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► **To cite this version:**

Jean-Michel André, Philippe Jonnard. Effective mass of photons in one dimensional photonic crystal. Physica Scripta, 2011, 84, pp.035708. 10.1088/0031-8949/84/03/035708 . hal-00631235

**HAL Id: hal-00631235**

**<https://hal.science/hal-00631235>**

Submitted on 11 Oct 2011

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# Effective mass of photons in one dimensional photonic crystal

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## Abstract

Photons propagating within photonic crystals can be regarded as quasi-particles having an effective mass. Methods of calculation of this mass from the photonic density of mode are presented for the case of one-dimensional photonic crystal, both from infinite and finite structure. The model is implemented to calculate the influence of the number of unit cells and of absorption, for bilayered Bragg structure used as reflectors in the soft-x-ray domain. The physical meaning of the effective photon mass concept is discussed.

PACS numbers: 78.67.Bf, 78.67.Pt.

## 1. Introduction

Photons propagating within photonic crystals (PCs) [1] can be regarded as quasi-particles having an effective mass similar to the one of electrons in a crystal. The nature of this effective mass can appear somewhat scheming and it is exciting to imagine experiments revealing this effective photon mass. Gorelik has studied the effective photon mass in globular photonic crystals [2] and more recently, reported experimental results establishing the existence of heavy photons in PCs [3]. The concept of effective photon mass appears also in the microcavities [4] such as these ones implemented to obtain the Bose-Einstein condensation of polaritons [5]. The calculation of effective photon mass can be performed from band structure computations by means of codes using expansion in Fourier series of the dielectric function; these codes are available in the literature [6]. In principle such calculations assume infinite structure. Extension of the coupled-mode theory applied to deep optical grating should also provide the group velocity and the group-velocity dispersion, that is the inverse effective mass of photon, in one-dimensional photonic crystal [7].

In this communication we focus on calculations of the effective photon mass in one-dimensional crystal (1D-PC), especially Bragg reflector, based upon the calculation of the photonic density of mode (DOM). We consider the case of infinite and finite structure. The paper is organized as follows: section 2 is devoted to the formalism of the effective photon mass (epm) in PCs and its relationship with the photonic DOM. Section 3 presents the calculation of the epm in an infinite 1D-PC and in section 4, we consider the case of a finite 1D-PC. Numerical examples are given in section 5 for the case of bilayered Bragg structure used as reflectors in the soft-x-ray domain. Finally in section 6, the physical foundation of the concept of epm is discussed and perspectives are presented.

## 2. Effective mass of photons in PCs and density of mode

The analogy between electromagnetism in a PC and quantum mechanics of solid-state physics has been reviewed in details in [1]. The propagation of a photon in a PC is governed by the following master equation deduced from Maxwell equations:

$$\hat{\Theta} \mathbf{H}(\mathbf{r}) = \Omega \mathbf{H}(\mathbf{r}) \quad (1)$$

where  $\mathbf{H}(\mathbf{r})$  is the spatial component of the harmonic magnetic field  $\mathbf{H}(\mathbf{r}, \omega) = \mathbf{H}(\mathbf{r}) \exp(-i\omega t)$ .

$\hat{\Theta}$  stands for the following linear operator:

$$\hat{\Theta} = \nabla \times \left( \frac{1}{\epsilon(\mathbf{r})} \nabla \times \right) \quad (2)$$

This operator for a PC is periodic since the dielectric constant  $\epsilon(\mathbf{r})$  has the periodicities of the PC lattice. The equation (1) forms a traditional eigenvalue problem similar to the Schrödinger equation that the electron satisfies in a crystalline solid. The eigenvalue  $\Omega$  is analogous to the electron energy and is proportional to the squared frequencies  $\omega$  of the harmonic modes:

$$\Omega = \left( \frac{\omega}{c} \right)^2 \quad (3)$$

By virtue of the periodicity of  $\hat{\Theta}$ , the Bloch-Floquet theorem applies to Eq.(1). The solutions are Bloch waves:

