Omnidirectional band gaps in quasiperiodic photonic crystals in the THz region

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Abstract

In this work we calculate the emittance spectra of the electromagnetic radiation normally and obliquely incident (s- and p-polarized modes) on a one-dimensional multilayer quasiperiodic photonic structure made up by layered system of positive (SiO₂) and negative (LiTaO₃) refractive index materials organized in a quasiperiodic (Fibonacci-like) fashion. We model the negative refractive index material by an effective medium, whose electric permittivity ε(ω) is characterized by a phonon-polariton frequency dependent dielectric function, while for the magnetic permeability μ(ω) we have a Drude-like frequency-dependent function. The emittance spectra are determined by means of a well known theoretical model based on Kirchhoff’s second law, together with a transfer matrix formalism. Our results shows that the omnidirectional band gaps appear in the THz regime, in well defined frequency intervals independently of the electromagnetic radiation’s polarized modes.

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1. Introduction

Photonic crystals (PCs) are structures characterized by the periodic spatial variation of their refractive index and the consequently periodic spatial variation of their dielectric function [1]. These PCs can generate spectral regions, named photonic band gaps (PBGs), where the electromagnetic waves with frequencies falling within the PBG regime cannot propagate through them. In other words, like electrons that cannot exist in a stable state within regions of forbidden energy of an ionic crystal, due to the periodicity of the electronic potential, light of a certain wavelength cannot propagate in photonic crystals, due to the periodicity of their refractive index. A large number of recent studies utilize the unique features of these modulated structures to control and improve the optical and radiative properties for specific applications, opened up opportunities for controlling the absorption and radiation spectrum of man-made materials through various physical effects. Among them, we can cite surface plasmons [2], resonant-cavity enhancement [3], Bragg reflection [4–6], and modification of photonic density of states [7].

A very interesting example of a photonic crystal are the so-called metamaterials, artificial materials engineered to have properties that may not be found in nature. Usually these properties come from their structure rather than their composition, using small inhomogeneities to create effective macroscopic behavior. There are many types of metamaterials [8], the most famous of them being the electromagnetic metamaterials, which are materials with negative refraction index (NRI) [9]. They can be artificially fabricated with periodic metallic structures, whose length of the period is smaller than the wavelength at which the non-usual properties occur [10]. In the optical domain, these materials should have dimensions in the micrometer range or less, and they can be fabricated easily in the microwave region [11,12]. Besides, they have exotic properties, like negative refraction in the Snell’s law, reversed Doppler shift, reversed Cherenkov radiation, etc.

On the other hand, since the discovery of quasicrystals by Shechtman et al. [13], the physical properties of a new class of artificial materials, the so-called quasiperiodic structures, have attracted a lot of attention, mainly in the last two decades. These quasicrystals are formed by the superposition of two (or more) incommensurate periods, so that they can be defined as intermediate systems between a periodic crystal and the random amorphous solids. A common (and more fascinating) feature of these structures is a fractal spectra of energy, forming a Cantor set, which is their basic signatures (for a review see Ref. [14]).

Theoretical and experimental studies on the propagation of light through periodic and quasiperiodic photonic crystals containing NRI materials, have shown the existence of a zero effective phase gap, which is omnidirectional and insensitive to disorder [15–17]. In these works, in general, the material with NRI is modeled by a plasmonic (Drude-like) frequency-dependent electrical permittivity ε and magnetic permeability μ function, leading to band gaps that are restricted to the GHz frequency...
Looking for an emittance spectrum in the THz region, instead of in the GHz region already discussed in previous publication [33], we model each layer of the NRI material by an effective medium formed by a periodic array of metallic split ring resonators, characterized by a polaritonic medium LaTiO₃, whose electric permittivity \( \varepsilon \) is a phonon-polariton frequency-dependent function, keeping the Drude-like function for the magnetic permeability response \( \mu \) [34,35]. The emission spectra of the thermal radiation in these multilayered structures are determined by using a theoretical model based on Kirchhoff's second law, together with a transfer matrix formalism, which simplify enormously the algebra [33].

This paper is organized as follows: in Section 2 we present the theoretical calculation based on the transfer matrix method to generate the thermal radiation spectra in the multilayered photonic structures. The numerical results are discussed in details in Section 3, while the conclusions are summarized in Section 4.

