## Photonic Crystals at Near-Infrared and Optical Wavelengths

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### ABSTRACT

As demonstrated for the example of a diamond and zinc blende structure of dielectric spheres, small inclusions of a low absorbing metal with the volume fraction $f_m$ can have a dramatic effect on a complete photonic band gap (CPBG) between the 2nd-3rd bands. For example, in the case of silica coated silver spheres, the CPBG opens for $f_m \approx 1.1\%$ and exceeds $5\%$ for $f_m \approx 2.5\%$. Consequently, any dielectric material can be used to fabricate a photonic crystal with a sizeable and robust CPBG in three dimensions. Absorption in the CPBG of $5\%$ remains very small ($\leq 2.6\%$ for $\lambda \geq 750$ nm). The structure enjoys almost perfect scaling, enabling one to scale the CPBG from microwaves down to ultraviolet wavelengths.

### INTRODUCTION

Photonic crystals are structures with a periodically modulated dielectric constant [1]. In analogy to the case of an electron moving in a periodic potential, certain photon frequencies in a photonic crystal can become forbidden, independent of photon polarization and the direction of propagation - a complete photonic bandgap (CPBG) [1, 2, 3]. In the last decade, photonic crystals enjoyed a lot of interest in connection with their possibilities to guide light and to become a platform for the fabrication of photonic integrated circuits [4, 5]. Despite the research activities of a large number of experimental groups, achievement of a CPBG below infrared wavelengths for both two- and three-dimensional photonic structures is still elusive, mainly because the required dielectric contrast $\delta$ to open a CPBG is rather high. Even for the best geometries $\delta \approx 5$ is required [2, 6]. Already this threshold value of $\delta$ excludes the majority of semiconductors and other compounds and materials, such as (conducting) polymers, from many useful photonic crystal applications. However, the required $\delta$ is even higher. For applications one needs a sufficiently large CPBG to leave a margin for gap-edge distortions due to omnipresent defects. Let us define the relative gap width $g_w$ as the gap width-to-midgap frequency ratio, $\triangle\omega/\omega_c$. Then in order to achieve $g_w$ larger than $5\%$, $\delta \geq 9.8$ and $\delta \geq 12$ is required for a diamond [6] and face-centered-cubic (fcc) structure [7], respectively. This leaves only a couple of materials for photonic crystals applications at near infrared and optical wavelengths [8]. Surprisingly enough, there is a way to create a sizeable and robust CPBG with just any dielectric material, be it silica glass or a polymer. A price to pay is to accept a small volume fraction $f_m$ of a low absorbing metal, the actual amount of which depends on an available material dielectric constant $\varepsilon$. Obviously, small
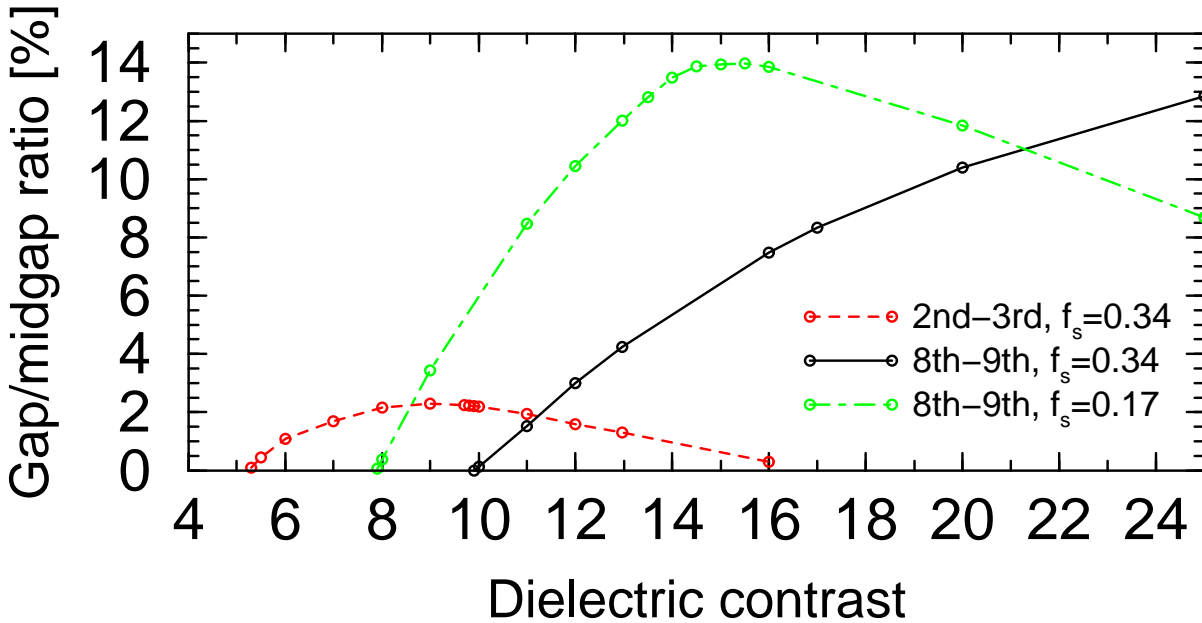
Figure 1: Gap width to midgap frequency ratio for a diamond lattice of dielectric spheres as a function of the dielectric contrast.

