

Towards two-dimensional complete photonic bandgap structures below infrared wavelengths

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Abstract. Bandgaps in two- and three-dimensional photonic crystals are hard to achieve due to the limited contrast in the dielectric permeability available with conventional dielectric materials. The situation changes for periodic arrangements of scatterers consisting of materials with a Drude-like behaviour of the dielectric function. We show for two-dimensional square and triangular lattices that such systems have in-plane complete photonic bandgaps (CPBGs) below infrared wavelengths. Of the two geometries, the optimal one for ideal Drude-like behaviour is a square lattice, whereas for Drude-like behaviour in silver, using experimental data (Palik E D 1991 *Handbook of Optical Constants of Solids* vol 1 (San Diego: Academic)), the optimal geometry is a triangular lattice. If the lattice spacing is tuned to a characteristic plasma wavelength, several CPBGs open in the spectrum and their relative gap width can be as large as 36.9% (9.9% in a nonabsorptive window) even if the host dielectric constant $\epsilon_h = 1$. Such structures can provide CPBG structures with bandgaps down to ultraviolet wavelengths.

Keywords: Photonic bandgap materials, fibre waveguides, wave optics, nonlinear optical materials, integrated optics

1. Introduction

There has been a growing interest in photonic crystals, i.e. structures with a periodically modulated dielectric constant. Such structures open up new ways of manipulating electromagnetic wave emission and propagation processes [1]. In fact, there is a common belief that, in the near future, photonic crystal systems will allow us to control light in much the same way as electrons can be controlled in ordinary crystals [1]. They also promise to become a laboratory for testing fundamental processes involving interactions of radiation with matter under novel conditions. In analogy with an electron moving in a periodic potential, propagation at certain frequencies can become impossible inside a photonic crystal, independent of photon polarization and the direction of propagation—a complete photonic bandgap (CPBG) [2, 3]. The presence of a CPBG severely modifies the quantum electrodynamics as compared with the vacuum case. This offers the possibility of controlling the spontaneous emission of embedded atoms and molecules in volumes much greater than the emission wavelength [5]. For many technological applications it is enough to achieve a photonic bandgap (PBG) for in-plane propagation and, for applications involv-

ing highly polarized light sources, it can be sufficient to obtain a PBG for a single polarization only. (Note that for in-plane propagation, the two photon polarizations do not mix and Maxwell's equations reduce to two scalar equations, one for each polarization.) Numerous applications have been suggested involving two-dimensional (2D) photonic structures, i.e. new designs for light-emitting diodes [6], polarizers [7], high transmission through sharp bends [8], efficient bandpass filters, channel drop filters, and, in one dimension, waveguide crossing without cross-talk [9].

In the following, we shall focus on 2D photonic structures. For such structures, only an in-plane CPBG can ensure light propagation control whatever the in-plane light propagation. Unfortunately, fabrication of photonic crystals with such a gap poses a significant technological challenge for 2D structures already in the near-infrared [10], not to mention three-dimensional (3D) photonic structures [11]. A 2D photonic crystal can be thought of as a 2D periodic arrangement of scatterers with a dielectric constant ϵ_s embedded in a host with a dielectric constant ϵ_h . In view of the scale invariance present in Maxwell's equations it makes sense to introduce the relative gap width g_w as the gap width-to-midgap frequency ratio, $\Delta\omega/\omega_m$. Practical crystals are expected to have g_w larger than a few per cent—to leave a margin for gap–edge distortions due to omnipresent

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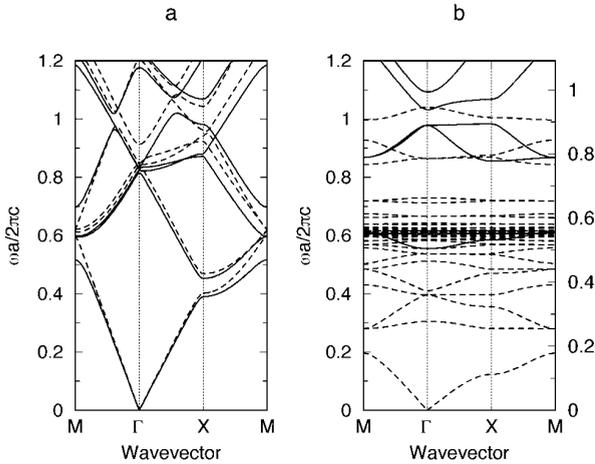