2. General theory

Consider the quasiperiodic multilayer structure, as depicted in Fig. 1. Layer A, with thickness \( d_A \), is fulfilled by SiO\(_2\), and is characterized by a positive refractive index \( \varepsilon_A = \sqrt{\varepsilon_{S0}\mu_A} \) and an impedance \( Z_A = \sqrt{\mu_A/\varepsilon_A} \), both constants. Layer B, with thickness \( d_B \), is fulfilled by the polaritonic metamaterial LaTiO\(_3\), and is characterized by a negative refractive index \( \varepsilon_B = \sqrt{\varepsilon_{S0}\mu_B} \) and an impedance \( Z_B = \sqrt{\mu_B/\varepsilon_B} \).

The multilayer structure is grown on an absorbing substrate S, with a constant refractive index \( \varepsilon_C \). The entire structure is embedded in a transparent medium C (considered to be vacuum) with a constant refractive index \( \varepsilon_C \).

A suitable transfer matrix method is employed to calculate the spectral properties of the optical quasiperiodic multilayer, organized in accordance to the Fibonacci quasiperiodic sequence [4]. This method consists of relating amplitudes of the electromagnetic fields in a layer with those of the previous one, by successive applications of Maxwell's electromagnetic boundary conditions at each interface along the multilayer system. Therefore, the transfer matrix relates the electromagnetic incident field amplitudes \( (A_{1C}^0, A_{2C}^0) \) of one side of the multilayer system (at \( z < 0 \)), with the

range [18]. Unfortunately, this type of model does not allow us to extend the frequency range for the THz regime by a simple change of scale, being necessary to consider another model for the NRI material, like a phonon-polariton response for the electric permittivity \( \varepsilon \).

Furthermore, the terahertz (THz) gap between high-frequency electronics (up to roughly 100 GHz) and low-frequency optics (down to roughly 10 THz) has stimulated intense investigation due to their potential applications, including imaging, security, spectroscopy and optical communication [19–21]. The first PC in the THz range was realized by Wu et al. [22]. Since then, PCs in the THz range have been intensively studied both experimentally [23–26] and theoretically [27,28]. In particular, THz photonic band gaps (PBGs) and interference filters in the one-dimensional PCs have attracted intense research, such as the tunability of the PBGs and the defect modes in the Terahertz PBG. On the other hand, omnidirectional terahertz mirrors [29], optical filters [30], optical switches [31], etc. Recently, Dai et al. [32] have studied a thermally tunable and omnidirectional THz photonic band gaps in the one-dimensional PCs, while the conclusions are summarized in Section 4.
transmitted amplitude $A_{21}^{n}$ of the electromagnetic field in the other side, at $z > 1$, $L$ being the size of the multilayer system (see Fig. 1), by means of the product of the interface matrices $M_{21}$ (with $\alpha, \beta$ being any $AB$ and $C$ media) and the propagation matrices $M_{i}$ ($i = A, B$ and $S$), as following [36]:

$$
\begin{pmatrix}
A_{11}^{n} \\
A_{21}^{n}
\end{pmatrix} = M_{C}M_{A}M_{AB}M_{B} \cdots M_{SB}M_{S} \begin{pmatrix}
A_{11}^{0} \\
0
\end{pmatrix},
$$

(1)

where

$$
M_{21} = \frac{1}{2} \begin{pmatrix}
1 + Z_{A}/Z_{B} & 1 - Z_{A}/Z_{B} \\
1 - Z_{A}/Z_{B} & 1 + Z_{A}/Z_{B}
\end{pmatrix},
$$

(2)

$$
M_{i} = \begin{pmatrix}
\exp(-ik_{i}d_{i}) & 0 \\
0 & \exp(ik_{i}d_{i})
\end{pmatrix},
$$

(3)

with $k_{ij} = \eta_{ij}c/\epsilon$.

The above matrices were obtained for the normal incidence case. For the oblique incidence one, we should replace $Z_{A} \rightarrow Z_{A}/\cos \theta_{s}$ for $s$-polarization or $TE$ mode, and $Z_{B} \rightarrow Z_{B}/\cos \theta_{p}$ for $p$-polarization or $TM$ mode in the interface matrices $M_{21}$, as well as $\eta_{i} \rightarrow \eta_{i}\cos \theta_{i}$, for both TE and TM polarizations in the propagation matrices $M_{i}$. Here $\theta_{s,p}$ is the angle of incidence of the light beam in the layers $a,b$, with respect to the $z$-axis.