metal inclusions do not open a CPBG in every dielectric structure. For example, a simple face-centered-cubic (fcc) lattice of spheres with a metal core requires $f_m \approx 50\%$ to open a CPBG [9, 10, 11, 12]. For a fcc lattice of metal-coated dielectric spheres the required metal filling fraction $f_m$ is slightly lower but still very high ($\approx 40\%$ [12]). Therefore, not surprisingly, when going further to shorter and shorter wavelengths, one is facing an increasing absorption: at $\lambda \approx 600$ nm the absorption exceeds $10\%$ even within a CPBG [12]. Although such a metallo-dielectric fcc structure could provide a CPBG [9, 10, 11, 12] at near infrared, the extension to visible is difficult. We show that a zinc-blende and diamond structures of metallo-dielectric spheres [2, 13] can display much better properties. Photonic band structures are calculated using the photonic Korringa-Kohn-Rostocker (KKR) method [7, 14]. The KKR method can be used for scatterers of arbitrary shape [15] but is optimized for lattices of spheres. In our case convergence of bands was achieved well below $1\%$.

**PURELY DIELECTRIC ZINC BLENDE PHOTONIC STRUCTURES**

It turned out to be necessary to recalculate the earlier results of Ho, Chan, and Soukoulis [2] on the photonic band structure of a diamond lattice of nonoverlapping spheres with di-
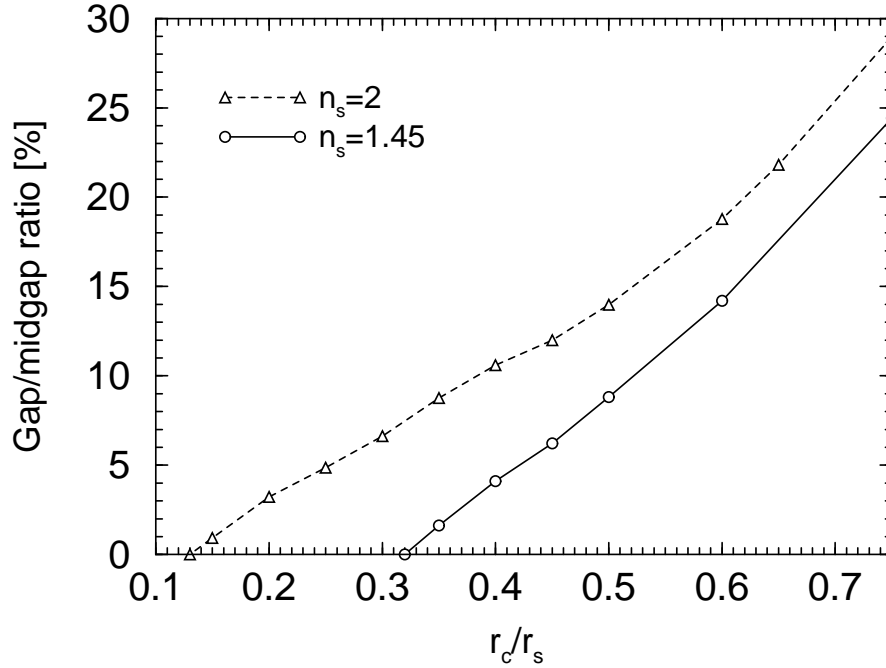
**Figure 2:** Gap to midgap frequency ratio $g_w$ of the 2nd-3rd CPBG for a close-packed diamond lattice of dielectric $n_s = 1.45$ (silica) and $n_s = 2$ (ZnS) coated silver spheres of radius $r_s = 80$ nm in air. $g_w$ is plotted as a function of the metal core radial filling fraction $r_c/r_s$. Metal volume fraction is then $f_m = 0.34 \times (r_c/r_s)^3$.