$$\mathbf{H}(\mathbf{r}) = \mathbf{h}_{\mathbf{K}}(\mathbf{r}) \exp(i\mathbf{K}\mathbf{r}) \quad (4)$$

where  $\mathbf{K}$  is the so-called Bloch wave-vector and the quantities  $\mathbf{h}_{\mathbf{K}}(\mathbf{r})$  have the periodicities of the PC lattice. The eigenvalue  $\Omega$  is a function of the Bloch wave-vector  $\mathbf{K}$ , so that the mode frequency  $\omega$  depends on  $\mathbf{K}$ :

$$\omega = \omega(\mathbf{K}) \quad (5).$$

This relationship called dispersion equation, can be explicitly found by inserting Eq.(4) in the master equation.

To the Bloch vector  $\mathbf{K}$ , one can associate a quasi-impulse  $\mathbf{P}$  by the relationship:

$$\mathbf{P} = \hbar \mathbf{K} \quad (6)$$

This quantity is important for the photon propagation in the PC because it satisfies the law of momentum conservation. Similarly by virtue of Planck's equation, one can find the photon energy  $E = \hbar \omega(\mathbf{K})$  which is also a function of the quasi-impulse:

$$E = E(\mathbf{P}) \quad (7)$$

This photon energy defined by Eq.(7) satisfies the law of energy conservation.

From Eq.(7) one can introduce the concept of effective photon mass. If  $\mathbf{P}_0$  is an extremum point of  $E(\mathbf{P})$ , one can expand this function in Taylor series:

$$E(\mathbf{P}) = E(\mathbf{P}_0) + \sum_{t=1}^{\infty} \left( \frac{d^t E(\mathbf{P})}{d\mathbf{P}^t} \right)_{\mathbf{P}_0} \frac{(\mathbf{P} - \mathbf{P}_0)^t}{t!} \quad (8)$$

For  $t = 1$ , the corresponding term is a vector and for  $t=2$ , the corresponding term is a 2-rank tensor. Since by assumption  $\mathbf{P}_0$  is an extremum, the derivative of rank 1 vanishes so that, in terms of quasi-impulse, one has the expansion:

$$E(\mathbf{P}) = E(\mathbf{P}_0) + \frac{d^2 E(\mathbf{P} - \mathbf{P}_0)^2}{d\mathbf{P}^2} + \dots \quad (9)$$

From Eq.(9) one introduces the effective mass tensor  $m^*$  by:

$$\mathbf{m}^* = \left\{ \frac{d^2 E}{d\mathbf{P}^2} \right\}^{-1} \quad (10)$$

where  $\{\}^{-1}$  denotes the inverse tensor. Provided that the higher terms of the expansion are negligible, the dispersion function  $E(\mathbf{P})$  takes the parabolic shape:

$$E(\mathbf{P}) = E_0 + \frac{1}{\mathbf{m}^*} \frac{(\mathbf{P} - \mathbf{P}_0)^2}{2} \text{ with } E_0 = E(\mathbf{P}_0) \quad (11)$$

The first term  $E_0$  of the expansion is nothing else but the photon energy of a “free” photon given by Planck’s law.

For a 1D-PC, the Bloch vector and the quasi-impulse become mere scalar quantities so that the effective photon mass is also a scalar. One writes:

$$m^* = 1 / \frac{d^2 E}{dP^2} = \hbar / \frac{d^2 \omega}{dK^2} \quad (12)$$

In the following we shall only consider 1D-PC. In this case, it is convenient to introduce the concept of photonic DOM  $\rho(\omega)$  defined by

$$\rho(\omega) = \frac{dK}{d\omega} \quad (13)$$

where  $K$  stands for the Bloch wave number. This quantity which is analogous to the inverse of a group velocity, can be calculated by different way as shown in the following sections.

Simple calculus shows that the scalar epm  $m^*$  can be expressed by means of the DOM from the following relationship:

$$m^* = \frac{\hbar \rho^3}{\rho'} \quad (14)$$

where the prime denotes derivative with respect to  $\omega$ .

