

**Toward Plasmonic UC-PBG Structures based SWCNTs for Optoelectronics
Applications
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Abstract

In this paper, the possibility of performing UC-PBG layers that is constructed from a forest of Single Wall Carbon Nanotubes (SWCNT) are aligned vertically on a thin flat film of quartz is studied. Such study is concerned in plasmonic optoelectronic applications in the visible regime. The study is conducted to the numerical simulations based Finite Element Method (FEM), then, compared with measurements. Remarkable benchmarks are found in the performance of the proposed UC-PBG which can be summarized as: 1- excellent ability of focusing the light over a wide range of the visible bands, 2- low effective losses, 3- a miniaturized size of the numerical a preacher, 4- no spherical apparition due to the flat geometry. It is found the proposed UC-PBG shows an effective refractive index varies from 10 to 20 in Lorentz-Drude manner. The maximum induced power of the proposed UC-PBG is found to be around 450 nm. Nevertheless, the size of the proposed UC-PBG layer is 200nm×200nm. Finally, the obtained results are compared to another numerical analysis based on Finite Integral Technique (FIT). Excellent agreements are found between the two invoked numerical methods.

Key words: FIT, FEM, UC-PBG, SWCNT.

دراسة امكانية بناء هياكل حزم الفجوات الضوئية من مصفوفات انابيب الكربون النانوية الاحادية الجدران نحو تطبيقات الكهرو بصريات

طه احمد عليوي

قسم الاتصالات - كلية المأمون الجامعة - بغداد - العراق

الخلاصة

في البحث تم دراسة امكانية بناء وتصميم طبقات الـ(UC-PBG) من الأنابيب الكربونية النانوية ذات الجدران الاحادية الـ(SWCNT) والمصفوفة عموديا على طبقة رقيقة من الكوارتز. هذه الدراسة تصب في تطبيقات الكهرو بصريات بظاهرة الانتقال البلازمي. لقد أجريت الدراسة باستخدام المحاكاة العددية القائمة على طريقة الـ(FEM)، ثم مقارنتها مع القياسات العملية باستخدام التحليل الطيفي. لقد وجد عدة امور مهمة في أداء الـUC-PBG التي يمكن تلخيصها على النحو التالي: 1- قدرة ممتازة لتركيز الأشعة خلال حزم واسعة من ضمن النطاق الضوء المرئي، 2- الخسائر الناجمة من هذه المصفوفات كانت منخفضة جداً، 3- حجم الفتحة العددية مصغرة جداً، 4- لا وجود للزيغ الكروي بسبب الشكل المسطح. تم احتساب معامل الانكسار والذي كان يتراوح من 10 إلى 20. ان أعلى حد لنفاذ الاشعاع كان عند 450nm. ومع ذلك، فإن مساحة طبقة الـUC-PBG هو 200nm×200nm. وأخيراً، تم مقارنة النتائج التي تم الحصول عليها باستخدام تحليل عددي آخر قائم على أساس تقنية الـ(FIT) حيث وجد اتفاق جيد جداً بين الطريقتين.

الكلمات المفتاحية : التكامل العددي المتناهي، التفاضل العددي المتناهي، حزم الفجوات الضوئية، انابيب الكربون النانوية.

Introduction

In differ from small carbon fibers of conductive properties that are treated by traditional manufacturing techniques with limited availability and expensive costs [1]. Moreover, these difficulties are engaged to high dispersion degrees that continue to the carbon nanotube composites manufacturing challenges [2]. Currently, most conductive carbon nanotube solutions are performed in laboratories using chemical evaporation methods [3-6]. The solutions and curing agents properly vary with different polymer matrices [7]. Generally, this procedure includes dissolving polymers to form a solution mixed with carbon nanotubes diluted by the aid of ultra-sonication to create casting films or solid parts then subjected to a curing process [8]. However, most of these techniques reduce the real advancements in the

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electromagnetic properties of the SWCNTs when they are treated as bulk films not as ballistic conductors [1]. Therefore, to achieve more uniform SWCNTs dispersion in array forms and get the advantage of their ballistic properties at the individual ones, vertically aligned forests are subjected to the research [9-12]. In [9], electron beam evaporation on a thermal oxide layer of silicon substrate is used to grow the SWCNTs vertically with the aid of chemical vapor deposition plasma system. A controlled atomic diffusion-induced catalyst evolution on an aluminum thin-film substrate was introduced in [10] to grow vertically aligned carbon nanotube arrays by a conventional low-pressure thermal chemical vapor deposition. Vertical SWCNT arrays of a uniform distribution were grown by combining chemical vapor deposition and block copolymer lithography [11]. Synthesizing vertically aligned SWCNT arrays using a decoupled method that facilitates control of the growth efficiency of the heights to several millimeters was developed in [12].

