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Band structure of one-dimensional photonic crystal with graphene layers using the Fresnel coefficients method

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In this paper, we have calculated the band structure of an instance of one-dimensional photonic crystal (1DPC) composed of double-layered dielectrics via the Fresnel coefficients method. Then, we supposed the addition of a thin layer of graphene to each dielectric layer and the given photonic crystal (PC) composed of dielectric–graphene composites. The effects of graphene layers on the PC band structure were evaluated. We found out that according to the effective medium theory unlike the TE polarization, the electric permittivity of the dielectric layers changed at TM polarization. As such, the band structure of PC for TM polarization changed, too. Moreover, instead of bandgap related to "zero averaged refractive index" an approximately omnidirectional bandgap appeared and a related bandgap to "$\varepsilon = 0$" disappeared. In addition, a new angular gap branch appeared at a new frequency at TM polarization in which the width of gap increased as the angle increased.

Keywords: Photonic crystals; band structure; Fresnel coefficients method; effective medium theory; graphene.

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1. Introduction

Photonic crystals (PCs) are composed of periodic dielectric layers that affect the propagation of electromagnetic waves in a way similar to that by which a periodic potential affects electrons in semiconductors. Metamaterials (MMs) are a new class of materials that possess a negative refractive index. The "zero averaged refractive index" gap appears in multi layers composed of conventional materials with

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positive refractive index and MMs with negative refractive index. Because of periodicity of the refractive index in PCs, the specific areas of wavelength that cannot be propagated within the crystal are known as PC bandgap wavelengths.[1–5] One-dimensional (1D) PCs can be fabricated from accumulated layers. Two-dimensional (2D) PCs can be fabricated via photolithography or by drilling holes in an appropriate substrate. The fabricated methods for three-dimensional (3D) PCs are drilling at different angles and stacking multiple 2D layers on top of one another.[1–5] The interest in PC bandgaps stems from their application in various researches and technological areas such as filters, waveguides, optical switches and cavities.[6–11] The PC concept was introduced by Yablonovitch and John in 1987.[12,13] In many previous papers, the band structure of different PCs has been calculated by transfer matrix method. A few points on omnidirectional bandgaps in 1D PCs were provided.[14] Differential transfer matrix method for photonic band structure of 1D nonuniform distribution plasma PCs was discussed.[15] Photonic band structure solved by a plane wave-based transfer-matrix method was carried out.[16] Ultra-wide low-frequency bandgap of 1D superconducting PCs containing MMs was also investigated.[17] Zero permeability and zero permittivity bandgaps in 1D MM PCs were studied[18] along with the omnidirectional gap and defect mode of 1D PCs with single-negative materials.[19] The terahertz (THz) technologies with applications in biosensing, forensic investigations and imaging have attracted significant attention.[20,21] Most natural materials basically absorb THz radiation and thus are not appropriate for THz applications. Contrariwise, MMs can offer better solutions for THz applications.[22,23] MMs are composed of periodically placed resonating metal–dielectric composites with unit cells much smaller than the operating wavelength. In this paper, we have calculated the band structure of an instance of 1D PC composed of double-layered dielectrics with specific optical characteristics by Fresnel coefficients method. Then, we extended our calculations on a band structure in the presence of a thin layer of graphene which is added to each layer of dielectrics and the given PC composed of dielectric–graphene composites. We suppose these composites as a quasihomogeneous medium. Under these circumstances, we consider the aforementioned PC as a PC with graphene layer. Among both scientific and engineering communities, research on graphene has been expanded because of its unique electron transport and extensive applications in optics, electronics and nanomechanics.[24–28] Carbon atoms in graphene are arranged in a planar honeycomb lattice based on a 2D atom-level-thick sheet. So, charge transport in graphene can be characterized as a 2D electronic system.[29–31] We have evaluated the effect of graphene layer on the PC band structure. We know that according to the effective medium theory, the presence of graphene layers change the electric permittivity of dielectric layers.[32] We found out that in the presence of graphene layers, the band structure of PC is changed at TM polarization. But at TE polarization, no changes are observed.

This paper consists of four sections; in Sec. 2, we mention the basic considerations of Fresnel coefficients method for calculating the PCs band structure. In the

third section, we calculate and compare the band structure of a PC composed of double-layered dielectrics by considering the effect of a graphene layer added to each dielectric layer. The paper concludes in Sec. 4.