### 3. Case of an infinite 1D-PC

An 1D-PC has a periodic structure of period  $d$ , along one axis (say  $z$ -axis), and consequently the dielectric constant  $\epsilon(z)$  of an infinite 1D-PC can be expanded in Fourier series:

$$\epsilon(z) = \sum_{l=-\infty}^{\infty} \epsilon_l \exp(i l g z) \quad (15)$$

where  $g = 2\pi/d$ ,  $d$  being the period of the PC along  $z$ . It has been shown [8] that in this case, the dispersion equation  $\omega = \omega(\mathbf{K})$  can be expressed by means of an infinite determinant as follows:

$$\sin^2 \left( \mathbf{K} \frac{d}{2} \right) = \Delta(0) \sin^2 \left( \frac{\omega}{c} \sqrt{J_0} \frac{d}{2} \right) \quad (16)$$

where  $\Delta(\mathbf{K})$  is the following infinite determinant:

$\Delta(K) =$

$$\left( \begin{array}{cccc} 1 & \frac{J_{-1} k^2}{J_0 k^2 - (K - g)^2} & \frac{J_{-2} k^2}{J_0 k^2 - (K - g)^2} & \frac{J_{-3} k^2}{J_0 k^2 - (K - g)^2} \\ \frac{J_1 k^2}{J_0 k^2 - K^2} & 1 & \frac{J_{-1} k^2}{J_0 k^2 - K^2} & \frac{J_{-2} k^2}{J_0 k^2 - K^2} \\ \dots & \dots & \dots & \dots \\ \frac{J_2 k^2}{J_0 k^2 - (K + g)^2} & \frac{J_1 k^2}{J_0 k^2 - (K + g)^2} & 1 & \frac{J_{-1} k^2}{J_0 k^2 - (K + g)^2} \\ \dots & \frac{J_q k^2}{J_0 k^2 - (K + q g)^2} & \dots & 1 \end{array} \right) \quad (17)$$

and  $J_l$  are the components of the Fourier expansion of  $J(z) = \frac{k_z(z)}{k}$  where  $k_z(z)$  is the modulus of the normal component of the wave-vector associated with the two counter-propagating plane waves propagating in the whole structures [8,9].

Let us now consider a mere Bragg bilayered structure consisting in  $N$  bilayers made up with two layers 1 and 2 of thickness  $d_1$  and  $d_2$  and dielectric constant  $\epsilon_1$  and  $\epsilon_2$ , respectively. If the structure is infinite, then  $N$  tends towards infinity and in this case, the dispersion equation  $K(\omega)$  is given by [9,10]:

$$\cos(Kd) = \frac{1}{1 - r(\omega)^2} (\cos\Phi - r(\omega)^2 \cos\Delta) \quad (18)$$

with  $d = d_1 + d_2$ ,  $r(\omega)$  is the Fresnel coefficient of reflection at the interface 1,2;  $\Phi$  and  $\Delta$  are the sum and the difference of the phase in the medium 1 and 2, respectively:

$$\begin{aligned} \Phi &= k_{\perp 1} d_1 + k_{\perp 2} d_2 \\ \Delta &= k_{\perp 1} d_1 - k_{\perp 2} d_2 \end{aligned} \quad (19)$$

where  $k_{\perp j}$  are the modulus of the normal component of the wave-vector associated with the two counter-propagating plane waves propagating in the layer  $j=1, 2$ .

From Eq.(16) and (17), one can calculate the DOM for an infinite 1D-PC and then by means of Eq.(14), one deduces the epm.

Let us emphasize that the Eq.(16) makes it possible to deal with the problem of any 1D-PC while Eq.(18) is restricted to the case of bilayered structure.

