Analytical description of band gaps in a ternary metallo-dielectric stack

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ABSTRACT

Metallo Dielectric Photonic Crystals formed by same periodicity metallic inserts in a Dielectric Photonic Crystal show three kind of band gaps, those at the well know dielectric band gap, the ones attributed to the absorption of metal to low frequencies and a new class of metallic bandgaps. Numerical studies have confirmed that while the dielectric band gap width is basically described by the refraction index contrast, the width of the metallic band is described by the thickness of the metal inserts. In this work we carry on the corresponding analytical analysis of both band gaps for this one dimensional ternary dielectric-dielectric-metal structure. The stack that we are proposing is a quarter-wave for the dielectrics and the thickness of the metallic layers is changed as a free parameter. Using standard transfer matrix formalism, we find a closed form of the dispersion relation and from it; we have analytically demonstrated the formation and width of the dielectric band gap and its metallic perturbation, as well as those of the additional metallic band gap.

Keywords: Photonic crystal, band gap, metallic layers

1. INTRODUCTION

Dielectric Photonics Crystals have greatly benefited from the practical experience learned with thin films as the early One Dimensional Photonic Crystals. We inherited practical rules of the thumb such as the Refraction Index Contrast dependence of the Photonic Band Gap width. Such simple, but useful knowledge for Metallo Dielectric Photonic crystals is not available and some preliminary analytical results are described in this article, to corroborate our early numerical findings[1]. Metallic Photonic Crystals (MPC) did not have such clear start because of the metal loss, there are two outstanding contributions. The first one by Kuzmiak and Maradudin[2], using dispersion relations and perturbation theory, they produce approximate solutions for a single metal-single dielectric PC. Well beyond the perturbation regimen, thicker metallic inserts, Yablonovitch and co-workers[3] studied PC and showed clearly non perturbative features in the equivalent dielectric crystal.

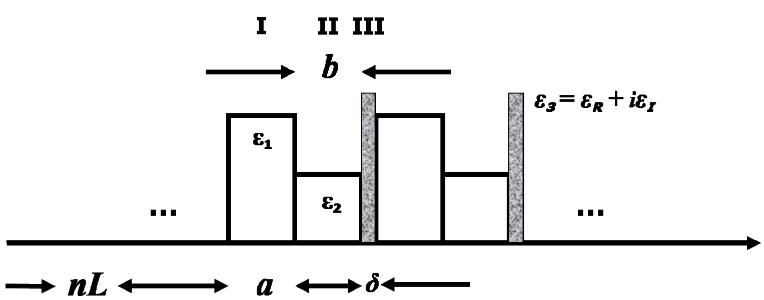

Figure 1. Schematic representation of the MDPC stack.

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22nd Congress of the International Commission for Optics: Light for the Development of the World,
edited by Ramón Rodríguez-Vera, Rufino Díaz-Uribe, Proc. of SPIE Vol. 8011, 801167
2011 SPIE · CCC code: 0277-786X/11/$18 · doi: 10.1117/12.902977

Our earlier works have shown that we are looking at opposite limits of the same problem[2-6], we have explored a model where both dielectric and metal features can be clearly differentiated, a Metallo Dielectric Photonics Crystal build from a basic Dielectric Photonic Crystals as the supporting structure with the metallic inserts keeping the same periodicity, (see Fig. 1), conforming a ternary stack dielectric-dielectric-metal Metallo Dielectric Photonic Crystal (MDPC). We have demonstrated that these structures show three kinds of band gaps, the first one that shows primarily the dielectric features and centered at the Bragg frequencies, and due to the metal component: a band gap at low frequencies and a metallic band gap, due primarily to the metal and located between Dielectric band gaps in a PC, this can be appreciated in Fig. 2, where stop gaps for the transmittance of the crystals are shown. Here, we are showing transmittance curves instead of band diagrams because the "metallic" band gaps are easier appreciated and the transmittance can be calculated faster than the band diagrams for high frequencies (a discussion about when this comparison is valid can be consulted in a previous work[7]). However, our calculations will be done on the bases of the dispersion relation and band diagrams terminology. Our goal in this work is to describe analytically the localization and thickness of this band gap.

