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Reflection peaks variations in multiwall carbon nanotube photonic crystal array

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ABSTRACT

In this paper we analyze the effects of material characteristics (metallic behavior) and the periodicity of dielectric function, on the reflection peaks in a defected two-dimensional multiwall carbon nanotube (MWCNT) photonic crystal, for photon frequencies up to 10 THz. The simulation results show that, the second peak amplitude depends on both material and periodicity changes of the structure, whereas the previous report shows the mentioned dependence only on the material characteristics of structure. It should be noted that, the first and third (Bragg) peaks are dependent only on the material characteristics and the dielectric periodicity, respectively.

1. Introduction

Photonic crystals (PCs) are composed of a periodic dielectric constant that affects the propagation of electromagnetic waves by defining allowed and forbidden photonic frequency bands [1]. The forbidden bands known as photonic band gaps (PBG) occur when the period of the PC structure is comparable to the incident light wavelength (Bragg scattering). The PBGs are due to strongly varying dielectric constants of the structure [2]. Due to the multiple light scatters a spectral gap may unfold where light is forbidden to propagate into the PC.

Carbon nanotubes (CNTs) have been of large interest in recent nanotechnology researches. These researches result in developing applications of CNT's optical, mechanical and electrical properties. Multi-wall carbon-nanotubes (MWCNTs) consist of multiple rolled layers of graphene [3]. Graphene has a two-dimensional "honeycomb" structure, made of sp^2-bonded carbon atoms [4]. Graphite (multiple rolled layers of graphene) has a layered structure and its optical properties are highly nonlinear and strongly anisotropic [5,6]. According to similarities of carbon bonds in the graphite and carbon nanotube structures, their dielectric functions are very similar [7]. The electric field oscillating perpendicular to the *c*-axis of graphite layer, has the same dielectric response function as of the electric field polarized along the nanotube axis. It should be noted that, in both cases, the electric field is perpendicular to the graphite optical axis. The dielectric response function of single-wall carbon-nanotubes (SWCNTs) is heavily dependent on the chirality (direction that graphite screen is rolled), while the MWCNTs have random chiralities [3].

In this work, we have presented a new approach for the analysis of the effects of material characteristics and the dielectric function periodicity in a two-dimensional MWCNT photonic crystal, on the ref lection peaks, in which the dependence of second reflection peak on both mentioned behaviors has been cleared.

The paper is organized as follows: Section 2 describes the theory of model. Section 3 presents the simulation results and the related discussions. Finally at Section 4, the main conclusions are presented.

2. Model

Taking into account the nonlinearity and photonic response of a 2D MWCNT square array, the finite-difference time-domain (FDTD) method [3,8] is used to evaluate the reflection and effective medium theory [9] in order to study the optical properties. The MWNTs are considered infinitely long and the incident light is assumed to be transverse magnetic (TM) polarized, in which the propagated light is perpendicular to the CNT's axis and parallel polarized w.r.t. it. With the TM polarization, the photonic band gap can be better opened in our MWCNT array structure [10]. Moreover, in the TM polarization, only the vertical component of dielectric function $\varepsilon_{\perp}(\omega)$ will be intended, which is used for the modeling of MWCNT dielectric function [3]. This modeling approach is a collection of several group works and is consistent

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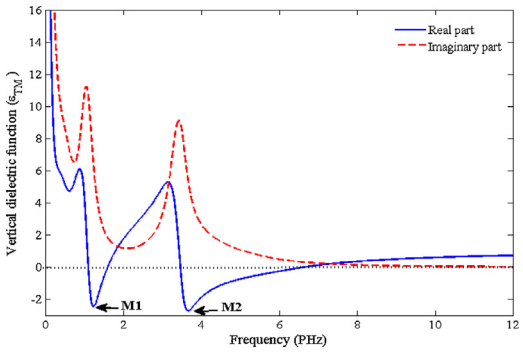

Fig. 1. The dielectric function of graphite for TM polarization.

with the Kramers–Kronig circumstances. These results have been fitted with a Drude–Lorentz model [11]

$$\varepsilon_{\perp}(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\omega/\tau} + \sum_{m=1}^{M} \frac{\sigma_m^2}{\omega_m^2 - \omega^2 - i\omega\gamma_m} \quad (1)$$

where ω_p is the free electron plasma frequency, τ is the relaxation time, ω_m is the transition frequency, σ_m is the oscillator strength and γ_m is the decay rate for Lorentz terms. The first term in (1) represents the Drude free electron and the second term shows the Lorentz oscillators corresponding to the inter-band transitions. To fit the parameters in (1) with the numerical method, a fitting with the static decay rates using $M = 7$ has been adopted from [8], which the related result for the dielectric function $\varepsilon_{\perp}(\omega)$ is shown in Fig. 1.

In our analysis that will be discussed in the next section, we have focused on the frequency range with Re $\{\varepsilon_{\perp}\}$ <0, which is related to the metallic bands. It should be noted that, the valleys of these bands are occurred at the transitions $M1$ and $M2$ in Fig. 1 which are ceased at the plasma frequencies of 1.6 and 6.6 PHz respectively, where at these points we have Re $\{\varepsilon_{\perp}\}$ =0.