Now with the current technologies, this paper discusses the hypothesis of constructing UC-PBG layers and the possibility of having them as the next generation in the optoelectronics applications. Nevertheless, this hypothesis is established very well by discussing the primary results and compares them to the published measurements for validations.

Electromagnetic Properties of an Individual SWCNT

The electromagnetic spectroscopy at the optical ranges for an individual SWCNT were studied experimentally as in [13-14] for an armchair SWCNT_{10,10} and SWCNT_{21,21}. In those results, the demonstration of a clear plasmonic signature due to the electrons transitions was reported. Now, to retrieve the dispersive refractive index, $n(\lambda)$, that to be used in this study, the same two suggested scenarios in [1-2] are used. However, the main difference, here, is the classical Sellmeier dispersion model without including any quantum effects accept the realistic geometry of an individual SWCNT_{10,10} is considered. The 3D bulk refractive index model based the third order Sellmeier dispersion model used is given as [15]:

$$n(\lambda) = \sqrt{1 + \sum_j \frac{(A_j/\lambda_j^2)}{(\frac{1}{\lambda_j^2}) - (\frac{1}{\lambda^2})}} \quad (1)$$

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A_j is the complex fitting parameter of materials [15]. To compute the required fitting parameters to obtain $n(\lambda)$, a Matlab retriever code is developed in this research based on an analytical calculation, [16], of the Scattering Cross Section (SCS) profile amplitude of the peak, spectral width, and the center wavelength at the maximum peak. For the actual geometry of an armchair SWCNT_{10,10} of radius of 0.678 nm, the HFSS and CSTMWS software packages are invoked to evaluate SCS in arbitrary unit (a.u.) and compare them with measured values. Nevertheless, the applied study of the SCS is independent of the plasmonic scatters length as proofed in [2]. In Figure (1), it is found an excellent agreement between the obtained results and measurements.

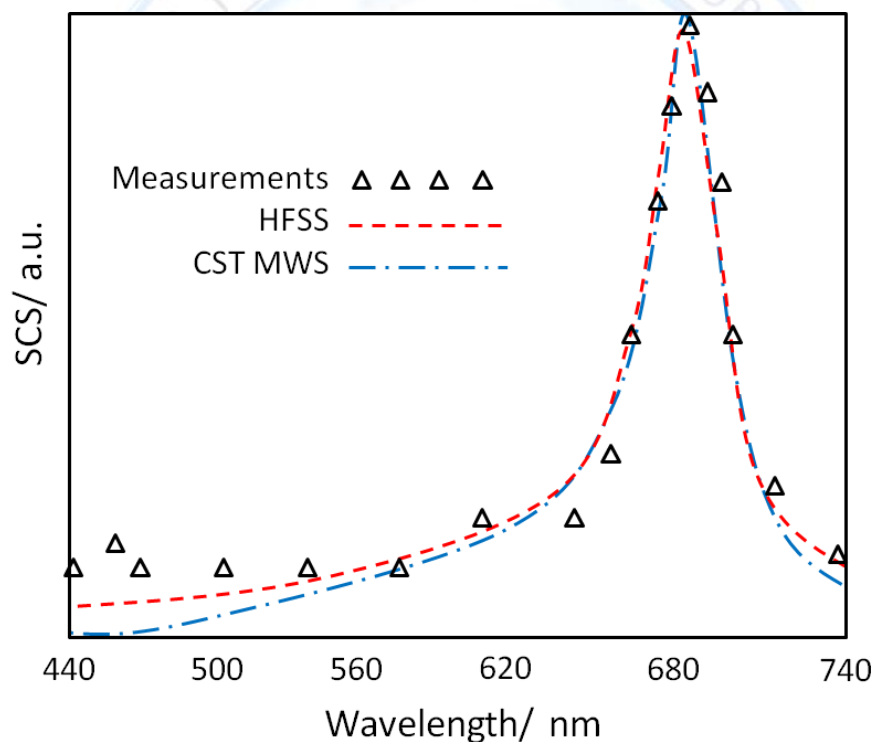


Figure 1: The numerical results of SCS verses measurements

The curve fitting parameters are: $A_1 = 0.2 - j0.34$, $A_2 = 1.6 + j0.45$, and $A_3 = -0.40 - j0.34$ that valid in the visible range only. The SWCNT length that used in this study is considered 10 nm.

