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IMPORTANT PARAMETERS ANALYSIS OF THE SINGLE-WALLED CARBON NANOTUBES COMPOSITE MATERIALS

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ABSTRACT

This paper aims to present the mathematical analysis for the single-walled carbon nanotube (SWCNT) composite material, in order to derive its effective conductivity model and its plasma frequency formula. This composite material consist of SWCNT coated by other materials. The effect of average thickness of coating layer on the model of an effective conductivity of SWCNT composite material, will be investigated and discussed. Meanwhile, present the effect of using different coating materials with different radii of SWCNTs on the plasma frequency and effective conductivity model of this composite material. The results of this work represent a theoretical study for the properties of SWCNT composite material, which is useful for the antenna application. The parameters of this composite material extracted in this work can be utilized to designing and implementing the dipole antenna, in order to estimate the electromagnetic properties of SWCNT composite material.

Keywords: SWCNT composite materials, effective conductivity model. plasma frequency.

INTRODUCTION

Since carbon nanotubes (CNTs) were exploited by (Iijima, 1991), it has been considered an efficient candidate material in many applications due to their unique electrical and physical properties. Therefore, a lot of research has been focused on CNTs as a candidate material in nano-applications (Huang *et al*., 2008), (E.Ali *et al*., 2014). The main structure of CNTs is a graphene sheets rolled up to configure a cylinders have nanometer radius scale dimension and up to several centimeters in length. The CNTs was classified into metallic and semiconducting material, based on its structure (Hoenlein *et al*., 2004). The number of tubes that constructs the CNTs was adopted to classify the CNTs into SWCNTs and multi-walled carbon nanotubes (MWCNTs) (Hanson, 2005), (Hanson and Jay A. Berres, 2011). The SWCNTs consist of one cylinder, while the MWCNTs consist of several numbers of concentric cylinders. In this paper, the metallic-SWCNT will be adopted as a basic material.

The CNTs-composite materials are promising to revolutionize the various fields of applications of material science. The CNTs-composite material were constructed, based on two approaches to obtain on new material with improved properties. First approach, mixed the CNTs (SWCNTs and MWCNTs) with the other materials through different chemical procedures, in order to construct new materials based CNTs (Arash *et al*., 2014), (Kunmo Chu and Sung-Hoon Park, 2015), (Jianghua Fan *et al*., 2013), (Lavanya *et al*., 2011), (Syed Bava Bakrudeen, 2013). Second approach, coating the CNTs by other materials, in order to enhance the CNTs surfaces properties. Where, the coating approach is one of the several fabrication approaches which are used for handling the surface problems of CNTs. Also, the coating approach was applied to produce a good candidate materials which can be utilized in various fields of sciences including biosensors, semiconductors, electrochemical sensors, microelectrodes, nanowire, and biomedicine. This new composite materials have upscale properties and can be fabricated by coating the SWCNTs with various materials. To date, miscellaneous composite SWCNTs structures could be successfully produced from deposited the nanoparticles of metallic, semiconducting and insulating materials onto the surface of SWCNTs, based on different coating methods (Wei-Qiang, Han and A. Zettl, 2003), (H. Li *et al*., 2009), (Y. Su *et al*., 2011). The main target of coating approach is to take a turn for the better for the electrical and mechanical properties of the new SWCNTs composite materials.

The coating methods of CNTs can be classified into several kinds, depending on the original structures of CNTs. First, methods for coating the MWCNTs (L. Qunqinq *et al*., 1997), (L. Zhu *et al*., 2007), (Y. Morihisa *et al*., 2008), (Y. Peng, and Q. Chen, 2012), (Y. Peng, and Q. Chen, 2012). Second, methods for coating SWCNTs (H. Li *et al*., 2009), (L. Zhu *et al*., 2007), (S. Inoue, and Y. Matsumura, 2009). On the other hand, for studying the mechanical properties of SWCNTs coated with metal, many research had been presented, based on used the Molecular Dynamic (MD) software package simulation (S. Inoue, and Y. Matsumura, 2009), (Y. Chen *et al*., 2012), (H. Liao *et al*., 2012), (Y. Chen *et al*., 2012). In their works, the Nickel (Ni) atoms were used as a metal for coating the SWCNTs to produce the SWCNT-Ni

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composite material. The coating techniques make the SWCNTs composite materials are among many rousing materials that have been explored in recent years. This paper focuses on the SWCNTs composite materials by depending on the simple mathematical technique to analyze and present the effective conductivity model and the plasma frequency formula for these materials. The previous works that reported in this literature and other related works were not presented a study about the electrical conductivity of the CNTs composite materials. Therefore, the main objective of this work is to analyze the SWCNTs composite materials, in order to derive the effective conductivity models and the plasma frequency formula for these composite materials. The dependence of these parameters on the radius of SWCNTs, average thickness of coating layer and conductivity of various kinds of coating material, will be investigated and discussed.