Figure 1. If, in a conventionally etched 2D square lattice of air cylinders in silica, the holes are filled with a material showing a Drude-like behaviour, the band structure changes drastically from (a) showing no CPBG to (b) that showing four CPBGs with $\omega_m \approx 0.25, 0.65, 0.69, 0.79$ and $g_w \approx 35\%, 2.9\%, 5.4\%$ and 11.4% , respectively. In both cases the lattice parameters are the same, with cylinder filling fraction $f = 65\%$ and $\varepsilon_h = 2.16$. In the second case, $a/\lambda_p = 1.1$. In addition, note a bandgap for TM polarization (s-polarization; \mathbf{E} parallel to the cylinder axis) below the first band in part (b), which is characteristic for 2D structures with metallic components [7]. For TE polarization \mathbf{E} is perpendicular to the cylinder axis.

impurities and yet to have a CPBG useful for applications. Then, the dielectric contrast $\delta = \max(\varepsilon_h/\varepsilon_c, \varepsilon_c/\varepsilon_h) \approx 8$ is required to open a CPBG with $g_w = 6\%$ [12]. Unfortunately, this required dielectric contrast is rather large and strongly limits the choice of available materials in the visible.

The main goal of this paper is to demonstrate that practical CPBGs can already open for the simplest lattice and scatterer geometries, as long as the scatterer dielectric function is correctly chosen. Therefore, we shall only discuss square and triangular lattices of infinitely long cylindrical scatterers with circular cross section and with one cylinder per lattice unit cell. Even then, for instance in a 2D square lattice of cylinders for a cylinder filling fraction of 65% in a silica host (see figure 1), several CPBGs open, one of them larger than 11.4% and another larger than 35%, provided that cylinders are made out of material with a Drude-like dielectric function [13, 14]

$$\varepsilon_s(\omega) = 1 - \omega_p^2/\omega^2, \quad (1)$$

where ω_p denotes the plasma frequency. Note that the Drude-like dielectric function is zero for $\omega = \omega_p$ which makes δ infinite and enables one to avoid the restrictions on the dielectric contrast. This approach has been shown to also work for 3D photonic structures [15].

A Drude-like behaviour of $\varepsilon_s(\omega)$ is typical for metals and semiconductors. For notational simplicity we shall often refer to a scatterer having such a dielectric function (1) as a metallic one, although we are aware that: (i) not all metals show a Drude-like behaviour and (ii) such a behaviour can also be found in new artificial structures [16]. Consequently, the proposed structures could be realized by introducing, for instance by electrochemical deposition, a Drude-like material

into the holes of a periodic structure of air holes in a dielectric, a structure that has no CPBG without the Drude-like material inserted (see figure 1).

Metals can be quite lossy at optical frequencies. Nevertheless, the absorption can be rather small in a certain frequency window, where the metal behaves as a highly dispersive dielectric. Typically, the plasma wavelength $\lambda_p = 2\pi c/\omega_p$, where c is the speed of light in vacuum, is closer to the short-wavelength edge of the nonabsorptive window, since for shorter wavelengths there is a higher probability of inducing electronic interband transitions. We restricted our investigation mainly to the ‘nonabsorptive’ window ($0.5\omega_p \leq \omega \leq 1.1\omega_p$ for the ideal Drude behaviour; 310–520 nm for silver [17]) which explains why the main part of the band structure shown in our figures is below the plasma frequency. Fortunately, this is also the region where one finds most of CPBGs. In real systems, such as silver, a deviation from the ideal Drude behaviour occurs, in particular in the proximity of the zero-crossing of $\text{Re } \varepsilon$ at some λ_z ($\lambda_z = 328$ nm for silver). Such a λ_z is red-shifted compared with λ_p ($\lambda_p \approx \lambda_z/1.9$ for silver) [17] and the band structure between λ_z and λ_p can be modified as compared with the ideal Drude behaviour (1). We studied both square and triangular lattices, the Bravais lattices that have Brillouin zones that come closest to a circle, and are hence expected to give rise to the biggest bandgaps. We find that for an ideal Drude-like material a square lattice leads to the biggest gaps of the two lattice types studied. However, the deviation of the dielectric function of silver from the ideal Drude behaviour means that silver triangular lattices result in bigger CPBGs than square lattices. In both cases, i.e. ideal Drude/square and silver/triangular, a CPBG with $g_w \approx 10\%$ is even found for a host dielectric constant ε_h as low as $\varepsilon_h = 1$.