#### 4. Case of a finite 1D-PC

We consider now the case of a 1D-PC made with  $N$  unit cells. The unit cell can be any multilayered stack although the most common stack are bilayered or trilayered. An efficient strategy to calculate the epm in this case is to compute the DOM using the method proposed by Bendickson *et al.* [11] generalized to lossy media in [12]. This strategy is based upon the use of the transmission coefficient  $t_N$  of the whole structure:

$$t_N = \sqrt{T_N} \exp(i\varphi_N) \quad (20)$$

$T_N$  being the transmittance and  $\varphi_N$  being the total phase accumulated as the radiation goes through the  $N$  unit cells of the PC. Hence one can introduce the effective wave-number  $k_N$  and can write

$$\varphi_N = k_N d \quad (21)$$

Following [9,10], we define the N-unit cell DOM as:

$$\rho_N = \frac{dk_N}{d\omega} = \frac{1}{d} \frac{d\varphi_N}{d\omega} \quad (22)$$

Simple calculations show that

$$\rho_N = \frac{1}{d} \frac{z'_N}{1+z_N^2} \text{ with } z_N = \text{Arc tan}(\varphi_N) \quad (23)$$

the prime standing for the derivate with respect to  $\omega$ . It has been shown in [11,12] how to calculate  $\rho_N$ , then  $\varphi_N$  using Eq.(23), by means of the transfer matrix method.

Let us outline that  $\rho_N$  differs from  $r$  but that these two quantities can be related as shown hereafter. To obtain the photonic DOM  $\rho$  defined by Eq.(13) from  $\rho_N$ , one makes use of:

$$\rho = \rho_N \frac{dK}{dk_N} \quad (24)$$

$K$  being the Bloch wave-number of an infinite 1D-PC introduced in section 3. To get the derivative  $\frac{dK}{dk_N}$ , one can use the following formula [11]:

$$z_N = \arctan(k_N d) = z \tan(NK) \cot g(K) \quad (25)$$

with  $z = \tan(\varphi)$ ,  $\varphi$  being the phase accumulated through a unit cell. Some manipulations give:

$$\frac{dK}{dk_N} = z \cos(dk_N) \left( N \frac{\cot g(dK)}{\cos^2(dKN)} - \frac{\tan(dKN)}{\sin^2(dK)} \right) \quad (26)$$

so that the photonic DOM reads:

$$\rho = \rho_N \cot g(\varphi) \cos^2(\varphi_N) \left( N \frac{\cot g(dK)}{\cos^2(dKN)} - \frac{\tan(dKN)}{\sin^2(dK)} \right) \quad (27)$$

From Eq.(7) and Eq.(14), it is possible to calculate the epm  $m_N^*$  of a N-unit cell 1D-PC.

## 5. Numerical results

In this section we calculate the epm  $m^*$  for a periodic stack of N bilayers forming a Bragg reflector for the soft-x-ray domain. We consider a mirror consisting of unit cells made up with a Mo layer of thickness  $d_1= 1.41$  nm and of  $B_4C$  of thickness  $d_2= 1.976$  nm designed to reflect at the first Bragg order a radiation of vacuum wavelength 6.77 nm (or photon energy 182 eV) at an incident angle of  $30^\circ$  corresponding to the first diffraction order. The materials are supposed to be absorbing and their complex optical indices are taken from [13]. This kind of device is now standard for x-ray optics [9].

We first consider the infinite case that is, N tends towards infinity. In this case the dispersion equation is given by Eq.(18). Figure 1 shows the normalized photonic DOM  $\bar{\rho}$  versus photon energy E between 180 and 210 eV. Note that the normalization consists in choosing  $\bar{\rho}$  equal to unity outside the Bragg domain (180 eV for instance). Figure 2 presents on the same energy domain the epm  $m^*$  given in kg. The epm is cancelled in the Bragg domain, is negative in the low energy domain before the Bragg gap and is positive in the high energy domain after the gap. This kind of behaviour was also reported by Gorelnik [3] who used the same theoretical approach.