METHODOLOGY

The current development in the new technologies is rely on the new material that available with good properties. The CNTs composite materials can be considered the novel material for nanotechnology applications. The CNTs composite materials have a several undetected potential applications in wide range of technological areas.

This paper aims to analyse the SWCNTs composite materials, in order to estimate the effective conductivity and the plasma frequency, as well as studying the influences of different parameters on their behaviours. In this section, the progress is presented as follows: First, analyze the layer geometry of the SWCNTs composite material. Second, derive the effective electrical conductivity model. Finally, derive the plasma frequency formula for this composite material.

Analysis the layer geometry of the SWCNTs composite material

The SWCNTs composite material that adopted in this work is consist of SWCNT coated by a thin layer of another material. As is known, the SWCNT has one layer of the carbon atoms which can be coated by single or multi layers of different materials atoms. The coating of SWCNT by another material leads to build and construct a new thick rod, as illustrate in Figure-1. The new rod will be characterized by properties differ than the properties of the original materials (SWCNT and coating material).

Furthermore, the final structure of this new rod that illustrated in Figure-2, was utilized by nanowire and other applications (Y. Suet al., 2011). In this figure, r represents the radius of SWCNT, and t represents the average thickness of coating layer.

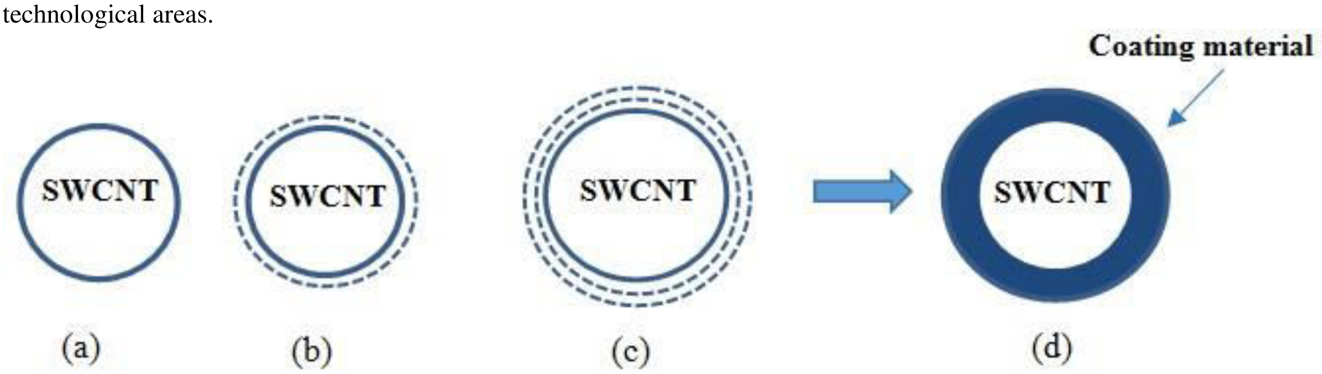

Figure-1. (a) SWCNT without coating, (b) SWCNT coated by single layer of coating material atoms, (c) SWCNT coated by several layers of coating material atoms, (d) Thick rod of SWCNT coated by thin layer of coating material.

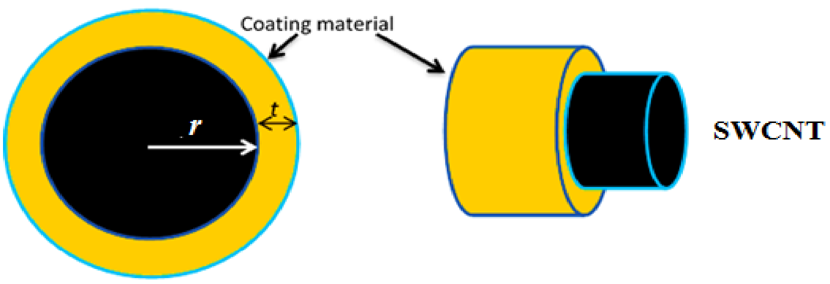

Figure-2. Structure of new rod (SWCNT coated by other material).