electric constant $\varepsilon_s$ in air, which were not converged (see [6] for more details). According to Figure 1, for a sphere filling fraction $f_s$ varying from 0 till the close-packed case $f_{cp} = 0.34$, two CPBGs can occur simultaneously, between the 2nd-3rd bands, and, as in an inverted fcc case, between the 8th-9th bands [6]. Contrary to previous calculations [2], the lower CPBG is not the dominant one (for its optimal $f_s = f_{cp}$ it does not exceed $2.3\%$ (for $\varepsilon_s = 9$), only persists for $\varepsilon_s \in [5.2, 16.3]$, and closes already for $f_s = 32\%$) [6]. The dominant CPBG is the upper one. For $\varepsilon_s = 12.96$, the upper CPBG persists down to $f_s = 4\%$. For $f_s = 17\%$ and $\varepsilon_s = 12.96$ it can reach $12\%$, however, the threshold value of $\varepsilon_s$ for its opening is 7.9, comparable to that for an inverted fcc lattice [7]. Unlike the case of a simple lattice (one scatterer per lattice primitive cell) [7], for the case of a diamond lattice of dielectric spheres, even when using the plane-wave method based MIT ab-initio program [16], one has to take a much higher number of plane waves than expected to reach a convergence comparable with the photonic KKR method. To reach convergence of the photonic band structure of a diamond lattice of dielectric spheres within $1\%$ the number of plane waves $N_c$ has to exceed 32768 (cf. Ref. [2]) and still an extrapolation $N \to \infty$ [17] has to be performed [18]. Relatively smaller differences were found [6] when compared to the results of Simeonov, Bass, and McGurn for zinc blende structures [13].
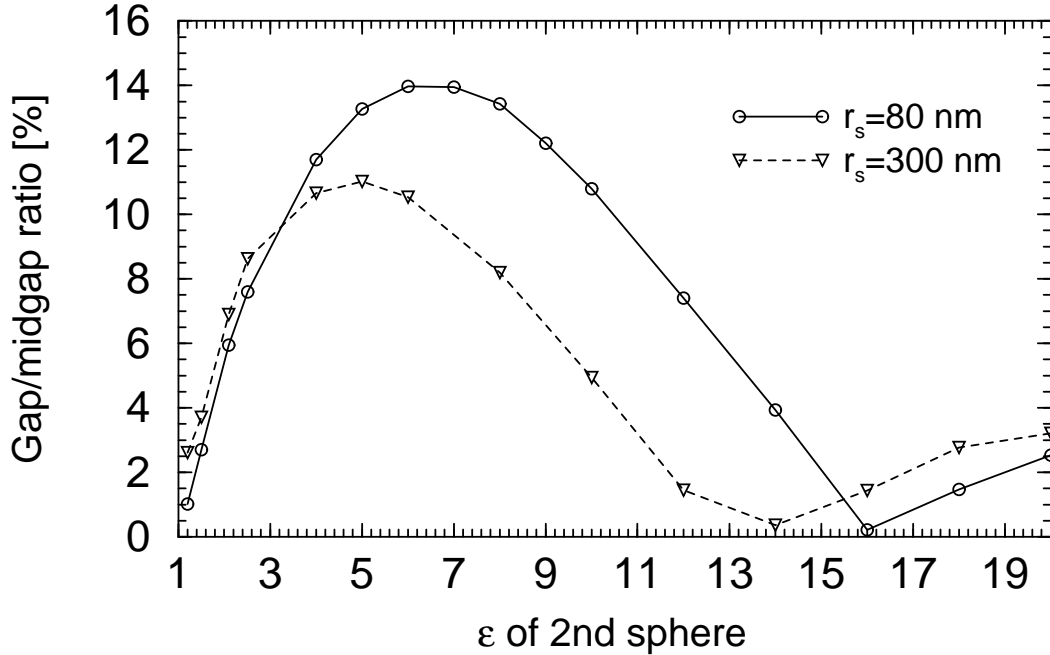
Figure 3: Gap to midgap frequency ratio $g_w$ of the 2nd-3rd CPBG for a close-packed metallo-dielectric zinc blende lattice of spheres in air with identical radii $r_s$. There are a silver core - silica ($n_s = 1.45$) shell sphere with $r_c/r_s = 0.75$ and a homogeneous dielectric sphere in the unit cell. $g_w$ is plotted as a function of the dielectric constant $\varepsilon_s$ of the 2nd sphere for the cases $r_s = 80$ nm and $r_s = 300$ nm.