SWCNT Arrays Electromagnetic Properties based Vertical Alignment

The electromagnetic properties in terms of the effective refractive index, n_{eff} , of the vertically aligned SWCNT arrays are retrieved in this section. The aim of that is to perform the effective surface that to be used later on to design the UC-PBG structure. Now, the SWCNT_{10,10} of length 10 nm are aligned in vertical arrays with a separation distance of 2 nm from center to center. This array is realized inside a virtual waveguide based on the effective medium theory [16] by applying the periodical boundary conditions along the length, where, the upper and lower faces are considered Perfect Electrical Conductor (PEC) and the other two sides are assumed Perfect Magnetic Conductor (PMC) as shown in Figure (2(a)). The excitations are applied at the two ends of the waveguide as wave ports. Figure (2(b)) displays the obtained scattering parameters, reflection and transmission, from both HFSS and CSTMWS.

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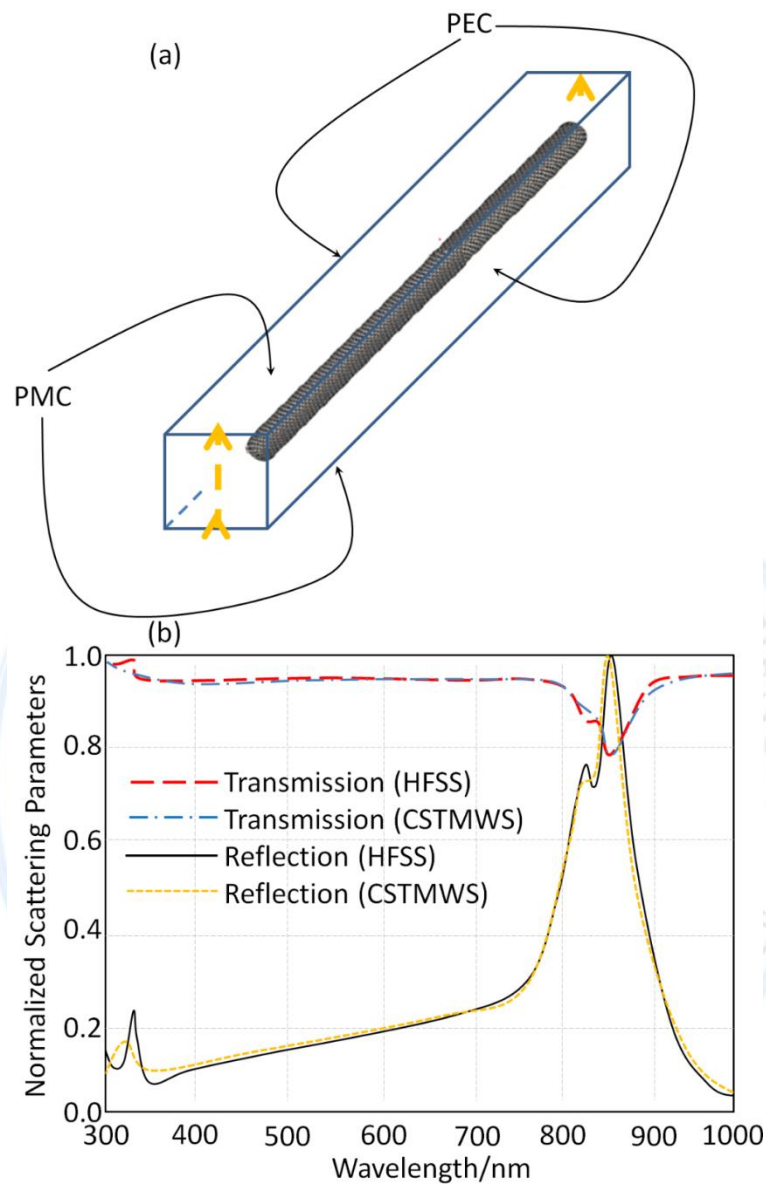


Figure 2: Vertical array of SWCNTs based HFSS and CSTMWS simulations; (a) The numerical setup, where, the yellow arrows are the excitation ports and (b) The obtained scattering parameters

Now, retrieving n_{eff} of the formed surface from the SWCNT arrays is presented in terms of real and imaginary parts as seen in Figure (3). It is found that n_{eff} of the proposed array follows Lorentz-Drude model during the visible range.