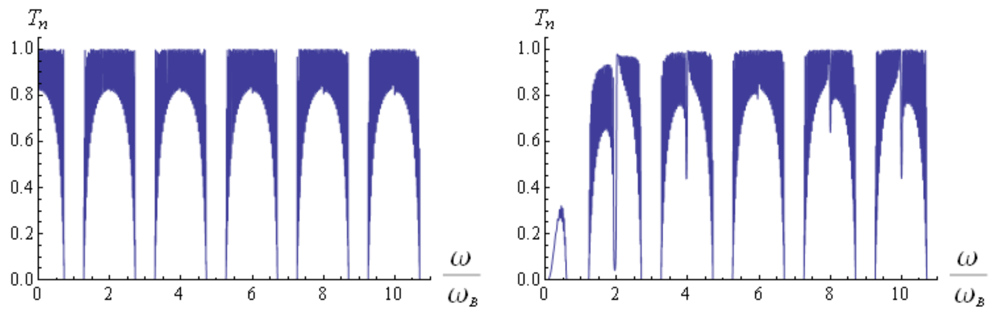

Figure 2. Left, stop gaps for a quarter-wave PC. Right, stop gaps for a MDPC.

We design the MDPC as follows. The thickness of the dielectrics will be λ/4 for each layer and for the case of the metallic inserts the thickness will be changed as a parameter δ. Thus, a period or unit cell of the crystal will be $L = a + b + \delta$, as we can see in Fig. 1.

2. ANALYTICAL RESULTS

We will start by recapitulating the well known dispersion relation for a 1D PC:

$$\cos(kL) = \cos(k_1 a)\cos(k_2 b) - \frac{k_1^2 + k_2^2}{2k_1 k_2}\sin(k_1 a)\sin(k_2 b), \tag{1}$$

where κ is the Bloch wave vector, k_1 and k_2 are the wave vectors in the respective medium. The band diagram for the Eq. (1) is shown in Fig. 3, the axes have dimensionless units.

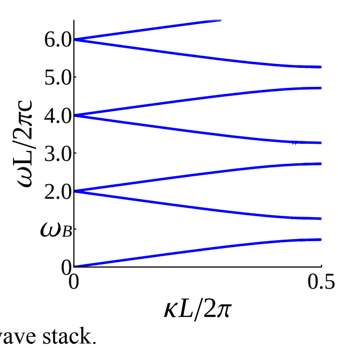

Figure 3. Band diagram for a quarter-wave stack.

In the Brillouin zone boundaries $\mathrm{Re}\{\kappa\} = \pi / L$, therefore

$$\kappa L = \pi \pm ix, \tag{2}$$

which means that the real part of the cosine function in the left part of Eq. (1) is close to 1 and the imaginary part x (absorption) will change in the band gap region, but in the boundaries will be cero. Also, there is a particular frequency ω_B (the Bragg frequency) that satisfies

$$k_1 a = k_2 b = \frac{1}{2}\pi. \tag{3}$$

It is located exactly at the middle of the band gap for a quarter-wave stack and because our normalization in the odd numbers in "x" axis (see the left graph in Fig. 2 or Fig. 3 at the end of the Brillouin zone). Using conditions (2) and (3) in the dispersion relation (1), yields

$$x = \operatorname{arccos} h\left(\frac{n_1^2 + n_2^2}{2n_1 n_2}\right). \tag{4}$$

Eq. (4) gives the maximum value for the absorption in the middle of the band gap.

On the other hand, if we take a small displacement from the central frequency in the band gap ω_B, and renormalizing as follows

$$y = \frac{\omega - \omega_B}{c} n_1 a = \frac{\omega - \omega_B}{c} n_2 b. \tag{5}$$

Again substituting in Eq. (1) the conditions (2) and (5), we arrive to

$$\cosh x = \frac{n_1^2 + n_2^2}{2n_1 n_2} \sin^2 y - \cos^2 y \tag{6}$$

and in the boundaries of the first Brillouin zone $x = 0$. Thus

$$y = \pm \arcsin\left(\frac{2\sqrt{n_1 n_2}}{n_1 + n_2}\right) \tag{7}$$

and the total width of the band gap in our original dimensionless units will be:

$$\Delta\omega_{Dgap} \sim 2 \arcsin\left(\frac{2\sqrt{n_1 n_2}}{n_1 + n_2}\right). \tag{8}$$

The previous procedure was discussed before by Yeh[8], and clearly can be extended for our MDPC but that will be published elsewhere.

Now, we will discuss the MDPC new features. We are considering the metal layers with a refractive index depending on the frequency. This is described trough the Drude model:

$$\varepsilon_3(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)} \tag{9}$$

as usual[2, 3], ω_p = 1.6 x 10^{16} rad/s, is the plasma frequency and $\gamma = 0.001\ \omega_p$ is the damping coefficient. When the metallic inserts are considered the dispersion relation is given by

$$\cos(\kappa L) = \left[\cos(k_1 a)\cos(k_2 b) - \frac{1}{2}\frac{k_1^2 + k_2^2}{k_1 k_2}\sin(k_1 a)\sin(k_2 b)\right]\cos(k_3\delta)$$
$$-\frac{1}{2k_3}\left[\frac{k_1^2 + k_3^2}{k_1}\sin(k_1 a)\cos(k_2 b) + \frac{k_2^2 + k_3^2}{k_2}\cos(k_1 a)\sin(k_2 b)\right]\sin(k_3\delta). \tag{10}$$