Modeling the effective conductivity of SWCNTs composite materials

The electrical conductivity plays an important role in the properties of the SWCNT composite materials. As well as, the total influences of the SWCNT and the coating layer are important for the electrical conductivity of these composite materials. Therefore, the estimation of the electrical conductivity for these materials is very important for different mathematical representations and different simulation modeling approaches. In this work, the effective electrical conductivity of the SWCNT composite materials (SWCNT coated by other different materials) is named by ($\sigma_{composite}$). While, the conductivity of a coating material is named by (σ_{coat}). Then, the effective conductivity of the SWCNT composite material can be derived as follows:

$$\sigma_{composite} = \sum_{j=1}^{k} m_j \sigma_{xj} \quad (1)$$

Where, k is the number of materials that construct the composite material. In this work (k = 2) which is equivalent to SWCNT material and coating material. And, the mj represent the volume fraction factor of the jth material. The effective conductivity model can be written as below

$$\sigma_{composite} = P\sigma_{SWCNT} + A\ \sigma_{Coat} \quad (2)$$

Based on the physical structure of SWCNT (hollow cylinder), the *P* is the circumference of SWCNT ($P = 2\pi r$); and *A* is the average radial cross-section area of coating layer depending on the average thickness of coating layer (*t*). Then the mentioned equation (2) can be written by a new formula below:

$$\sigma_{composite} = \frac{(2r)\sigma_{SWCNT} + t^2\sigma_{Coat}}{(r+t)^2} \quad (3)$$

The formula in equation (3) represent the effective conductivity model of the SWCNT composite material. Then by substituting the conductivity of the SWCNT (Hanson, 2005) (that mentioned in equation (4)), the final formula of the effective conductivity model for SWCNT-composite material is demonstrated by the equation below

$$\sigma_{SWCNT}(w) = -j\frac{2e^2V_f}{\pi^2 hr(w - jv)} \quad (4)$$

$$\sigma_{composite}(w) = \frac{1}{(r+t)^2}\left[-j\frac{4e^2V_f}{\pi^2 h(w - jv)} + t^2\sigma_{Coat}\right] \quad (5)$$

Where σ_{SWCNT} is the surface conductivity of the SWCNT, *e* is the electron charge, *h* is the reduced Plank's constant ($h = 1.05457266\times10^{-34} J.s$), V_f is the Fermi velocity of CNT ($V_f = 9.71\times10^5$ m/s), *v* is a phenomenological relaxation frequency ($v = 6T/r$), where (*T*=300) is temperature in kelvin, so, $F_v = v/2\pi$, and *w* is the angular frequency.

Plasma frequency of the SWCNT composite material

In addition to the effective conductivity model of the SWCNT composite material, the plasma frequency is very important parameters for the purpose of electromagnetic modeling and simulation of the SWCNTs composite material in different 3D electromagnetic simulation software packages like; CST (MWS) and HFSS for antenna applications. Based on the effective conductivity model that mentioned in equation (5) and the bulk conductivity model presented in (Hanson, 2005), the plasma frequency of the SWCNT composite material ($W_{P,composite}$) is deduced as below

$$W_{P,composite} = \frac{e}{\pi(r+t)}\left[\frac{4V_f + \pi^2 hD}{h\varepsilon^{\circ}}\right]^{1/2} \quad (6)$$

$$D = \left(\frac{t^2\ v\ \sigma_{Coat}}{e^2}\right) \quad (7)$$

Where, the conductivity of coating material can be estimated from the standard conductivity formula of materials (Sophocles, J. Orfanidis, 2010).

$$\sigma_{coat} = \frac{e^2 N^D_{coat}}{2m_e v_{coat}} \quad (8)$$

Where $v_{coat} = 1/\tau_{rlxcoat}$, at $\tau_{rlxcoat}$ is the relaxation time of coating material. The N^D_{coat}, is the number of electrons per (m^3) of coating material. These parameters (N^D_{coat}, v_{coat}) are useful to distinguish the materials from others.