## ZINC BLENDE PHOTONIC STRUCTURES WITH METALLIC INCLUSIONS

On purely experimental grounds, only the case of metal cores is investigated here. Indeed, a metal shell around dielectric core is formed by an aggregation of small metallic nanoparticles. The shell has to be around 20 nm thick before it becomes complete [19]. With emphasis on photonic structures in the visible and near infrared, the 20 nm shell thickness then would mean rather high threshold value of the metal filling fraction $f_m$ (of the order of 5%). On the other hand, it is much easier to tune the metal filling fraction $f_m$ from zero to a few percent by coating small metal nanoparticles with a dielectric in a controlled way [20]. We have considered the close-packed diamond lattice (both spheres in the primitive cell are identical metal core-dielectric shell spheres) and its various close-packed zinc-blende deformations (one sphere in the primitive cell is a metal core-dielectric shell sphere and the second sphere is purely dielectric, both spheres having the same radius).

Photonic band structure calculations revealed two remarkable features of the metallo-dielectric structure. First, a strong increase of the CPBG between the 2nd and 3rd bands with $f_m$ (see Figure 2). For example, for a close-packed diamond lattice of silver spheres
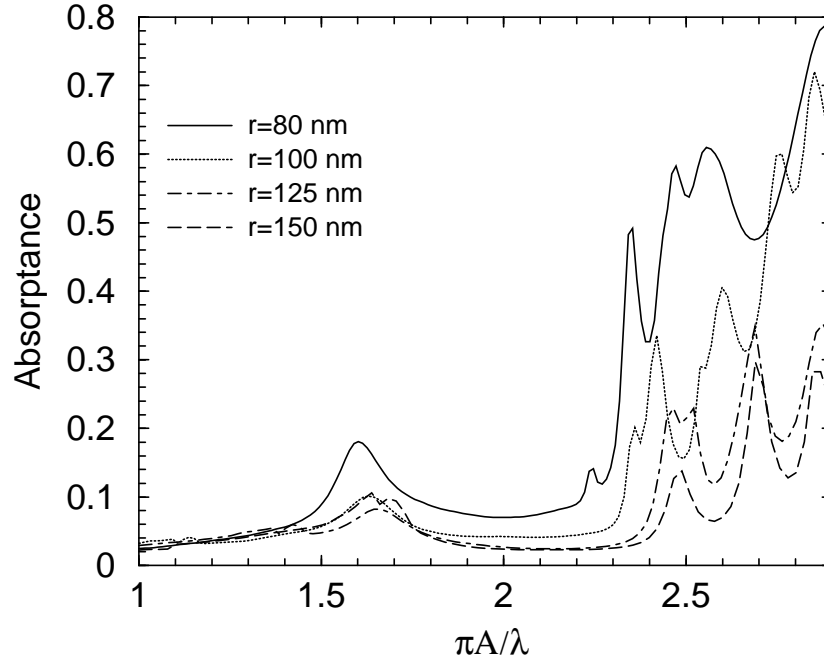
Figure 4: Absorptance of light incident normally on a two unit cells (12 planes) thick zinc blende lattice of spheres in air stacked in the (111) direction. One of the two spheres in the primitive cell is silica coated silver sphere ($n_s = 1.45$) with $r_c/r_s = 0.75$, whereas the other is a ZnS core-silica shell sphere with $r_c/r_s = 0.60$ of the same radius. Dimensionless frequency is used on the $x$-axis, where $A$ is the unit cell size, to emphasize the scaling-like behavior - in all cases, the 2nd-3rd CPBG lies between $\approx 1.7$ and 2.2.