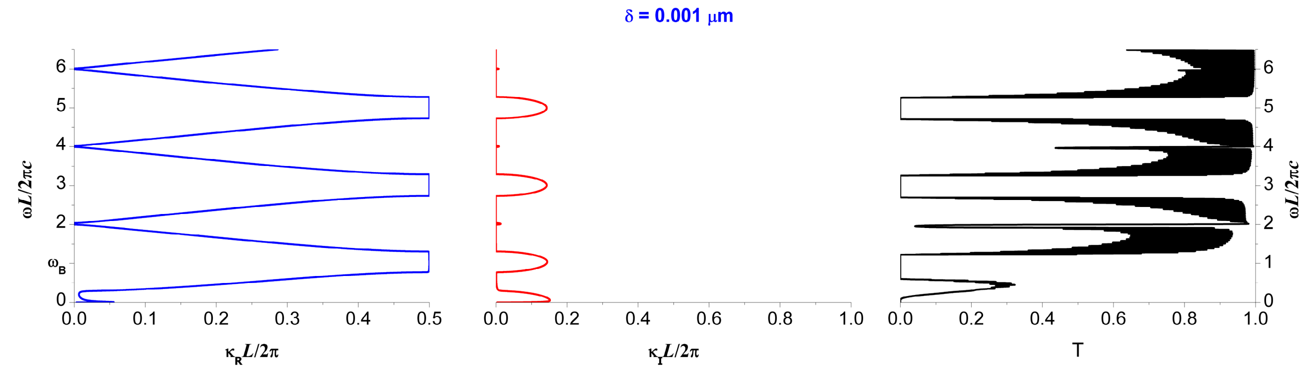

Figure 4. Band diagram, absorption and the transmitance for the MDPC with metallic layers of thickness δ = 0.001 μm.

We are aware that the wave vectors of the metal are complex numbers with real (imaginary) part k_{3R} (k_{3I}) and therefore the Bloch wave number κ_R (κ_I) as well. As we can see from Fig. 2, there is an unexpected additional stop gap just between two consecutive dielectric stop gaps. This can also be appreciated in the band structure, Fig. 4 is the plot of the MDPC dispersion relation Eq. (10). This means that, in this case the relation (3) should be modified to

$$k_1 a = k_2 b = \frac{1}{2}\pi + \pi = \frac{3}{2}\pi, \tag{11}$$

as long as δ is small. In the same way Eq. (2) should be changed to

$$\kappa L = \frac{\pi}{2} \pm ix \tag{12}$$

and substituting this last relation and Eq. (11) in Eq. (10), yields

$$\cos\left(\frac{\pi}{2} + ix\right) = -\frac{1}{2}\frac{k_1^2 + k_2^2}{k_1 k_2}\left[\cos(k_{3R}\delta)\cosh(k_{3I}\delta) - i\sin(k_{3R}\delta)\sinh(k_{3I}\delta)\right]. \tag{13}$$

Separating the last relation into real and imaginary parts, and evaluating them on the boundaries of the first Brillouin zone ($x = 0$), we arrive to

$$-\frac{1}{2}\frac{k_1^2 + k_2^2}{k_1 k_2}\cos(k_{3R}\delta)\cosh(k_{3I}\delta) = 0 \tag{14}$$

and

$$-i\sinh x = \frac{i}{2}\frac{k_1^2 + k_2^2}{k_1 k_2}\sin(k_{3R}\delta)\sinh(k_{3I}\delta). \tag{15}$$

From the real parts relation, we find

$$k_{3R}\delta = \frac{3\pi}{2} + 2\pi(n-1) \quad (n \in \mathbf{N}), \tag{16}$$

where the $\pi/2$ solutions were discarded because they correspond to the stop gaps associated to the pure dielectric stack. Whereas the imaginary part has the solution

$$x = \operatorname{arc\,sinh}\left(\frac{1}{2}\frac{k_1^2 + k_2^2}{k_1 k_2}\left[\sinh\left(k_{3I}\delta\right)\right]\right), \tag{17}$$

which represents the maximum absorption from the metal in the middle of the band gap.