SIMULATION RESULTS AND DISCUSSION

These simulation results is present the influences of different parameters on the effective conductivity model of the SWCNT composite material, based on equation (5). Therefore, several simulations can be carried out. The simulation results show that, dependence the conductivity model of SWCNT composite material on the alteration of the factors *r*, *t*, and σ_{Coat}. Figure-3 shows effects of changing the radius of SWCNT on this conductivity model. Where, the average thickness of coating layer is (*t* = 2 nm). Figure-4 shows the influence of increases the thickness of coating layer on this conductivity model, at the radius of SWCNT is (*r* = 2.71 nm). In the simulation results presented in Figures-3 and Figur-4, the coating material that used to construct this composite material is graphite material. On the other hand, the influences of using different coating layers on this effective conductivity model is presented in Figure-5, at average thickness of coating material (*t* = 2nm). Based on using different material like; copper, gold, and graphite, the influences of variation the radius of SWCNTs on this effective conductivity model at frequency 50 GHz is demonstrated in Figure-6, at radius of the SWCNT is (*r* = 2.71 nm) and the average thickness of coating layer is (*t* = 2 nm).

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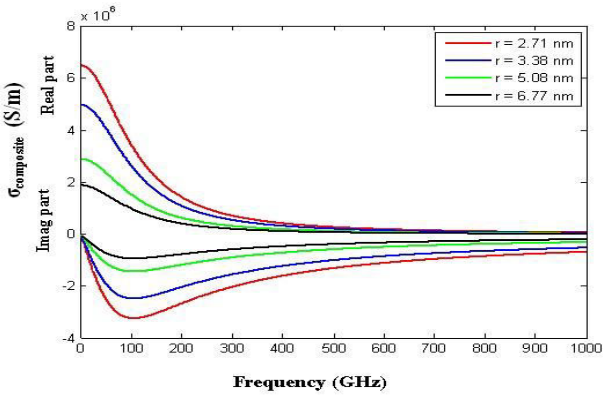

Figure-3. The effective conductivity model of the SWCNT composite material affected by several radii of SWCNT, at SWCNT coated by graphite material and the average thickness of coating layer t = 2 nm.

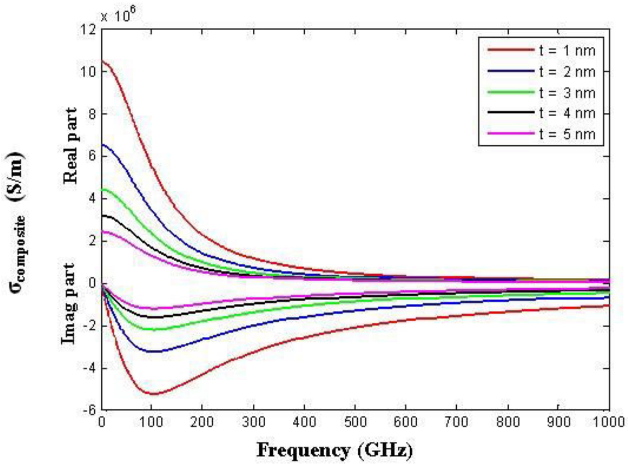

Figure-4. The effective conductivity model of the SWCNT composite material affected by several values of the average thickness of coating layer, at radius of SWCNT r = 2.71 nm.

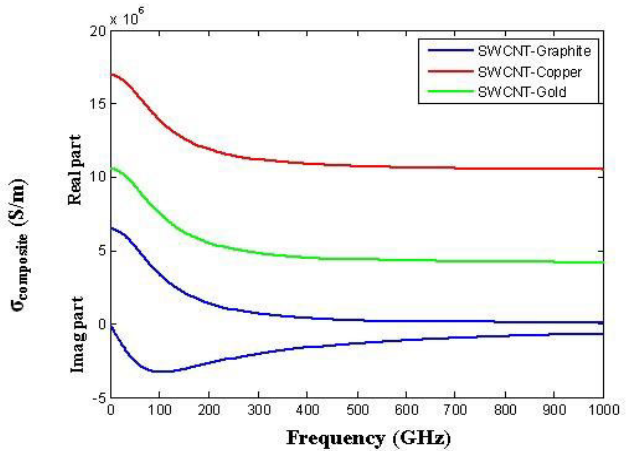

Figure-5. The effective conductivity model of the SWCNT composite material affected by the conductivity of different coating materials (Graphite, Copper and Gold material), at average thickness of coating material t = 2 nm.

