# Towards two-dimensional complete photonic-bandgap structures below infrared wavelengths

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## Abstract

Band gaps 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 complete in-plane photonic band gaps (CPBG's) 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[20], the optimal geometry is a triangular lattice. If the lattice spacing is tuned to a characteristic plasma wavelength, several CPBG's 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 $\varepsilon_h = 1$. Such structures can

provide CPBG structures with bandgaps down to ultraviolet wavelengths.

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## I. 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 crystals 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 of 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 to 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 involving 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 (1D), 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 speak about 3D photonic structures [11]. A 2D photonic crystal can be thought of as a 2D periodic ar-

rangement of scatterers with a dielectric constant $\varepsilon_s$ embedded in a host with a dielectric constant $\varepsilon_h$. 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, $\triangle\omega/\omega_m$. 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 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 the present article is to demonstrate that practical CPBG's can already open for the simplest lattice and scatterer geometries, as long as the scatterer dielectric function is rightly chosen. Therefore, we shall discuss only 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 two-dimensional square lattice of cylinders for a cylinder filling fraction of 65% in a silica host (see Fig. 1), several CPBG's 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],

$$\varepsilon_s(\omega) = 1 - \omega_p^2/\omega^2, \tag{1}$$

where $\omega_p$ is called the plasma frequency. Note that the Drude-like dielectric function is zero for $\omega = \omega_p$ which makes $\delta$ infinite and enables one to avoid the restrictions on the dielectric contrast. This approach has been shown to work also for three-dimensional (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]. Then 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 Fig. 1).

Metals can be quite lossy at optical frequencies. Nevertheless, the absorption can be rather 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 to induce 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 CPBG's. In real systems, such as silver, a deviation from the ideal Drude behaviour occurs in particular in the proximity of the zero crossing of Re $\varepsilon$ at some $\lambda_z$ ($\lambda_z = 328$ nm for silver). Such a $\lambda_z$ is red-shifted compared to $\lambda_p$ ($\lambda_p \approx \lambda_z/1.9$ for silver) [17] and the band structure between $\lambda_z$ and $\lambda_p$ can be modified as compared to 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 hence are expected to give rise to the biggest band gaps. We find that for an ideal Drude-like material a square lattice leads to the biggest gaps of the two studied lattice types. However, the deviation of the dielectric function of silver from the ideal Drude behaviour makes that for silver triangular lattices result in bigger CPBG's than square lattices. In both cases, i.e. ideal Drude/square and silver/triangular, a CPBG with $g_w \approx 10\%$ is found even for a host dielectric constant $\varepsilon_h$ as low as $\varepsilon_h = 1$.

## II. 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 for either polarization. This polarization decoupling is specific to 2D and obviously is not

the case for 3D photonic structures where a truly vectorial KKR method is required [19]. Given a plasma frequency $\omega_p$, we performed calculations for frequencies from $\approx 0.5\omega_p$ up to $1.1\omega_p$, assuming $\varepsilon_h$ is constant in this frequency region. In contrary to the plane-wave method [4,7], dispersion does not cause any difficulties to the KKR method and 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 10 as compared to the plane-wave method [7].

## III. 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 3D [15]. The plasma wavelength sets a characteristic scale, and, correspondingly, bandgaps only occur for certain values of $r_c/\lambda_p$, or, $a/\lambda_p$, where $r_c$ and $a$ is 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 $\varepsilon_h$ is as low as $\varepsilon_h = 1$. Other noteworthy points in case of $\varepsilon_h = 1$ are

1. no or only tiny CPBG's for $a/\lambda_p \leq 0.9$
2. no CPBG's bigger than 5% below $a/\lambda_p \leq 1$
3. for $f$ fixed, a CPBG $g_w$ grows rapidly with $a/\lambda_p$ 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 biggest $g_w$ 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 CPBG's mentioned above, we also found very big CPBG's at lower frequencies, outside the "nonabsorptive" window, typically at midgap frequencies of 20% of the plasma frequency. For instance, in case of the structure of Fig. 1b 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 CPBG's. However, the maximal $g_w$ found was 3.5%.