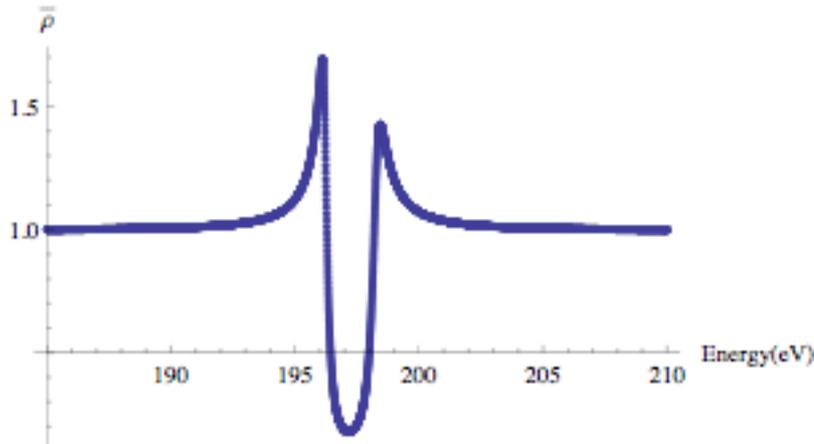


Figure 1: Normalized density of mode for the Mo/B<sub>4</sub>C Bragg reflector versus photon energy E with an infinite number of bilayers. The details of the Bragg reflectors are given in the text.

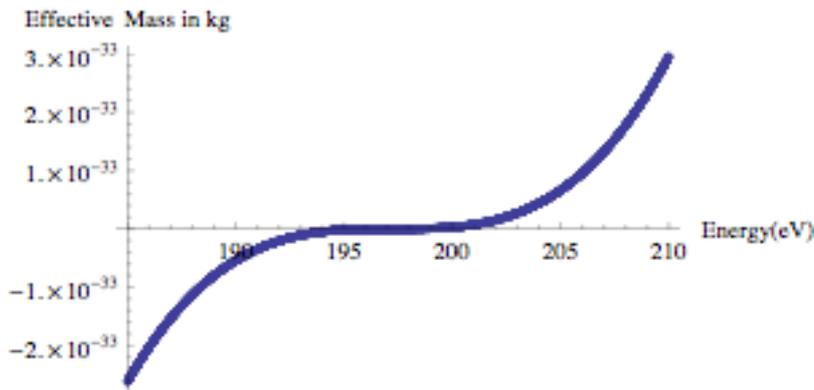


Figure 2: Effective photon mass for the Mo/B<sub>4</sub>C Bragg reflector versus photon energy with an infinite number of bilayers. The details of the Bragg reflectors are given in the text.

We now consider the case of finite structure. Figures 3-5 show the normalized DOM for  $N=20, 200$  and  $2000$  versus photon energy  $E$  and figures 6-8 present the corresponding variation of the epm  $m^*$ . First one notes that for large values of  $N$  (say  $2000$  in our example) our model of finite structure is in fair agreement with the infinite model. For small values of  $N$ , the infinite model fails and the shape of the curve  $m^*$  versus  $E$  changes considerably with the value of  $N$ . At intermediate (realistic) values of  $N$  that is typically between  $100$  and  $500$ , oscillations appear outside the Bragg gap which are due to interferences within the multilayer structures. For very low numbers of bilayers (see figure 6,  $N=20$ ), the epm curve presents “spikes” which correspond to the zeros of the DOM derivatives.

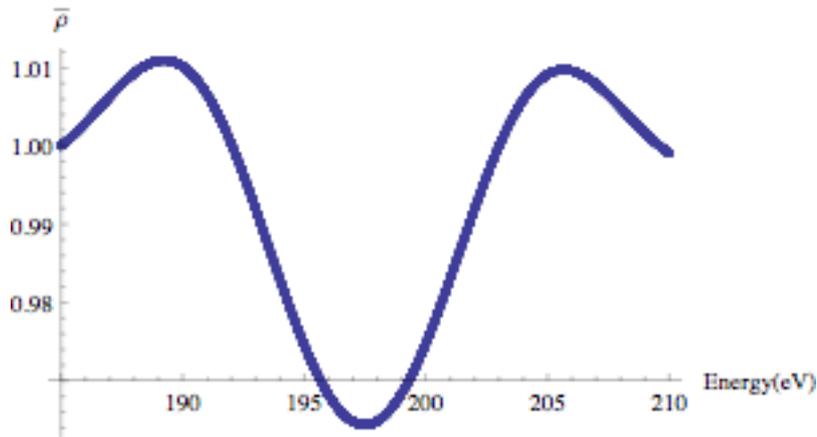


Figure 3: Normalized density of mode for the Mo/B<sub>4</sub>C Bragg reflector versus photon energy with a finite number of bilayers: N=20. The details of the Bragg reflectors are given in the text.