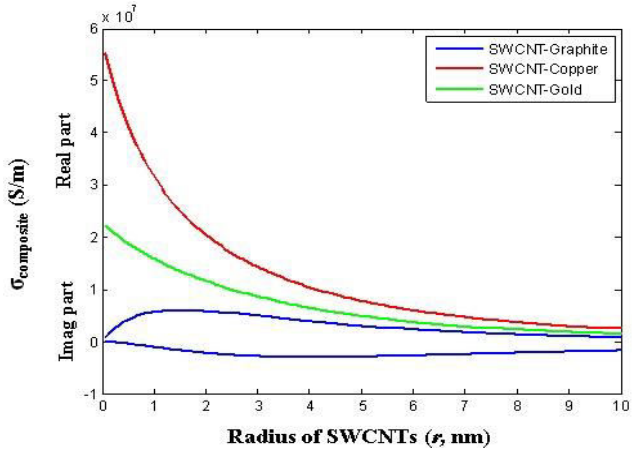

Figure-6. Effective conductivity model of the SWCNT composite materials versus the different radius of the SWCNTs with different type of coating materials, at average thickness of coating layer is t = 2 nm.

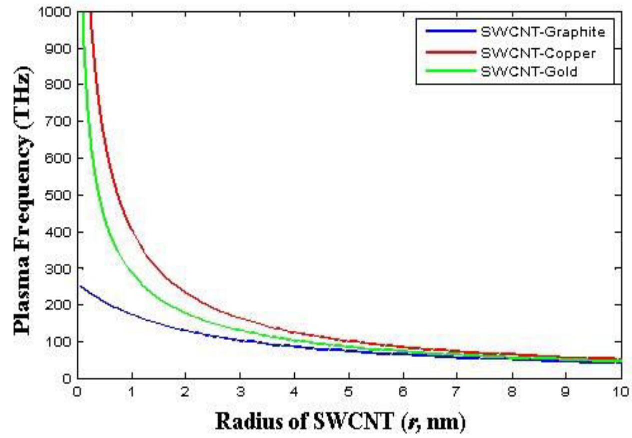

Figure-7. Plasma frequency of the SWCNT composite materials versus the different radii of the SWCNT with different type of coating materials, at average thickness of coating layer is t = 2 nm.

From these results, the effective conductivity model of SWCNT composite materials is inversely proportional for both the average thickness of coating layer and the radius of the SWCNT. As well as, the conductivity of the SWCNT composite materials increases by using coating material with high conductivity value. Therefore, to obtain the higher conductivity of SWCNT composite materials, the very small radius of SWCNT with a thin of average coating layer could be used, in addition to using coating material with high conductivity. From Figure-5., and mentioned equations (5 and 8) the real part of the effective conductivity of the SWCNT composite materials increases by adding the coting material, whereas the imaginary part was not affected.

The plasma frequency ($W_{P,\, composite}$) of the SWCNT composite materials was derived and estimated in this work. The behavior of this plasma frequency versus different radii of the SWCNTs with different kinds of coating materials, is illustrated in Figure-7. This result is presented based on equation (6) and related important equations. From Figure-7, the plasma frequency of SWCNT composite materials is inversely proportional to increases the radius of the SWCNT. As well as, it affected by the conductivity of the coating material. This plasma frequency was increased with increases the conductivity of coating material. Finally, the behavior of the plasma frequency for these composite materials is affected by the properties of SWCNT material. These properties were caused to make the plasma frequency of SWCNT composite materials has no finite value. This mean, the properties of SWCNT composite material are affected by the properties of SWCNT and the properties of coating materials; for instance graphite, copper and gold materials.

CONCLUSIONS

This paper presented the effective conductivity model and the plasma frequency formula for SWCNT composite material. The SWCNT composite material consist of SWCNT coated by a thin layer of other material. The simulation results showed, the effective conductivity of SWCNT composite material depend on several factors, based on its structure. Also, these results exhibited the requirements that should be available to get on the SWCNT composite materials have better conductivity; for instance, SWCNT has a smaller radius, the average thickness of the coating layer is very thin, coating layer has a high conductivity. On another context, the effective conductivity model of the SWCNT composite material is affected by the factors r, t, and σ_{Coat}. Hence, the new composite material properties are dependent on the properties of both SWCNT and coating material.

The SWCNT composite material can be used in places where the metals or other materials have typically been the materials of choice. There are many advantages of using the SWCNT composite material such as light-weight, resistance to erosion, and the ability to be easily adapted to the needs of a particular application. At the modern technologies, most of the potential applications of SWCNTs composite material depend on its electromagnetic properties. Therefore, at antenna applications, the theoretical and experimental studies of this composite material are very important.

Finally, the purpose of these mathematical analysis approaches, for the effective conductivity and plasma frequency, is to make possible to study the electromagnetic properties of SWCNT composite material with different coating material into different 3D electromagnetic simulation software packages.

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