2. Basic Considerations

We used the Fresnel coefficients method for calculating the PC band structure in our study. Unlike the transfer matrix method, we don't consider any hypothesis about the periodicity of the system. In Fresnel coefficients method, the refractive indices of each layer of dielectrics and the initial incident light angle are used to acquire the Fresnel coefficients. By using these coefficients, the transmission and reflection coefficients of the crystal can be determined. So, we can calculate the necessary and sufficient conditions for 100% reflection from crystal surface [Eqs. (1) and (2)]. Therefore, the band structure of the PC can be determined as follows[33-36]:

$$\frac{(\rho_1 - \rho_2)^2}{(1 - \rho_1^2)(1 - \rho_2^2)} \sin \Delta_1 \sin \Delta_2 > \cos^2 \left(\frac{\Delta_1 + \Delta_2}{2} \right), \tag{1}$$

$$\frac{(\rho_1 - \rho_2)^2}{(1 - \rho_1^2)(1 - \rho_2^2)} \sin \Delta_1 \sin \Delta_2 < -\sin^2 \left(\frac{\Delta_1 + \Delta_2}{2} \right), \tag{2}$$

where ρ is the Fresnel reflection coefficient from the dielectric upper layer and Δ is the single-path phase shift and is defined as

$$\Delta = 2\pi \left(\frac{d}{\lambda_0} \right) \sqrt{n^2 - \sin^2 \theta} \tag{3}$$

in which n and d are the refractive index and thickness of each dielectric layer, respectively, and θ is the initial incident angle on the crystal surface. In Eqs. (1) and (2), indices 1 and 2 in quantities ρ and Δ are related to the first and second layers of dielectrics, respectively. Using Fresnel reflection coefficients and Eqs. (1) and (2) we have

$$G_{s,p}(n_1, n_2, \theta) \sin \Delta_1 \sin \Delta_2 > \cos^2 \left(\frac{\Delta_1 + \Delta_2}{2} \right), \tag{4}$$

$$G_{s,p}(n_1, n_2, \theta) \sin \Delta_1 \sin \Delta_2 < -\sin^2 \left(\frac{\Delta_1 + \Delta_2}{2} \right), \tag{5}$$

where

$$G_s(n_1, n_2, \theta) = \frac{1}{4} \sqrt{\frac{n_1^2 - \sin^2 \theta}{n_2^2 - \sin^2 \theta}} + \frac{1}{4} \sqrt{\frac{n_2^2 - \sin^2 \theta}{n_1^2 - \sin^2 \theta}} - \frac{1}{2}, \tag{6}$$

$$G_p(n_1, n_2, \theta) = \frac{1}{4} \left(\frac{n_2}{n_1} \right)^2 \sqrt{\frac{n_1^2 - \sin^2 \theta}{n_2^2 - \sin^2 \theta}} + \frac{1}{4} \left(\frac{n_1}{n_2} \right)^2 \sqrt{\frac{n_2^2 - \sin^2 \theta}{n_1^2 - \sin^2 \theta}} - \frac{1}{2}. \tag{7}$$

Labels s and p are related to the TE and TM polarization of incident light. Equations (4)–(7) are the fundamental relations for calculating the band structure of 1D PCs by Fresnel coefficients method.

3. Results and Discussions

In this section, the band structure of the aforementioned PC is calculated, taking the graphene layers into consideration.

For the extension of our theory, we consider the optical characteristics of PC as follows:

$$
\left.\begin{array}{c}
\varepsilon_0 = \mu_0 = 1, \quad \varepsilon_2(f) = 1 + \dfrac{5^2}{0.9^2 - f^2} + \dfrac{10^2}{11.5^2 - f^2}, \quad \varepsilon_1 = \mu_1 = 1, \\[12pt]
\mu_2(f) = 1 + \dfrac{3^2}{0.902^2 - f^2}, \quad d_1 = 12 \text{ nm}, \quad d_2 = 6 \text{ nm},
\end{array}\right\}
\tag{8}
$$

where f is the incident light frequency in THz. d_1 and d_2 are the thickness of the first and second layers of dielectrics, respectively. At some frequencies the second layer of dielectrics becomes a MM. So, the "zero averaged refractive index" gaps appear in the PC band structure in both polarizations.

A monolayer graphene sheet is an infinitesimally thin conductive layer and its surface conductivity can be determined using a semiclassical quantum mechanical approach.[30,31]