2. Method

We performed band-structure calculations using a 2D analogue of the familiar Korringa–Kohn–Rostocker (KKR) method [18]. Since, for in-plane propagation, the two photon polarizations decouple, the calculation reduces to the use of the ordinary 2D scalar KKR method [19] for either polarization. This polarization decoupling is specific to two dimensions and is obviously not the case for 3D photonic structures where a truly vectorial KKR method is required [20]. Given a plasma frequency ω_p , we performed calculations for frequencies from $\approx 0.5\omega_p$ to $1.1\omega_p$, assuming ε_h is constant in this frequency region. In contrast to the plane-wave method [4, 7], dispersion does not cause any difficulties for the KKR method and the computational time is the same as without dispersion. Also (cf [7]), the calculation is not limited to the case of a small metallic volume fraction of $f \leq 1\%$ and one can safely proceed up to the case of closely packed metallic cylinders. Last but not least, there are no problems in obtaining convergence for the so-called flat bands first encountered in [7]. In order to ensure precision of around 0.1%, cylindrical waves were included with angular momentum up to $l_{\max} = 24$. This means that the size of a typical secular matrix is reduced by a factor of almost ten as compared with the plane-wave method [7].

3. Results for an ideal Drude metal

The qualitative behaviour of the band structure for a 2D periodic arrangement of Drude-like scatterers is similar to that in three dimensions [15]. The plasma wavelength sets a characteristic scale and, correspondingly, bandgaps only occur for certain values of r_c/λ_p , or, a/λ_p , where r_c and a are the cylinder radius and lattice constant, respectively. Of the two geometries studied, a *square* lattice is optimal for a Drude metal. Then, a CPBG with g_w nearly 10% opens even if ε_h is as low as $\varepsilon_h = 1$. Other noteworthy points in the case of $\varepsilon_h = 1$ are:

- (1) No or only tiny CPBGs for $a/\lambda_p \leq 0.9$.
- (2) No CPBGs larger than 5% below $a/\lambda_p \leq 1$.
- (3) For f fixed, a CPBG g_w grows rapidly with a/λ_p until $a/\lambda_p \approx 1.1$ is reached, with the optimal filling fraction being $60\% \leq f \leq 70\%$; for $a/\lambda_p \approx 1.1$ the gap width g_w increases only marginally and, beyond $a/\lambda_p \approx 1.47$, g_w decreases.
- (4) No CPBG with $g_w \geq 5\%$ exists for $a/\lambda_p \geq 2$.
- (5) A CPBG with $g_w \geq 5\%$ can be achieved for $43\% \leq f \leq 77\%$.

For $\varepsilon_h = 1$, the largest g_w is found to be 9.9% for $f = 65\%$ and $a/\lambda_p \approx 1.47$. When silica ($\varepsilon_h = 2.16$) is used as the host, the maximal gap width can be increased further. For example, a structure with $f = 65\%$, $\varepsilon_h = 1$, and $a/\lambda_p = 1.1$ exhibits a CPBG with $g_w = 8.7\%$, whereas for $\varepsilon_h = 2.16$ this CPBG width increases to $g_w = 11.4\%$.

Besides the CPBGs mentioned above, we also found very large CPBGs at lower frequencies, outside the ‘nonabsorptive’ window, typically at midgap frequencies of 20% of the plasma frequency. For instance, in the case of the structure presented in figure 1(b) for $\varepsilon_h = 2.16$, we found a CPBG with $g_w = 35\%$, at $\omega_m/\omega_p = 0.217$ ($g_w = 36.9\%$, at $\omega_m/\omega_p = 0.213$ for $\varepsilon_h = 1$).