The reflectance $R(\omega)$ and the transmittance $T(\omega)$ coefficients are simply given by

$$
R(\omega) = \left| M_{21} \right|^{2} \quad \text{and} \quad T(\omega) = \left| 1/M_{21} \right|^{2},
$$

(4)

where $M_{ij}$ $(i,j = 1,2)$ are the elements of the optical transfer matrix $M = M_{C}M_{A}M_{AB}M_{B} \cdots M_{SB}M_{S}$. As we can see, the ordering of these matrices in the product depends upon the generation number of the Fibonacci quasiperiodic structure. The transfer matrices of the Fibonacci structure considered here can be straightforwardly determined (for details see Ref. [6]).

If no absorbing material is introduced in the multilayer system (lossless medium), then $R(\omega) + T(\omega) = 1$ by conservation of energy. When we introduce a material with complex refractive index (material with absorption), $R(\omega)$ and $T(\omega)$ can be used to define a real absorbance by $A(\omega) = 1 - R(\omega) - T(\omega)$, which is again a statement of conservation of energy. However, from Kirchhoff’s second law, we know that the ratio of the thermal emittance $E(\omega)$ to the absorbance $A(\omega)$ is a constant, independent of the nature of the material, being the unity when the source is a perfect blackbody [37,38]. Hence, $E(\omega) = A(\omega)$, and therefore

$$
E(\omega) = A(\omega) = 1 - R(\omega) - T(\omega).
$$

(5)

In this way, by considering the Eqs. (1), (4) and (5), we can calculate the emittance $E(\omega)$ for any multilayer system with an absorbent substrate.

3. Numerical results

Considering the quasiperiodic multilayer structure in thermal equilibrium with its surroundings at a given temperature, we present now the numerical simulations for the spectral emissivity. The schematic geometrical representation of the multilayered photonic structure is shown in Fig. 1, considering medium $A$ as SiO$_2$, whose refractive index is $\eta_{A} = 1.45$, while medium $B$ (LiTaO$_3$) is an effective polaritonic metamaterial, considered to have a negative complex refractive index $\eta_{B} = \sqrt{\epsilon_{B} \mu_{B}}$. This multilayered photonic stack is embedded in the vacuum ($\eta_{v} = 1.0$), and is grown on an absorbing substrate 5, whose complex refractive index is given by $\eta_{S} = 3.0 + i0.03$. Its thickness is given by $d_{S} = 100\lambda_{0}/\eta_{S}$, $\eta_{S}$ being the real part of $\eta_{S}$. Here, the central wavelength $\lambda_{0}$ is considered to be 12.238 $\mu$m, that corresponds to the negative refractive index band central frequency for the LiTaO$_3$ [35].

A significant change in our results, compared with previous one, can be found if we use for the NIR medium the electrical permittivity of phonon-polariton character, defining a more realistic polaritonic medium and producing a much complex emission pattern, i.e.:

$$
\epsilon_{B}(\omega) = \epsilon_{B} \left(1 + \frac{\omega_{0}^{2} - \omega_{0}^{2}}{\omega_{0}^{2} - \omega^{2} + 1F(\omega)} \right),
$$

(6)

$\omega_{0}(\omega_{0})$ being the longitudinal (transverse) optical phonon frequency.

The magnetic permeability $\mu(\omega)$ can be defined as a Drude-like function [34]:

$$
\mu_{B}(\omega) = 1 - \frac{\omega_{p}^{2}}{\omega^{2} - \omega_{p}^{2} + i\Gamma(\omega)}.
$$

(7)

We have considered for LiTaO$_3$, a typical polaritonic material extensively used experimentally, the following physical parameters for its electrical permittivity [35]: $\omega_{0}/2\pi = 26.7$ THz, $\omega_{0}/2\pi = 46.9$ THz, $\epsilon_{c} = 13.4$ and $\Gamma = 0.6$ THz. Regarding its magnetic permeability, we considered that the fraction $F$ is determined only by the geometry of the lattice rather than by the charge, effective mass and density of electrons, as is the case in naturally occurring materials, whose value is $F = 0.56$, motivated by the experimental work of Smith et al. [11]. Also, $\omega_{p} = 2\pi\lambda/\lambda_{0}$, and $\Gamma = 0$ neglecting any damping term (when lossy metamaterial is considered, the damping factor can be defined as a fraction of the resonant frequency $\omega_{0}$).