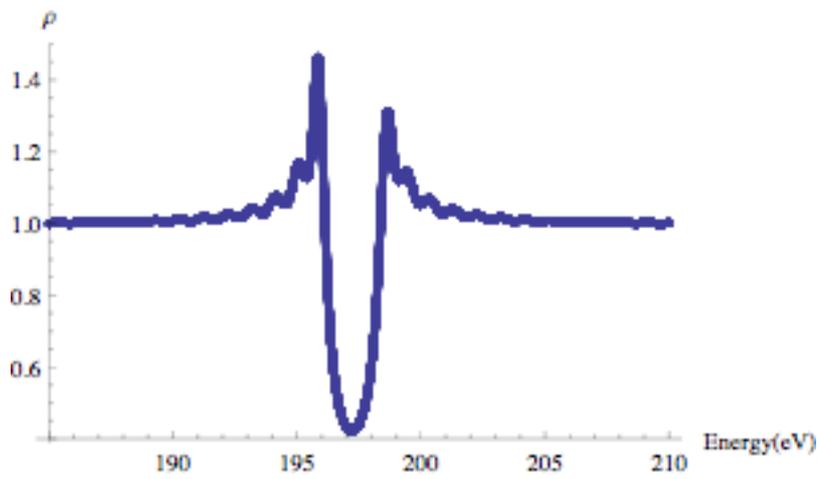


Figure 4: Normalized density of mode for the Mo/B<sub>4</sub>C Bragg reflector versus photon energy with a finite number of bilayers: N=200. The details of the Bragg reflectors are given in the text.

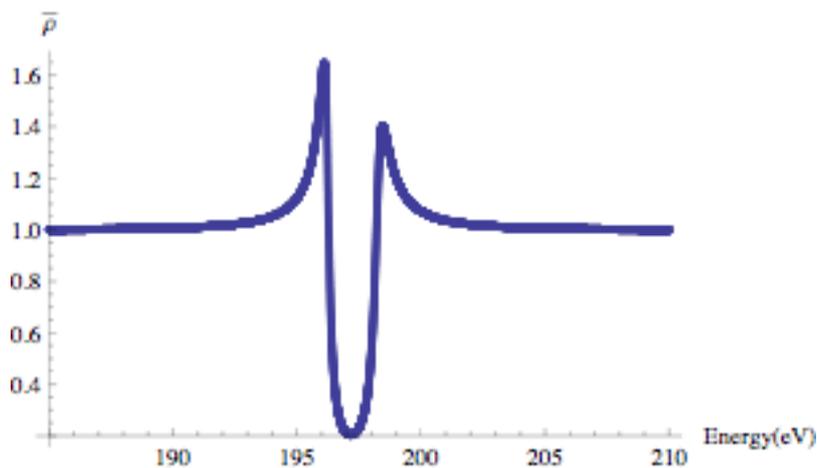


Figure 5: Normalized density of mode for the Mo/B<sub>4</sub>C Bragg reflector versus photon energy with a finite number of bilayers: N=2000. The details of the Bragg reflectors are given in the text.