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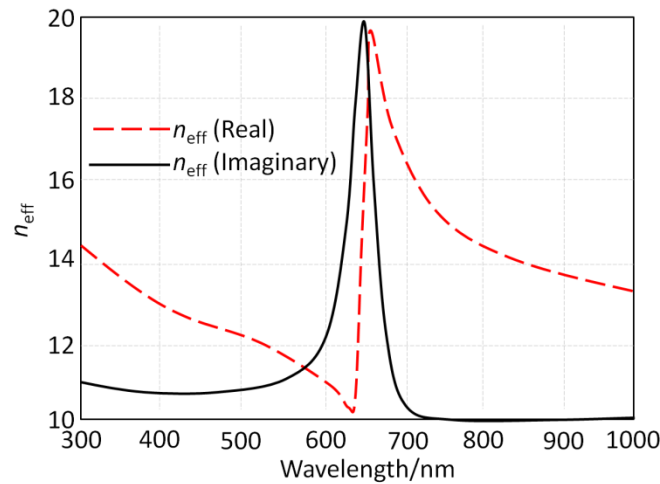


Figure 3: The retrieved n_{eff} of the vertical SWCNT array in terms of real and imaginary parts

UC-PBG Performance and Results Validations

The performance of the proposed UC-PBG structure based SWCNT arrays are characterized in terms of the scattering profiles, band gap, as well as transmission and absorption spectra. The proposed UC-PBG structure, see Figure (4), is constructed from three concentric circular eye patterns, these, eye patterns are constructed from eight eyes at 30 nm, 60 nm, 90 nm from the center, consequently. At the center, a circular eye is positioned. Therefore, each eye behaves as superposition source with a certain phase progressive with respect to the central one. Moreover, the curved edges are created to avoid the possibility of light diffractions [16].

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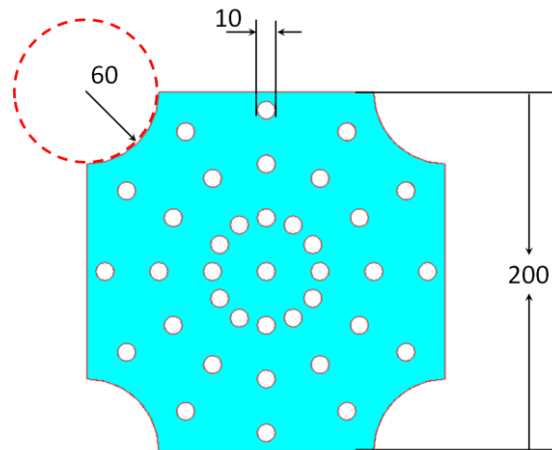


Figure 4: The proposed UC-PBG structure based SWCNT array

Now, to study the performance of the proposed UC-PBG structure, the scattering parameters in terms of extinction cross section spectra are computed using both HFSS and CSTMWS, see Figure (5), then, compared to each other. From the presented results in Figure (5), it is found that the proposed UC-PBG structure shows the maximum scattering around 400 nm, which it may be attributed to the Reighley scattering. In this observation, the scatterer dimensions are relatively comparable to the half incident wave length at 400 nm. In addition to the same manner, this is attributed to electrical resonance of the scatterer length with respect to the incident light. Finally, this observation is agreed with obtained results from both HFSS and CSTMWS.

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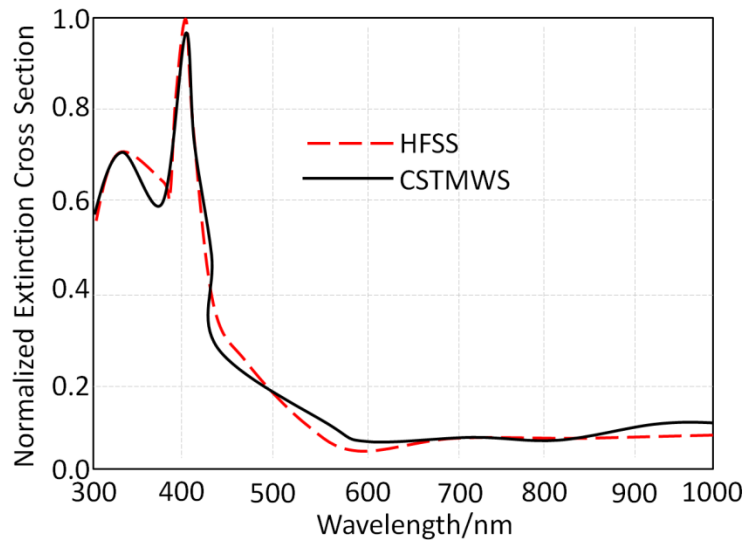


Figure 5: The extinction cross section spectra of the proposed UC-PBG structure

In a relative manner, the electromagnetic band gap location, at which the propagation through the UC-PBG structure is prohibited, is studied. The localization of the band gap around the lattice vertex (Γ , χ , M) is computed at the First Brillouin Zone. As illustrated in Figure (6), it is found that the proposed UC-PBG structure shows no a specific band gap at the visible spectra that is motivated the author to consider the proposed design for the optoelectronic applications.