According to [8], the comparison between the bulk graphite and MWCNTs for the reflection spectra clears that, both structures have peaks in the frequencies accompanied by $M1$ and $M2$ dips in the dielectric function of Fig. 1, such that these peaks are dependent only on the material characteristics (metallic behavior) of the MWCNT array. Also, the Bragg reflection peak has not been detected in the bulk reflection spectra and is clearly dependent on the photonic crystal arrangement. In this work, we have investigated the effects of metallic behavior and dielectric function periodicity on the mentioned three peaks of the reflection spectra.

3. Results and discussion

A 25 rows two-dimensional square array of MWCNT based photonic crystal with the lattice constant $a = 20$ nm has been considered for the analysis. For obtaining the periodic boundary condition, the MWCNTs are periodically repeated in the vertical direction. The input light is TM polarized and only $\varepsilon_{\perp}(\omega)$ in (1) is used to define the MWNTs optical properties.

Fig. 2 shows the reflection spectra for various outer radius values of MWCNTs. With the increase of outer radius, the filling ratio is increased and consequently, the reflection will be increased. The multiple scattering effects in the reflection spectra are occurred at the wavelength $\lambda \approx 2a < n >$ where $<n>$ is the average refractive index. For $a = 20$ nm, the Bragg scattering causes a Bragg reflection peak (third peak) nearly at $\lambda \approx 35$ nm which is corresponding to the frequency of ~8 PHz, and this result is consistent with the reported results in [8]. Regarding the two first peaks, it has been claimed that they are completely dependent on the MWCNTs metallization (substance). This means that the amplitudes of first and second

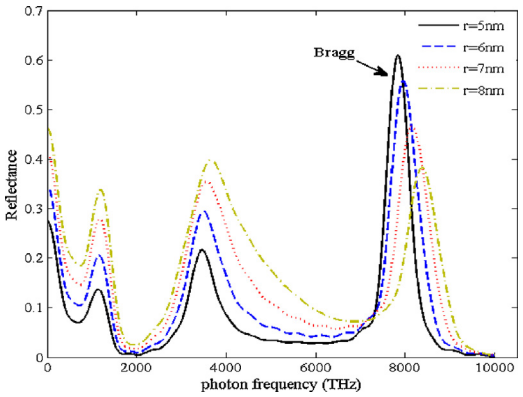

Fig. 2. The reflection spectra for a 25 rows MWCNT based photonic crystal with $a = 20$ nm and various outer radius values of MWCNTs.

reflection peaks will be constant for a fixed filling ratio because the percentage of metal in the lattice is not changed. Also since the periodicity of dielectric function is not changed, the Bragg peak amplitude will be unchanged.

In our simulations, the precision and correctness of above claim is investigated. With the change of dielectric function periodicity at constant filling ratio, the dependence of each peak's amplitude on the lattice arrangement could be examined. For this purpose, we have reshaped MWCNTs cross sections from circle to ellipsoid to have a fixed cross section area. With this work, the total amount of material is constant, but the dielectric function periodicity of photonic crystal will be changed.

The experimental results reported in [12] show how we can reshape MWCNTs cross sections in the photonic crystal array from circle to ellipsoid. This purpose could be achieved with the radial deformation of adjacent nanotubes due to the van der Waals forces between them. Choosing a suitable value for the photonic crystal lattice constant in one direction (x or y) such that the spacing between adjacent MWCNTs is equal to the van der Waals distance (≈3.4 nm), the ellipsoidal cross sections for all nanotubes in one direction would be achieved. Fig. 3 shows this achievement schematically.

Also in [13], the flattening of nanotubes in a CNT crystal under the van der Waals attraction against each other for the diameters over 25 Å has been investigated.

For evaluating the dependence of peaks on both the material characteristics (metallic behavior) and the periodicity of $\varepsilon_{\perp}(\omega)$ (ε_{TM}), a line defect is inserted into the lattice, which the related schematic view and the reflection spectra are shown in Fig. 4. As is cleared from Fig. 4(b), all of three peaks amplitudes will be changed with the insertion of line defect. This observation leads us to persuade for accepting that, the variations of material and $\varepsilon_{\perp}(\omega)$ periodicity leads to changes in the amplitudes of three discussed reflection peaks. Hereby, with the defect insertion, we have altered both the periodicity and amount of material.

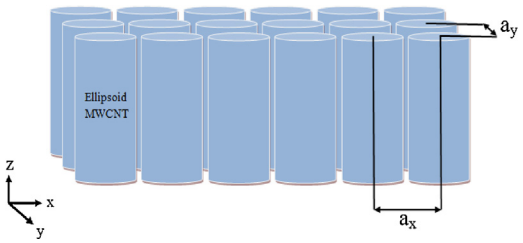

Fig. 3. The ellipsoidal cross sections for MWCNTs in the photonic crystal array using the radial deformation by the van der Waals forces.