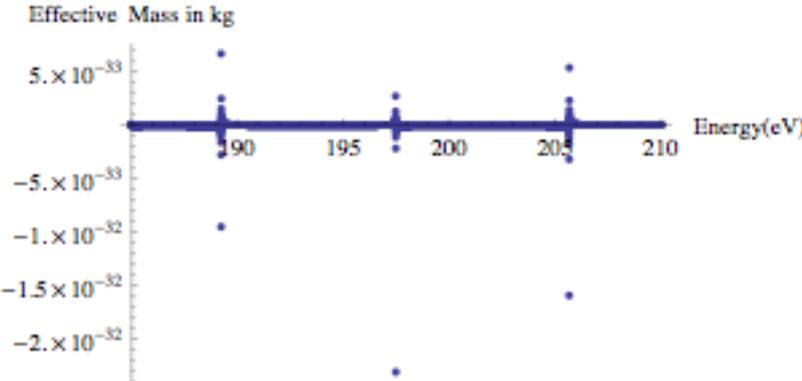


Figure 6: Effective photon mass for the Mo/B<sub>4</sub>C Bragg reflector versus photon energy with a finite number of bilayers: N=20. The details of the Bragg reflectors are given in the text.

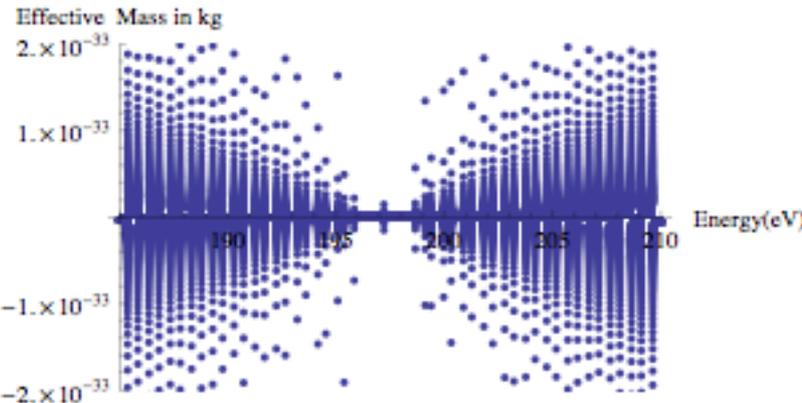


Figure 7: Effective photon mass for the Mo/B<sub>4</sub>C Bragg reflector versus photon energy with a finite number of bilayers: N=200. The details of the Bragg reflectors are given in the text.

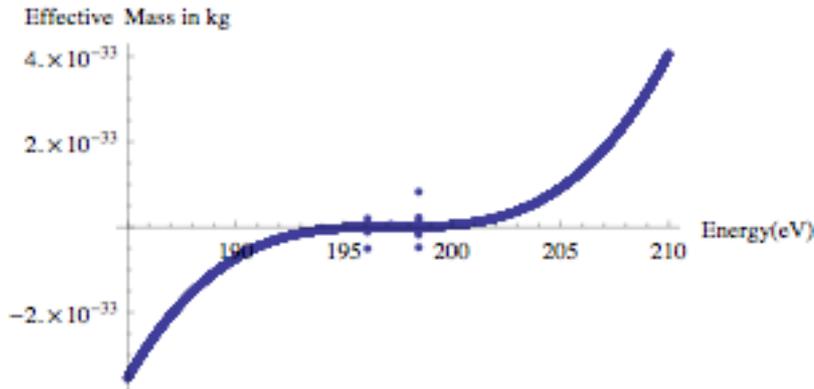


Figure 8: Effective photon mass for the Mo/B<sub>4</sub>C Bragg reflector versus photon energy with a finite number of bilayers: N=2000. The details of the Bragg reflectors are given in the text.

The influence of photon absorption is illustrated in Figures 9 and 10 by the case of a reflector with a large number of bilayers (N =2000) without absorption; to deal with this case, calculations are carried out with the imaginary part of the optical index enforced to zero. The transparency of the Bragg structure makes it possible to obtain strong interferences which are not attenuated by the photon attenuation. These interferences give rise to oscillations in the vicinity of the Bragg domain outside the bandgap both in the DOM and the epm curves. These oscillations are so closed that they are not resolved in the figures in spite of the huge number of points ( $10^5$ ) retained in the calculation. Let us mention that for an infinite structure these oscillations disappear and one obtains an epm quite similar to the one presented in figure 2.