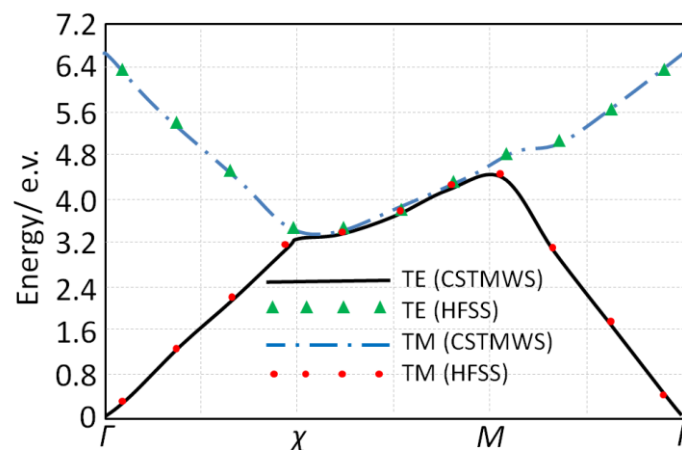


Figure 6: The dispersion diagram of the proposed UC-PBG structure

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Furthermore, the numerical analysis is conducted to study the normalized absorbed and transmitted power profiles in the visible range at the bore-sight directions. In Figure (7), it is found that the proposed UC-PBG structure shows insignificant chromatic apparitions in the range from 600 nm up to 900 nm. However, in the other bands shows chromatic certain apparitions. The surface electromagnetic distributions on the proposed UC-PBG structure are presented in Figure (8). From the absorption spectra, it is found that the UC-PBG layer shows no significant effects. The observed distributions are mostly Gaussian at the center that proofs that the proposed UC-PBG spherically shows no spherical apparitions.

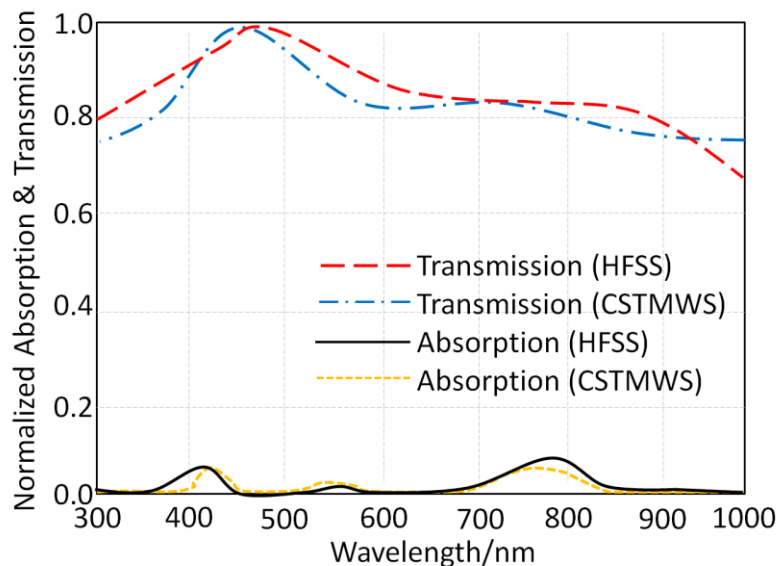


Figure 7: The normalized power of the absorption and transmission profiles of the proposed UC-PBG structure

It is good to mention; the field distribution is polarized in the same direction from 550 nm up to 800 nm. This is due to the fact of having almost insignificant spherical apparition within this band; however, the field distribution is affected between 400 nm and 500 nm due to the effect of the structure resonance as can be seen in Figure (8).

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Figure 8: The electromagnetic field distributions on the surface of the proposed UC-PBG structure

Conclusions

In this paper, the possibility of constructing UC-PBG layers based SWCNT arrays for optoelectronics applications are investigated and proofed. Therefore, a UC-PBG design based on a vertical SWCNT array of 10 nm in length is realized in this study. The electromagnetic properties of the SWCNT array are retrieved using effective medium theory and compared with published optical spectroscopy measurements in [2]. The retrieved effective electromagnetic properties are to create the effective surface that would be used for the UC-PBG construction. It is found the constructed UC-PBG shows a maximum transmitted power around 450 nm with insignificant chromatic apparitions. Nevertheless, the electromagnetic field distribution is found to be in the same direction for the most visible bands. Finally, the

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obtained results from FEM approach are compared against to the numerical simulation based FIT method for validation. An excellent agreement is achieved between the simulated and measured results for the SCS of an individual SWCNT.

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