coated with a dielectric with refractive index $n_s = 1.45$ (silica) and radius 80 nm, the CPBG between the 2nd and 3rd bands below 600 nm opens for $f_m \approx 1.1\%$ and reaches 5% already for $f_m \approx 2.5\%$ (see Figure 2). When the sphere refractive index $n_s$ increases, one comes closer and closer to the threshold refractive index contrast of $\approx 2.3$, for which the CPBG of the parent diamond structure of non-overlapping dielectric spheres begins to open [6]. Not surprisingly (Figure 2), the respective metal $f_m$s to open the 2nd-3rd CPBG and to have a CPBG of 5% rapidly decrease with increasing sphere refractive index $n_s$. However, quite counter-intuitively, the 2nd-3rd CPBG begins to narrow after the dielectric constant increases beyond a certain threshold (see Figures 1, 3).

For the diamond lattice of pure metallic spheres, only the CPBG between the 2nd-3rd bands opens and it can be huge. For silver spheres, depending on the sphere radius $r_s$, it can stretch from 60% ($r_s = 80$ nm) till 75% ($r_s \geq 300$ nm) [6, 11]. This is consistent with a previous estimate of $g_w \geq 60\%$ for the case of an ideal metal ($\varepsilon_s = -\infty$) [21]. A combination of the two limiting cases, i.e., purely dielectric (Figure 1) and purely metallic spheres, yields an indication of why only the lower CPBG (between the 2nd-3rd bands)
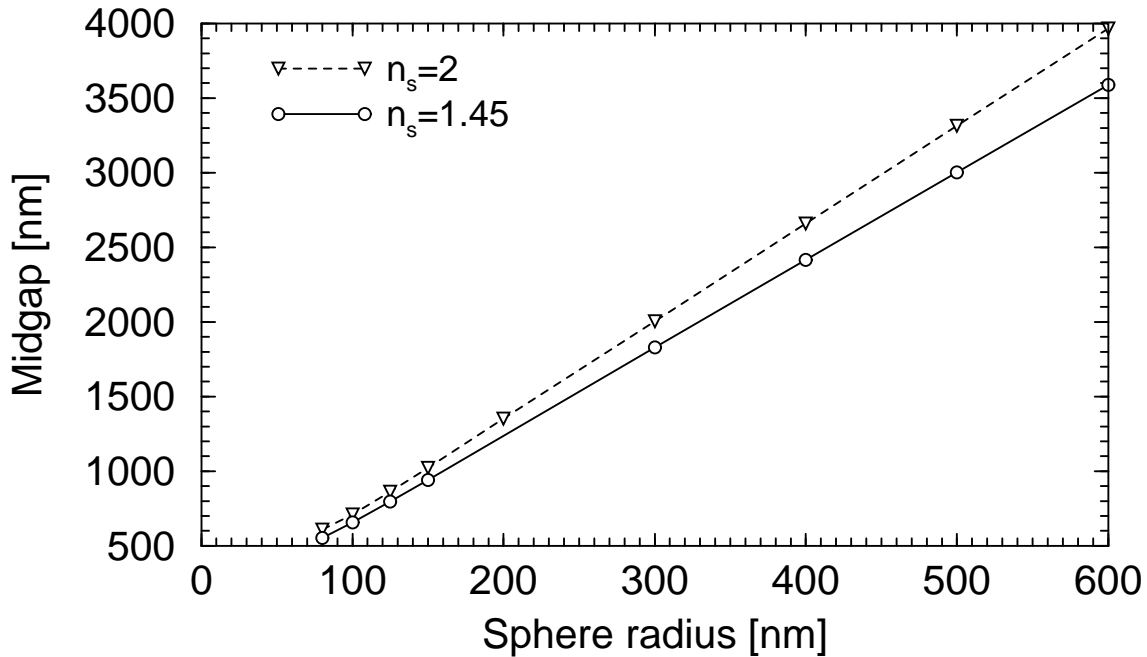
Figure 5: An example of scaling of the 2nd-3rd CPBG midgap wavelength for a close-packed diamond lattice of coated silver spheres in air with the sphere radius. Spheres are either $n_s = 1.45$ (silica) coated silver spheres with fixed $r_c/r_s = 0.6$, or, $n_s = 2$ (ZnS) coated silver spheres with fixed $r_c/r_s = 0.4$.