To identify the frequency region where layer $B$ (LiTaO$_3$) has negative refractive index, we showed in Fig. 2 the variation of its refractive index as a function of the frequency $\omega$ in THz. As it can be observed from this figure, the frequency region in which medium $B$ behaves as a metamaterial, with negative refractive index, is 161.64 $< \omega < 269.40$ THz.

Fig. 3 shows the calculated emittance spectra $E(\omega, \theta)$ for the periodic and quasiperiodic sequences as a function of the frequency $\omega$ and the incident angle $\theta = \theta_{0}$ (C is the vacuum where the light beam comes from). We have taken into account the same polarization, namely TE or $s$-polarized mode, in two distinct situations: the periodic case (Fig. 3a), and the ninth-generation of the Fibonacci quasiperiodic sequence (Fig. 3b), respectively. It is easy to see that the

![Fig. 2. Real and imaginary parts of LiTaO$_3$'s refractive index as a function of the frequency in THz.](image-url)
angular dependence for the periodic case presents one well defined band gap, with a spectrum more uniform than the quasiperiodic one. Observe that there exist two omnidirectional band gaps, i.e. gaps region where the emittance spectra $E(x, h)$ is zero. The first is characterized by a narrow region $231.68 < x < 284.79$ THz, for $h = 0/2$, where the band gap is greater than in the region $1.495 < x < 2.2$, for $h = 90/2$, showing that the width of the band gap depends on the angle. The second omnidirectional band gap is in a very thin frequency region $153.94 < x < 161.64$ THz. On the other hand, in the frequency region $0 < x < 153.94$ THz, we have a smooth dependence with the angle, going from the central top of the spectrum at $\omega = 15.39$ THz, $\theta = 0^\circ$ and $E(\omega, \theta) = 0.6$, to the bottom of the spectrum, at $\omega = 153.94$ THz, $\theta = 0^\circ$ and $E(\omega, \theta) = 0.02$.

For the quasiperiodic structure (Fig. 3b), we observe that there are two large regions exhibiting omnidirectional band gaps: the first one is in the frequency region $70.81 < x < 153.94$ THz, while the second one is in the frequency region $230.91 < x < 284.79$ THz. We can note that in the latter region the band gap is more narrow, for $\theta = 0^\circ$, when compared with the gap in the frequency region $230.91 < x < 338.67$ THz, for $\theta = 90^\circ$. Also we observe

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Fig. 3. TE mode ($s$-polarized electromagnetic wave) of the emittance spectra $E(\omega, \theta)$ as a function of the frequency $\omega$ (in THz) and the incident angle $\theta$, considering medium B with a frequency-dependent negative refractive index, whose dielectric function has a phonon-polariton character: (a) the periodic case; (b) the ninth-generation of the Fibonacci quasiperiodic sequence; (c) amplification of (b) in the frequency region $0 < \omega < 0.6$.

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a fragmented spectrum at the high-frequency region, totally distinct of the contour lines that defines the surface seen in Fig. 3a in the same region. Other interesting aspect of the emittance spectra \( E(\omega, \theta) \) for the quasiperiodic case can be observed in the region \( 0 < \omega < 70.81 \) THz where, differently of the periodic case, it is possible to see the existence of tiny gaps. A detailed amplification of this region can be seen in Fig. 3c. Note the existence of very narrow omnidirectional band gaps at low-frequency centered at \( \omega = 38.49 \) THz; 42.33 THz; 49.26 THz; 64.65 THz and 69.27 THz.

Besides, there is another larger omnidirectional band gap in the region \( 50.03 < \omega < 61.58 \) THz.