For a triangular lattice one encounters more CPBGs. However, the maximal g_w found was 3.5%.

4. Results for silver

For silver we used the experimental data from Palik [21]. The deviation from the ideal Drude behaviour, which occurs in the proximity of the zero-crossing of $\text{Re } \varepsilon$ at $\lambda_z = 328$ nm [17], means that for silver a triangular lattice leads to bigger CPBGs than a square lattice. For a fixed f , the relative gap width g_w increases with increasing a/λ_z (or with a/λ_p) until $a/\lambda_z \approx 2$ ($a/\lambda_p \approx 1.1$) is reached. Afterwards, CPBGs fall into a region of increased absorption. Interestingly, a/λ_m , where λ_m is the midgap wavelength, stays close to unity: $a/\lambda_m \approx 0.9$ for $a = 329$ nm and $a/\lambda_m \approx 1.1$ for $a = 650$ nm.

For a fixed lattice constant $a = 650$ nm we found the largest CPBG, with $g_w = 11.7\%$, for $f = 58\%$, with the entire CPBG still lying in the ‘nonabsorbing’ frequency window (see figure 2). Note that in this case the distance between the silver cylinders is ≈ 115 nm. Manufacturing of such a structure is realistic, since the minimal dielectric width between two cylinders technologically realized in semiconductors such as GaAs is 30 nm [22]. The dependence

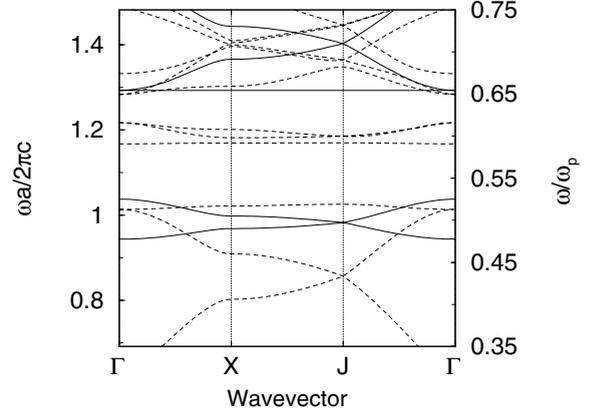


Figure 2. Calculated photonic band structure for a triangular lattice of silver cylinders in silica ($f = 58\%$, $a = 650$ nm, $a/\lambda_z = 1.98$, $\varepsilon_h = 2.16$). TM and TE bands are drawn with full and dashed curves, respectively. Note three CPBGs at $\omega_m \approx 1.10, 1.17, 1.25$ with $g_w = 11.7\%, 1\%$ and 5.4% , respectively.

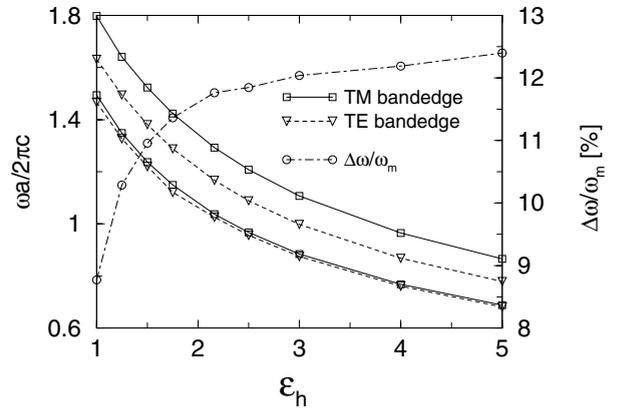


Figure 3. The dependence of band edges and g_w of the largest CPBG on the host dielectric constant ε_h for a triangular lattice of silver cylinders, $f = 58\%$, and $a/\lambda_z = 1.98$.

of the largest CPBGs bandgap edges and g_w on ε_h for $f = 58\%$ and $a = 650$ nm is shown in figure 3. The figure shows that as ε_h increases, g_w saturates at $\approx 12.5\%$.

For a square lattice, much smaller CPBGs are found with $g_w \leq 4\%$.