opens in the intermediate case of metallic inclusions for $n_s \leq 2.3$ and why the CPBG begins to contract after the dielectric constant increases beyond a certain threshold (Figure 3). The same reasoning also indicates why an order of magnitude higher metal volume fraction is required to open a CPBG in the case of a simple fcc structure [9, 10, 11]: in the purely dielectric case, an fcc lattice of spheres in air does not have any CPBG, irrespective of the sphere dielectric constant [7, 17]. Most crucially (see Figure 4), absorption within a CPBG of $5\%$ can be kept below $2.6\%$ for $\lambda \geq 750$ nm. (Absorption was calculated using the layer KKR method [22].) This should be tolerable in most practical applications.

A second remarkable feature of the metallo-dielectric structure is a surprising scaling-like behavior (see Figure 5), which is intrinsic only to ideal dispersionless structures. This scaling-like property is very useful from a practical point of view. It means that once a CPBG is found, with some midgap wavelength $\lambda_c$, the CPBG can be centered at any other wavelength by a simple scaling of all the sizes of a structure. Since metals are highly dispersive, the almost precise scaling behavior of the photonic structures is far from obvious, especially for a CPBG below 2 $\mu$m. It is true that a typical metal filling fraction $f_m$ which is considered here is $\leq 5\%$, i.e., rather small. Yet, as a counterargument, even with such a small metallic content, the effect on photonic band gaps turns out to be very strong (see Figure 2). For

sphere radii $r_s > 300$ nm the CPBG lies above 2 $\mu$m where the limit of perfect metal is approached. Here, the scaling becomes more and more precise, since it makes rather little difference if metal $\varepsilon = -200$ or $\varepsilon = -\infty$.

## CONCLUSIONS

For the example of a zinc blende structure of dielectric spheres it has been demonstrated that small inclusions of a low absorbing metal with volume fraction $f_m$ can have a dramatic effect on a CPBG between the 2nd-3rd bands. Surprisingly, the inclusions have the biggest effect for $\varepsilon \in [2, 12]$, which is a typical dielectric constant at near-infrared and in the visible for many semiconductors and polymers. For example, in the case of silica spheres, the 2nd-3rd CPBG opens for $f_m \approx 1.1\%$ of silver and exceeds $5\%$ for $f_m \approx 2.5\%$. Absorption in the 2nd-3rd CPBG of $5\%$ remains very small ($\leq 2.6\%$ for $\lambda \geq 750$ nm). The structure enjoys scaling-like behavior, enabling one to scale the 2nd-3rd CPBG from microwaves down to ultraviolet wavelengths. Our results imply that just any dielectric material can be used to fabricate a photonic crystal with a sizeable and robust CPBG in three dimensions. These findings (i) open a door for many other semiconductor and polymer materials to be used as genuine photonic crystal building blocks and (ii) significantly increase the possibilities for experimentalists to realize a CPBG in the visible. Moreover, due to a high sensitivity of a CPBG on $f_m$, one has the freedom to engineer $g_w$ from zero to more than $60\%$.

## ACKNOWLEDGMENTS

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