## IV. RESULTS FOR SILVER

For silver we used the experimental data from Palik [20]. The deviation from the ideal Drude behaviour, which occurs in the proximity of the zero crossing of Re $\varepsilon$ at $\lambda_z = 328$ nm [17], makes that for silver a triangular lattice leads to bigger CPBG's than a square lattice. For a fixed $f$, the relative gap width $g_w$ increases with increasing $a/\lambda_z$ (or with $a/\lambda_p$) until $a/\lambda_z \approx 2$ ($a/\lambda_p \approx 1.1$) is reached. Afterwards CPBG's fall into region of increased absorption. Interestingly, $a/\lambda_m$, where $\lambda_m$ 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 biggest CPBG, with $g_w = 11.7\%$, for $f = 58\%$, with the entire CPBG still lying in the "nonabsorbing" frequency window (see Fig. 3). Note that in this case the distance between the silver cylinders is $\approx 115$ 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 [21]. The dependence of the largest CPBG's band-gap-edges and $g_w$ on $\varepsilon_h$ for $f = 58\%$ and $a = 650$ nm is shown in Fig. 2. The figure shows that as $\varepsilon_h$ increases, $g_w$ saturates at $\approx 12.5\%$.

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

## V. DISCUSSION

We aimed at showing that practical in-plane CPBG's can open for the simplest 2D lattice and scatterer geometries, as long as the scatterer dielectric function is rightly 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 ultraviolet, whereas that of a semiconductor 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 6 orders of magnitude compared to 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 perfomance of the photonic crystal fibre designed by Knight et al [22]. The photonic crystal fibre [22] 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 center of the photonic crystal fibre, for instance by omitting one cylinder, such that it induces a transversaly 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 cladding has higher refractive index.

Although we have shown that one can achieve the relative gap width $g_w$ larger than 10%, one expects that the width can yet be enlarged 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 article.

We note 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]. Also the main interest was in microwave [16,26] or even in radiofrequency applications [27]. Surprisingly enough, no systematic search has been made to look for CPBG's 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 require mostly unrealistic values of the dielectric contrast $\delta$ 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, Cassagne and Jouanin [12]. For a graphite arrangement of dielectric cylinders with a dielectric constant $\varepsilon_c$ 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, Cassagne and Jouanin suggested the use of GaN [12]. However, this material is very hard and difficult 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 lengths of cylinders, provided that their aspect ratio, i.e. height/radius, is reasonably high ($\approx 10$).

From practical point of view there are, in addition to the possibility in obtaining a practical in-plane CPBG, several additional advantages in using metallo-dielectric structures. Since metals are known to possess high nonlinear susceptibilities [31], an 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 CPBG's 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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# Figure captions

**Fig. 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 CPBG's 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, $a/\lambda_p = 1.1$. Note also a band gap for TM polarization (s-polarization; **E** parallel to the cylinder axes) below the first band in part (**b**), which is characteristic for 2D structures with metallic components [7]. For TE polarization **E** is perpendicular to the cylinder axes.

**Fig. 2 -** The dependence of band egdes and $g_w$ of the largest CPBG on the host dielectric constant $\varepsilon_h$ for a triangular lattice of silver cylinders, $f = 58\%$, and $a/\lambda_z = 1.98$.

**Fig. 3 -** 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 line, respectively. Note three CPBG's at $\omega_m \approx 1.10$, 1.17, 1.25 with $g_w = 11.7\%$, 1%, and 5.4%, respectively.

FIG. 1.