In single-layer 2D PCs, it isn't necessary to consider the effective thickness of graphene layers. However, as the instance we have considered, in 1D double-layered PCs the thickness of graphene layers should be considered.[37] We suppose that the graphene layer has a finite thickness Δ. For which Δ is very small in comparison with the thickness of dielectric layers and it is ignorable. The incident light propagating inside the graphene layer follows $\mathbf{\nabla} \times \mathbf{H} = -i\omega\varepsilon_0\mathbf{E} + \mathbf{J} = -i\omega\varepsilon_0\varepsilon_g\mathbf{E}$, where the effective relative permittivity of graphene layer is ε_g and $\mathbf{J} = \frac{\mathbf{E}_{\parallel}\sigma}{\Delta}$. The $\mathbf{E}_{\parallel}$ is the component of electric field along the graphene surface and σ is the surface conductivity of graphene layers. It is known that the effective medium theory is an important approximate theory. Some of the fundamental requested approximations in this theory are quasistatic and linear approximations.[32] As it can be seen in Eq. (8), we suppose that the thickness of dielectric layers are in order of 10^{-8}, -10^{-9} and the thickness of graphene layers are in order of 10^{-10}. The dielectric layers are thick in comparison with graphene layers. So, there is no interaction between graphene layers. Also, the thicknesses of dielectric layers are smaller than the wavelength of the operating field. As a result, the effective medium theory can be used for the evaluation of multilayer graphene–dielectric composite.

According to the effective medium theory, by considering the fact that graphene sheets have negligible thickness compared to that of the dielectric layers, the added graphene layers will change the electric permittivity of dielectric layers as[32]

$$
\varepsilon'_{K\parallel} = \varepsilon_k + \frac{i\sigma}{\omega\varepsilon_0 d_k}, \quad k = 1, 2,
\tag{9}
$$

where $k = 1, 2$ refers to the layers of dielectrics. $\varepsilon'_{k\parallel}$ is the effective electric permittivity of the dielectric layers by considering the effect of added graphene layers for TM polarization of incident light. ε_k is the electric permittivity of layers without

considering the effect of graphene layers. d_k is the thickness of each layer of dielectrics. The surface current density of graphene layer depends on the component of electric field along the graphene surface. So, in TE polarization, the graphene layers don't change the electric permittivity of the dielectric layers.

According to the Drude–Boltzmann formula, Graphene's conductivity can be written as[38]

$$\sigma = \frac{2e^2 \kappa_B T}{\pi \hbar^2} \ln \left[2 \cosh \left(\frac{E_F}{2\kappa_B T} \right) \right] \frac{i}{\omega + i2\Gamma}, \tag{10}$$

where e is the electron's charge, κ_B is the Boltzmann's constant, T is the absolute temperature, $\hbar$ is the reduced Planck's constant, E_F is the Fermi energy in graphene, ω is the angular frequency and Γ is the phenomenological scattering rate. We suppose that $T = 300$ K and $\Gamma = 0.1$ meV.

In Figs. 1(a) and 1(b), we plotted the μ_2 and ε_2 as a function of the radiation field frequency, respectively.

Now, we calculate the band structure of PC using the optical characteristics of crystal and Eqs. (1) and (2) in both TE and TM polarizations.

The "zero averaged refractive index" gaps appear in the PC band structure for both TE and TM polarizations when $\mu(\omega)$ or $\varepsilon(\omega)$ change their signs. At frequencies where $\varepsilon = 0$, a gap occurs for TM polarized waves. Moreover, at the frequencies in which $\mu = 0$, a gap occurs for TE polarized waves.[39–42]

The initial frequencies of bandgaps related to $\mu = 0$ and $\varepsilon = 0$ in Fig. 2 are compatible with diagrams of ε_2 and μ_2 in Fig. 1.

In both TE and TM polarizations, the lower branch of bandgaps in Figs. 2(a) and 2(b) is related to "zero averaged refractive index". Although in TM polarization the width of this gap decreases as the angle increases, in the TE polarization case the width of the gap remains constant with angle variation.
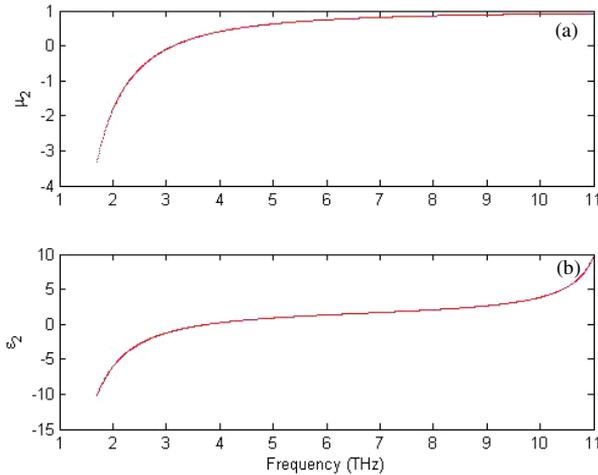

