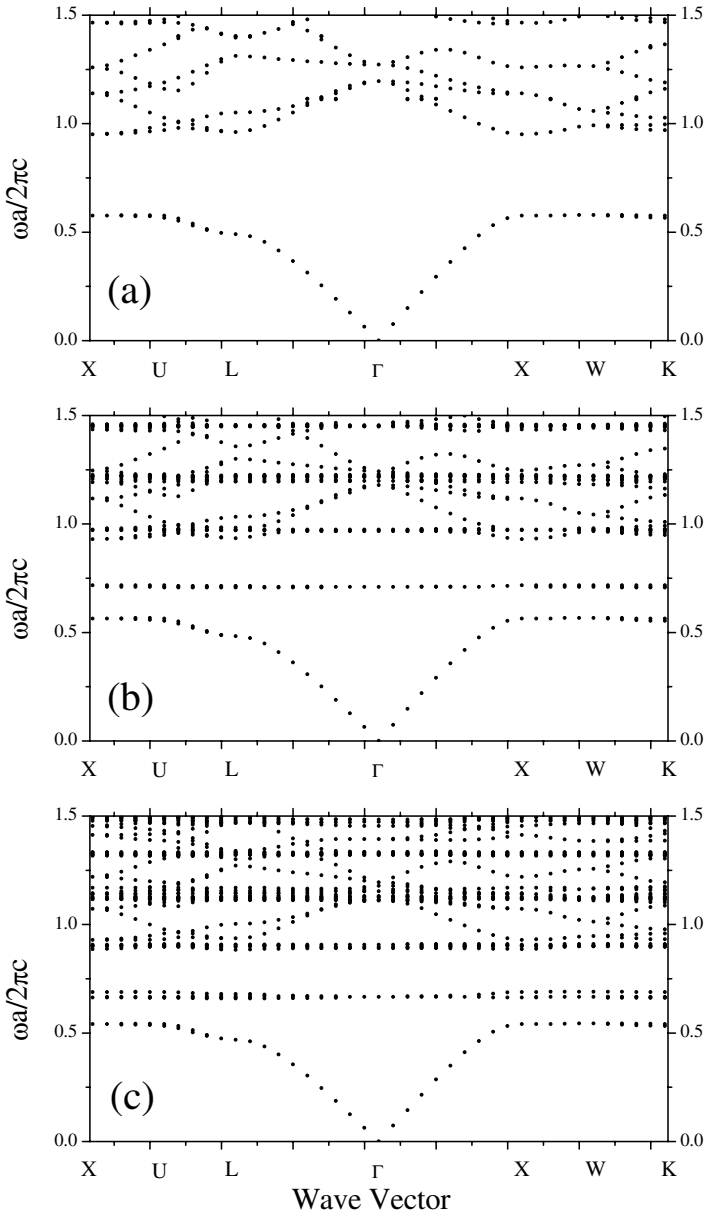

Figure 4. The photonic band structures of diamond crystals composed of metal-coated dielectric spheres in air; $\epsilon = 8$ for the inner dielectric spheres; $\omega_p a/2\pi c = 14.8$ for the metal-coating layer; the filling ratio of whole spheres is $f = 0.3$. The metal-coating layer thickness is (a) 15% of the total sphere radius; (b) 5% of the total sphere radius; (c) 3% of the total sphere radius.

the resonance modes are also coupled out as can be seen in figure 4(b). The frequencies of the in-gap states are $\omega a/2\pi c = 0.71$, 0.97, and 1.2 for angular momenta $l = 1$, 2, and 3, respectively. The dielectric constant of the inner dielectric spheres is also chosen such that the resonance mode for $l = 1$ is located roughly at the centre of the photonic gap. The bandwidth of the in-gap states becomes larger when the metal-coating layer thickness reduces to 3% of

the total sphere radius; the result is shown in figure 4(c).