For the TM or \( p \)-polarized mode, the emittance \( E(\omega, \theta) \) versus \( \omega \) and \( \theta \) are plotted in Fig. 4. We have taken into account the same two distinct situations considered for the \( s \)-polarization case, namely the periodic case (Fig. 4a), and the ninth-generation of the Fibonacci quasiperiodic sequence (Fig. 4b), respectively. In Fig. 4a, the angular dependence presents a well-defined omnidirectional band gap, with a spectra more uniform than the quasiperiodic case depicted in

**Fig. 4.** Same as in Fig. 3 but for the TM mode (\( p \)-polarized electromagnetic wave).
Fig. 4b, but very similar to the s-polarized mode (see Fig. 3a). It is also observed a narrow gap in the frequency region 230.91 < ω < 284.79 THz, for θ = 0°, in comparison with the high-frequency region 230.91 < ω < 323.247 THz, for θ = 90°. On the other hand, in the region 0 < ω < 153.94 THz, we have two peaks with the maximum emittance, corresponding to E (0.25,60°) = 0.98, and E(0.25,−60°) = 0.98, respectively, decreasing smoothing until its minimum value, corresponding to E(0,θ) = 0, for ω = 153.94 THz, and θ = 90°. The quasiperiodic emittance spectrum have also two omnidirectional band gaps with similar characteristics, concerning to the angular dependence. In the frequency region 0 < ω < 89.29 THz, it is possible to observe the existence of tiny gaps.

The amplified detail of the narrow regions at low frequencies, centered at the middle of the frequencies ω = 80.82 THz and 86.98 THz, and the band gap localized in the frequency region 63.12 < ω < 73.89 THz, are depicted in Fig. 4c. Comparatively, Figs. 3 and 4 present differences with respect to the polarizations, mainly in the low-frequency region. Note that for the p-polarized mode, the emission spectrum is much intense than the s-polarized mode. Besides, the spectra are completely distinct in the frequency region 46.18 < ω < 92.36 THz. While the s-polarized mode is characterized by an absence of thermal emission in the region 50.03 < ω < 61.58 THz, the p-polarized mode, on the contrary, emits intensely in this frequency region. In the frequency range, 61.58 < ω < 73.89 THz the s-polarized mode shows an alternation of peaks and dips in the thermal emittance spectrum, while for the p-polarization mode there is a band gap in the same range of frequency, the alternation of peaks and dips being evident at 73.89 < ω < 89.29 THz.

In a general way, the periodic case shows qualitative difference between the s- and p-polarizations, which means that the spectra are very sensitive to the geometry of the structure. Moreover, the Fibonacci quasiperiodic structure presents a more fragmented spectrum in comparison with the periodic case, due to its higher degree of disorder (or fractality). By controlling the incidence angle on the structure, in the periodic case, we can tune the frequency range and the width of this omnidirectional band gaps, while in the quasiperiodic case we have an additional parameter to control the band gaps: the generation of the sequence, not explored here. In both case, we have an omnidirectional PBG that will offer many prospects for omnidirectional THz optical switches, optical filters and other optical devices. Finally, new devices based on periodic or quasiperiodic polaritonic crystals may be designed in a near future.

4. Conclusions

In summary, we have investigated the emittance behavior of light waves in one-dimensional multilayers photonic crystals, in which one of the layers is fulfilled by a NRI polaritonic materials, considering a periodic and a quasiperiodic arrangement. To model the NRI material we have proposed an effective medium model the NRI material we have proposed an effective medium. Considering a periodic and a quasiperiodic arrangement. To model the NRI material we have proposed an effective medium. Considering a periodic and a quasiperiodic arrangement.

band filters designed using hybrid periodic/quasiperiodic one-dimensional photonic crystals in microwave domain. Therefore, our result can be extended to include these hybrid systems in the THz regime. Besides, the periodic case shows only qualitative difference between the s- and p-polarizations, in regions out of the omnidirectional band gap, which means that the spectra are very sensitive to the geometry of the structure. Moreover, the ninth Fibonacci quasiperiodic generation presents a more fragmented spectrum in comparison with the periodic case, due to its higher degree of disorder (or fractality). By controlling the incidence angle on the structure, in the periodic case, we can tune the frequency range and the width of this omnidirectional band gaps, while in the quasiperiodic case we have an additional parameter to control the band gaps: the generation of the sequence, not explored here. In both cases, we have an omnidirectional PBG that will offer many prospects for omnidirectional THz optical switches, optical filters and other optical devices. Finally, new devices based on periodic or quasiperiodic polaritonic crystals may be designed in a near future.

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References

[34] H.V. Shadrivov, A.A. Sukhorukov, Y.S. Kivshar, Appl. Phys. Lett. 82 (2003) 3820.