

Simulation of the carbon nanotubes in the terahertz frequencies

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Abstract

Since little is known isolate a sheet of carbon-graphite one atom thick. This crystal is two-dimensional graphene has remarkable electronic transport properties, which are neither those of a metal nor those of a semiconductor. In this paper we have developed a novel structure electromagnetic bandgap (EBG), with a periodic arrays of carbon nanotubes presented, by introducing a multiwalled carbon nanotubes like a metallic viaholes. The electromagnetic bandgap (EBG) surface, also referred to as a photonic bandgap (PBG) surface, has attracted extensive studies, In the optical domain , microwave and millimeter-waveareas[1]. The method used is an integral method based on the concept of waves (WCIP).

Keywords: carbon nanotubes, EBG structure ,wcip method

1. Introduction

Molecular electronics is an emerging nano physics, promising to make new types of devices useful for both information storage quantum information. Among the nanostructures considered for the construction of a molecular electronics, the carbon nanotube is presented as a particularly promising candidate.

Since the articles reference S.Iijima early 90s, carbon nanotubes have been extensively characterized and found to be very interesting for the development of nanoelectronics due to their many remarkable properties.Nanotubes are nanometer diameter cylinders micron length, which can be seen as the winding of a sheet of graphite.

Their cylindrical shape and the particular electronic structure resulting make a rare experimental realizations of one-dimensional electronic system. The carbon nanotube is characterized by the helicity and he diameter of the tube, since these two parameters determine the periodic boundary conditions of the electronic wave functions. In this work we develop a new iterative method based

on wave concept (WCIP) to model a forest of multiwalled carbon nanotubes(MWCNT) fig-1.

2. Method and formulation

Multiwall carbon nanotubes sheet (MWCNT) consist of multiple graphene sheet (2 to 50) rolled

around each other. For this work, we chose multiwalled carbon nanotubes with diameters around of 2 and 25 nm.

The periodic structure have attracted much attention in recent years for promising application in the fields microelectronics, in this context and in order to respond to new needs of the modeling of planar circuits integrants passive elements that this work is situated.

Our approach will focus on the global modeling of periodic structure designed by carbon nanotubes, we introduce the iterative method denoted WCIP who is an integral method based on the concept of wave for solving electromagnetic scattering problems and analysis of planar circuits, it appeals to the fast fourier transform mode (FMT).

The passage between the spatial domain and the spectral domain is obtained by a 2D-FFT (also called Fast Modal Transform). This method depends on the manipulation of incident and reflected waves instead of electromagnetic field [2], [3].

Thus, method defines two operators in the spectral and spatial domain.

WCIP method uses easy equations to solve that with the integral method.

The main characteristic of periodic structures is to act as a device band-stop to remove undesirable electromagnetic waves in a certain frequency range Fig-1.



Fig-1 structure with via holes carbon nanotubes

The writing of electric field E_i and surface current density J_i in terms of incident and reflected waves are given by the following set of equations [2]:

$$E_i = \sqrt{Z_{0i}}(A_i + B_i)$$
 $J_i = \frac{1}{\sqrt{Z_{0i}}}(A_i - B_i)$ (1)

Where:

 A_i and B_i are two tangential vectors associated with the discontinuity interface $\boldsymbol{\Omega}$ Fig-2.

 J_i is the surface tangential current density.

- E_i is the tangential electric field.
- Z_{0i} is the intrinsic impedance of the two middles.

The nanotube structure is determined by the pair of integers (m, n) defining a feature vector of the winding called vector of chirality[4] [5]:

$$\overrightarrow{C_h} = n\overrightarrow{a_1} + m\overrightarrow{a_2}$$

$$d_t = \frac{C_h}{\pi} = a_{c-c} \frac{\sqrt{3}\sqrt{(n^2 + nm + m^2)}}{\pi} , \ a_{c-c} = 1.42 \text{ Å (2)}$$



Fig-2 Illustration of waves on both sides of the interface $\boldsymbol{\varOmega}$

3. Application

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In this study we present the influence of the number of carbon nanotubes(via holes) on the response of S-parameters and the influence of the distance between carbon nanotubes , to do this we chose to work with the number N of carbon nanotubes variant. The structure of geometric dimensions $a = b = 36\mu m$, the length of the carbon nanotube L = 16 μm and a diameter of 25nm Fig-4.



Fig-3 Scattering parameters for (L = $16\mu m$) and (L= $1\mu m$).

Fig-3 (a) shows the S-parameters as function of the frequency according to a structure formed by 1024

via holes the length of the via hole $L = 16\mu m$ and Fig-3 (b) chows the scattering parameters for $1\mu m$ of length.

We note in Fig-3 (b) no resonances in the frequency range of 2-20 THz this implies that more the length of the hole is small and more the resonant frequencies are away to above 20 THz values.

On Fig-4, we have the Scattering S parameters variation depending on the number of nanotubes present in the structure, however this number only affects the bandwidth so the diameter and the length of carbon nanotube can be considered as filter criteria.



Fig-4 Scattering parameters with variant number of nanotubes

4. Conclusion

In this article the EBG structure based on carbon nanotubes is characterized by an efficient numerical method based on wave concept iterative process (WCIP), mostly used for planar circuits. The simulation results obtained confirm that the parameters of the studied structure are filtering criteria.

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