In analogy with the dielectric calculation, we will proceed to calculate the width of the metallic band gap. If a small shift to the low frequencies is considered on the neighborhood of the Bragg frequency for the metallic stop gaps, then

$$k_1 a = k_2 b = k_{3R}\delta = \frac{3\pi}{2} + y \tag{18}$$

and again evaluating in the dispersion relation (10) in the boundaries of the first Brillouin zone, it reduces to

$$\begin{gathered}\left[1 - \frac{\left(n_1 + n_2\right)^2}{2n_1 n_2}\cos^2 y\right]\left[i\sinh\left(k_{3I}\delta\right)\cos y + \cosh\left(k_{3I}\delta\right)\sin y\right] \\ + \frac{n_1 + n_2}{2n_1 n_2 \left|n_3\right|^2}\left[n_1 n_2\left(n_{3R} - i n_{3I}\right) + \left|n_3\right|^2\left(n_{3R} + i n_{3I}\right)\right]\sin y \cos y\left[-\cosh\left(k_{3I}\delta\right)\cos y + i\sinh\left(k_{3I}\delta\right)\sin y\right] = 0.\end{gathered} \tag{19}$$

After some algebraic manipulation, taking only the real pat because the imaginary part is a redundant equation, we arrive to

$$\begin{gathered}-\frac{\left(n_1 + n_2\right)^2}{2n_1 n_2}\cosh\left(k_{3I}\delta\right)\cos^2 y \sin y + \cosh\left(k_{3I}\delta\right)\sin y + \\ + \frac{n_1 + n_2}{2n_1 n_2 \left|n_3\right|^2}\left[-\left(n_1 n_2 + \left|n_3\right|^2\right) n_{3R}\cosh\left(k_{3I}\delta\right)\cos y - \left(\left|n_3\right|^2 - n_1 n_2\right) n_{3I}\sinh\left(k_{3I}\delta\right)\sin y\right]\sin y \cos y = 0.\end{gathered} \tag{20}$$

Until this point we were working with exacts equations, but we need to make and approximation to find an analytical solution for y not so cumbersome. Then, we are taking the expansions of the sine and cosine functions to order cero:

$$\begin{gathered}-\frac{\left(n_1 + n_2\right)^2}{2n_1 n_2}\cosh\left(k_{3I}\delta\right) y + \cosh\left(k_{3I}\delta\right) y + \\ + \frac{n_1 + n_2}{2n_1 n_2 \left|n_3\right|^2}\left[-\left(n_1 n_2 + \left|n_3\right|^2\right) n_{3R}\cosh\left(k_{3I}\delta\right) - \left(\left|n_3\right|^2 - n_1 n_2\right) n_{3I}\sinh\left(k_{3I}\delta\right) y\right] y = 0\end{gathered} \tag{21}$$

which can be immediately solved

$$y = -\frac{\left(n_1^2 + n_2^2\right)\left|n_3\right|^2 + n_{3R}\left(n_1 n_2 + \left|n_3\right|^2\right)\left(n_1 + n_2\right)}{\left(n_1 + n_2\right)\left(\left|n_3\right|^2 - n_1 n_2\right) n_{3I}}\tanh\left(k_{3I}\delta\right). \tag{22}$$

Finally, the width of the metallic band gap will be

$$\Delta\omega_{Mgap} = \frac{L}{\pi n_1 a} y. \tag{23}$$

The width of the metallic band gap is plotted in Fig. 5. The lineal relation corroborate our early numerical results and show that they are a good approximations to describe for metallic inserts in the perturbative regimen, in our example a thickness should be less than $\delta = 0.01$ µm.

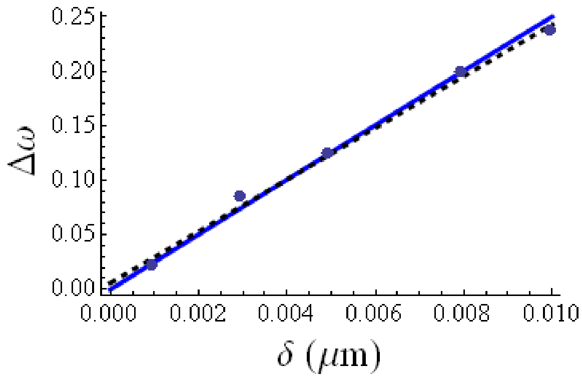

Figure 5. Solid line, the widht of the metallic band gap described by Eq. (23). Circles are numerical measurements and dashed line is a numerical fit.

3. CONCLUSIONS

We described analytically the position and width of a new band gap in a ternary one dimensional photonic crystal dielectric-dielectric-metal. Our results show that these band gaps are structural band gaps and they are different from the band gap formed before the plasma frequency in structures with metal and at the same time not attributed to the dielectrics band gaps well-known in 1D quarter-wave dielectric photonic crystals.

ACKNOWLEDGMENT

A. A. M. thanks National Council for Science and Technology from Mexico (CONACyT) for the scholarship with number 183001. This research was supported by CONACyT under contract CB-2008/101378.

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