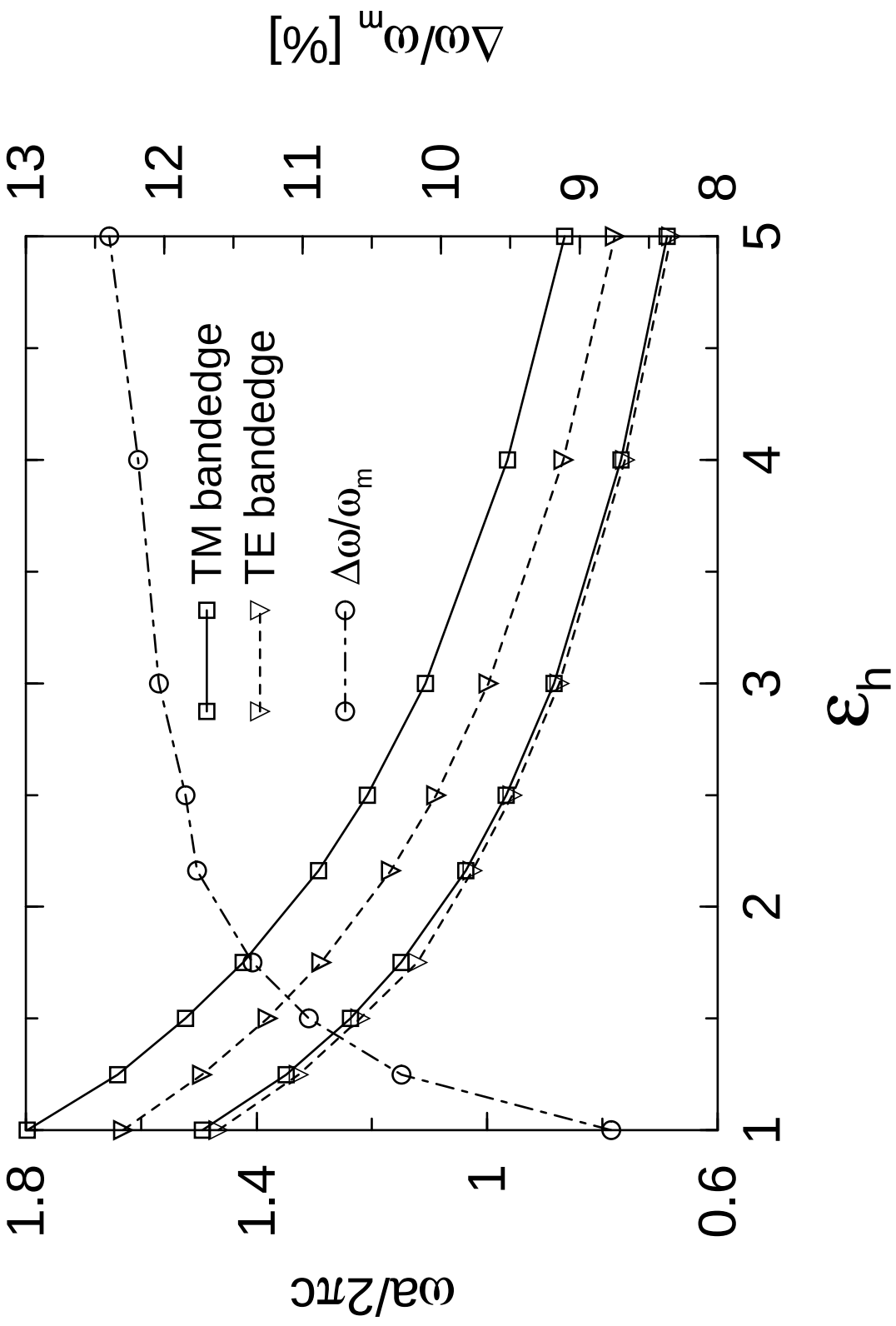
TM bandedge
TE bandedge
Δω/ω_m
ωa/2πc
ε_h
Δω/ω_m [%]
1.8
1.4
1
0.6
1
2
3
4
5
8
9
10
11
12
13

FIG. 2.

FIG. 3.