5. Discussion

Our aim was to show that practical in-plane CPBGs can open for the simplest 2D lattice and scatterer geometries, as long as the scatterer dielectric function is correctly chosen. Our proposal in using scatterers with a metallic Drude-like dielectric function (1) offers a new and promising way to fabricate 2D structures with a practical CPBG in the wide frequency range from GHz to ultraviolet. Indeed, a typical plasma frequency of a metal is in the ultraviolet, whereas that of a semiconductor is in the infrared. On the other hand, it has been shown [16] that a whole new class of artificial materials can be fabricated in which the plasma frequency may be reduced by up to six orders of magnitude compared with conventional materials, from UV down to GHz frequencies.

Correspondingly, the proposed structures can provide CPBG structures in this frequency range.

The observed magnitude and robustness of the in-plane CPBG of the metallo-dielectric structures allows one to speculate that an inclusion of metallic (silver) wires could also boost the performance of the photonic crystal fibre designed by Knight *et al* [23]. The photonic crystal fibre [23] is a 2D photonic periodic arrangement of thin cylindrical glass fibres where the light is sent along the cylinder axis. In lateral directions, the localization of light is achieved in complete analogy to the case of electrons: it is possible to introduce a defect at the centre of the photonic crystal fibre, for instance by omitting one cylinder, such that it induces a transversely localized mode with frequency within a 2D CPBG. The light can then propagate with that frequency along the cylinder axis even if the core of the photonic crystal fibre is air and if the cladding has a higher refractive index.

Although we have shown that one can achieve a relative gap width g_w larger than 10%, one expects that the width can be enlarged further by considering lattices with more than one scatterer per unit cell [23] or using more complicated scatterers such as cylinders with an ellipsoidal cross section [24] and coated cylinders, which were outside the scope of this paper. We also point out that the idea of using highly dispersive metallic and semiconductor components for photonic structures is not new [7, 16, 25–28]. Nevertheless, calculations using the plane-wave method [2] have often been restricted to an extremely low filling fraction, $f \leq 1\%$, of metallic components [7]. In addition, the main interest was in microwave [16, 26] or even in radiofrequency applications [27]. Surprisingly enough, no systematic search has been made for CPBGs with a Drude-like behaviour (1) of the dielectric function.

There have been many studies involving 2D structures since the pioneering work of Maradudin and collaborators [4]. However, these mostly require unrealistic values of the dielectric contrast δ to produce a CPBG below infrared wavelengths. The issue of the optimal 2D photonic structure with a CPBG below infrared wavelengths has only recently been addressed by Barra *et al* [12]. For a graphite arrangement of dielectric cylinders with a dielectric constant ϵ_c in air, they showed that the dielectric contrast $\delta \approx 8$ is enough to open a CPBG with $g_w = 6\%$ [12]. The required cylinder diameter to obtain a CPBG in the visible (around 500 nm) was 80 nm. Although this is technologically manageable, the required dielectric contrast $\delta \approx 8$ is large and strongly limits the choice of available materials in the visible. Barra *et al* suggested the use of GaN [12]. However, this material is very hard and problematic to etch (see, however, [29] for recent progress).

Throughout this work cylinders have been assumed to be infinitely long and we considered only in-plane propagation. However, as has been demonstrated by Labilloy *et al* [30], these facts do not preclude the application of our results to finite structures with finite cylinder lengths, provided that their aspect ratio, i.e. height/radius, is reasonably high (≈ 10).

From a practical point of view there are, in addition to the possibility of obtaining a practical in-plane CPBG, several additional advantages in using metallo-dielectric structures. Since metals are known to possess high nonlinear

susceptibilities [31], interesting possibilities such as optical switching and bistability [32, 33] can be achieved and studied in the presence of an in-plane CPBG. In addition, a nonzero electric conductivity can be used in pumping and/or in a fabrication of a new class of displays.

Finally, a few words about absorption. Since within CPBGs in the nonabsorptive window the size parameter of cylinders is $x = 2\pi r_c/\lambda \geq 5$, surface plasmon absorption is avoided and absorption is entirely determined by bulk properties and hence small. Such a moderate absorption has been shown to modify band structure only slightly [28]. Recently, a study of a 1D model showed that a certain degree of absorption can even be advantageous, since absorption turned out to widen some of the gaps by as much as 50% [34].

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