The corresponding transmission spectra are presented in figure 5 for different absorption values γ; the effect of the metal absorption on the resonance-induced in-gap states is the same as those discussed in relation to the FCC crystal: it drastically reduces the transmission intensity of the resonance-induced in-gap states. Thus, choosing the right metal-coating layer becomes vitally important. As was emphasized by Moroz [15], this can be done by making the appropriate choice of the metal element to ensure that the least absorptive frequency window coincides with the photonic gap region, and thus the photonic structures are not significantly altered [34]. The field intensity of resonance-induced in-gap states in the diamond-type crystal is also very localized and has a similar pattern to that in FCC crystal. Note that while the above

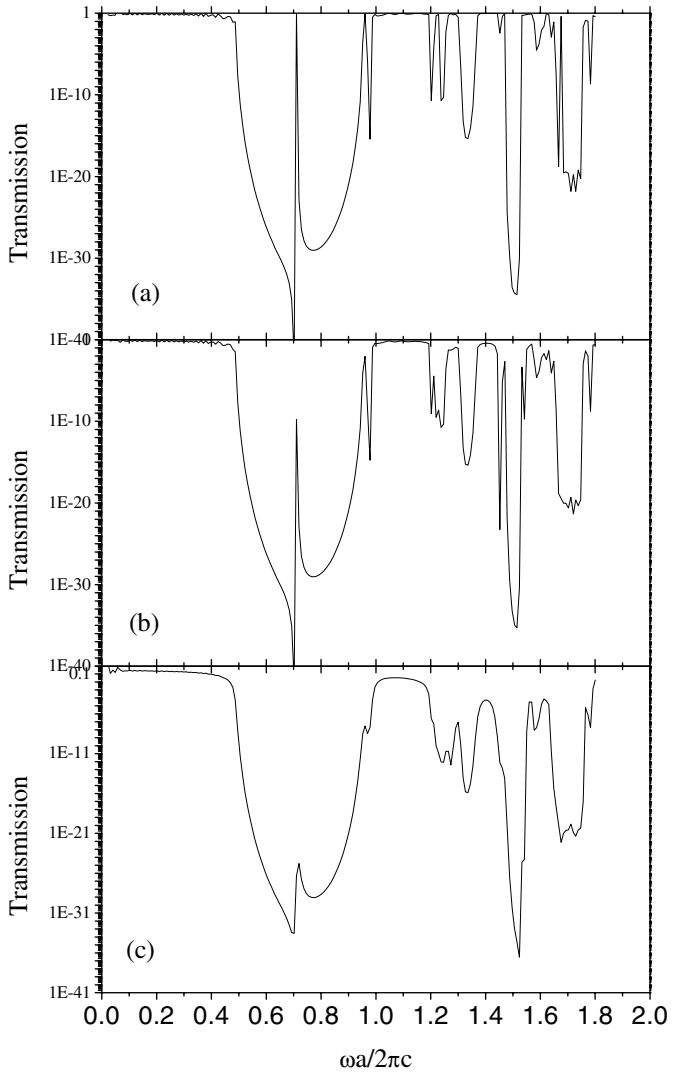

Figure 5. The transmission spectra along the (111) plane for diamond crystals with 32 double layers; the parameters are the same as for figure 4(b) but with different absorption coefficients. (a) $\gamma a/2\pi c = 0.0$; (b) $\gamma a/2\pi c = 0.01$; (c) $\gamma a/2\pi c = 0.1$.

calculation bas been done for metal-coated dielectric spheres in air, cases with other background dielectric media can be studied in the same way.

As the localized mode in the photonic band gap has a variety of applications in the design of optical devices, it is of great interest to verify experimentally these resonance-induced in-gap modes. While photonic crystal with diamond structure is very difficult to make in the laboratory, crystals with FCC structures can be assembled in electrorheological fluids of metal-coated spheres under suitable magnetic and electric fields [35]. In order to minimize the metal absorption, highly conductive metals such as silver and gold are highly recommended. The resonance-induced in-gap modes can be observed through transmission measurements.

In summary, the photonic band structures of metal-coated dielectric spheres can contain both a large photonic band gap and resonance-induced in-gap states if appropriate material parameters are chosen. The position of the resonance-induced in-gap states depends on the dielectric constant of the inner dielectric spheres while the bandwidth of the in-gap states depends on the metal-coating layer thickness. These features can be used to design band filters with different specifications. For a very narrow in-gap band, it may also be used to design a microcavity laser with a phase-coherent directional output.

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