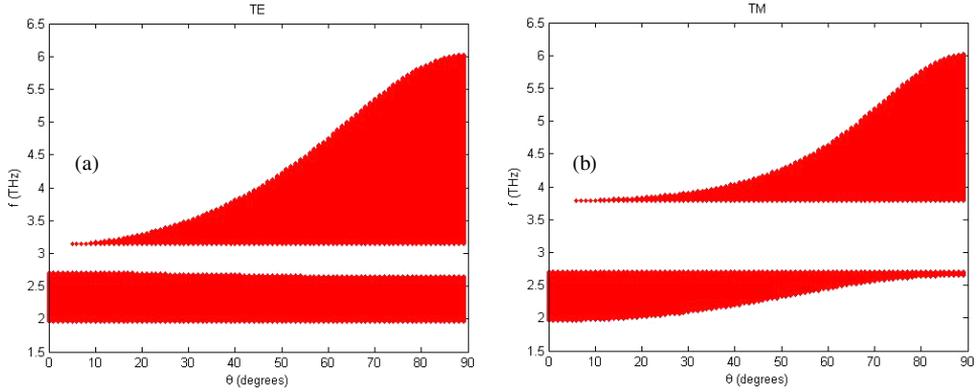Fig. 1. (Color online) Diagrams in terms of frequency for: (a) μ_2 and (b) ε_2.

Fig. 2. (Color online) The PC band structure for: (a) TE polarization and (b) TM polarization.

The upper branch gap relates to the "zero permittivity" in TM polarization for which the width of the branch increases as the angle increases. Instead of this gap, we observe a gap branch related to "zero permeability" in TE polarization where its width increases as the angle increases.

Now, we calculate the PC band structure by considering the effect of graphene layers. Regarding the optical characteristics of PC [Eq. (8)], just the amounts of both ε_2 and ε_1 change as Eq. (9).

As it has been mentioned concerning TE polarization, the addition of graphene layers does not change the electrical permittivity of the layers. Thus, according to Figs. 3(a) and 2(a), the PC band structure also does not change in this case. But in the case of TM polarization, the addition of graphene layers changes the electrical permittivity of the layers. The comparison of Figs. 3(b) and 2(b) shows that the PC band structure has changed. Instead of the "zero averaged refractive index" gap an approximately omnidirectional bandgap appears in the same frequency area
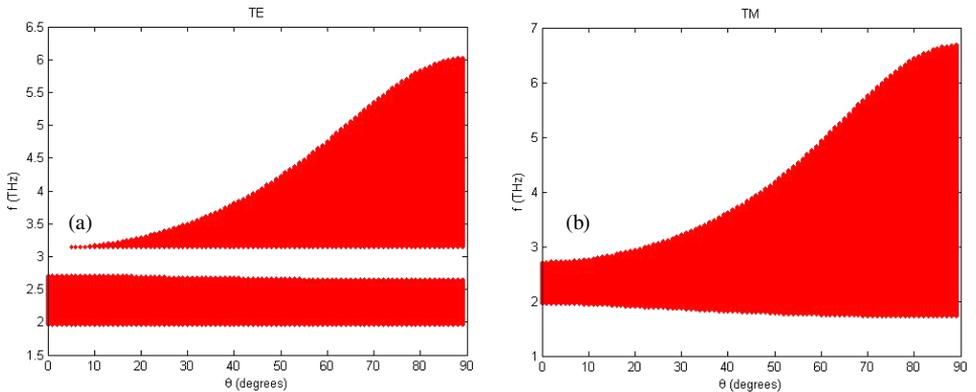

Fig. 3. (Color online) The PC band structure with the effect of graphene layers for: (a) TE polarization and (b) TM polarization.

in which the gap's width remains approximately constant with angle variations. The gap band related to "$\varepsilon = 0$" is omitted. A new branch of bandgap appears around 3 THz at TM polarization for which the gap's width increases as the angle increases. But at TE polarization there no change. As it can be seen in Fig. 3(b), the omnidirectional and angular branches of bandgaps are connected to each other.

4. Conclusions

In short, in this paper we have calculated the band structure of a 1D PC composed of double-layered dielectrics with specific optical characteristics, considering the graphene layers added to each layer of dielectrics. We have evaluated the effect of these added graphene layers on the PC band structure. Because of added graphene layers that change the electric permittivity of dielectric layers at TM polarization, the PC band structure also changes in this case. We found out that the gap related to "zero averaged refractive index" is replaced with an approximately omnidirectional bandgap. The gap related to "$\varepsilon = 0$" is eliminated while a new gap is created around 3 THz. As the angle increases, the width of this gap also increases. Moreover, the mentioned gap is connected to omnidirectional bandgap. At TE polarization, the added graphene layers don't affect the electric permittivity of dielectric layers. So, the band structure of PC at this polarization doesn't change at two states. We should mention that the aforementioned changes are true about the proposed specific PC not about the general ones.

Acknowledgments

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