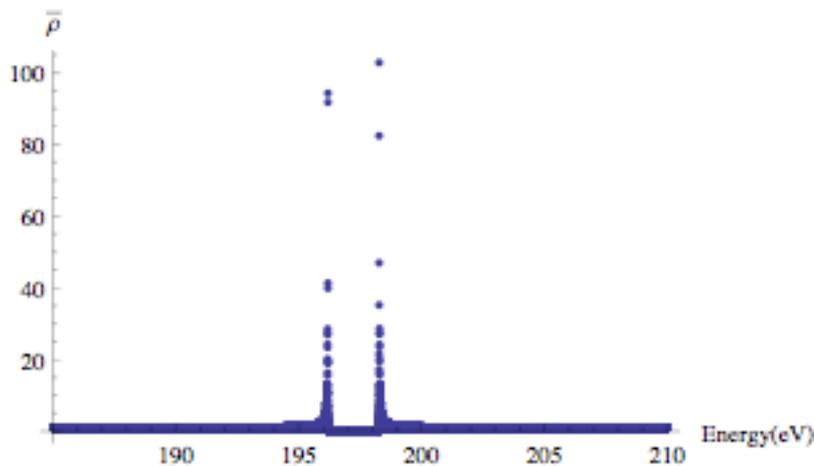


Figure 9: Normalized density of mode for the Mo/B<sub>4</sub>C Bragg reflector versus photon energy with a finite but large number of bilayers: N=2000 without absorption. The details of the Bragg reflectors are given in the text.

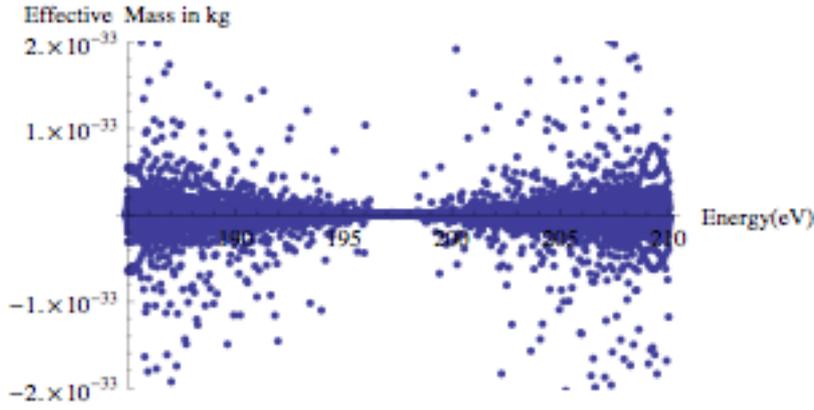


Figure 10: Effective photon mass for the Mo/B<sub>4</sub>C Bragg reflector versus photon energy with a finite but large number of bilayers: N=2000 without absorption. The details of the Bragg reflectors are given in the text.

## 6. Discussion and conclusion

It has been shown that for finite 1D-PC, accurate calculations of the epm required a model which takes into account the limited number of unit cells and the absorption in the media. This paper gives for the first time such a model. The Bendickson *et al.* model generalized to lossy media [11,12] appears to be an efficient method of calculation of  $m^*$  via the photonic DOM. We have applied it to pure periodic structure but it is important to mention that it works well for quasi-periodic one such as Fabry-Perot resonator where defect states can occur [1,12]. This case will be considered in a forthcoming paper.

The concept of epm is likely very useful when considering scattering processes involving photons propagating in PCs since it should be introduced in the law of energy conservation. Among the involved scattering processes, there is the Raman scattering in microcavity. Optical-phonon Raman scattering enhancement has been reported in semiconductor planar cavity [14] and Bragg-Raman scattering has been observed in the soft-x-ray domain with a La/B<sub>4</sub>C Bragg superlattice [15]. The main features of the latter process have been accounted for by considering the conservation of momentum and energy but the outgoing Raman photon was considered as a “massless” photon. A calculation done with the introduction of the epm of the outgoing Raman photon in the value of its energy (Eq.(8)) is under way. We guess that this study can be a test for the validity of the epm concept.

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