Optical Properties of Armchair Single Wall Boron Nitride Nanotubes

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Abstract

The optical properties of Armchair single wall Boron Nitride Nanotubes (ASWBNNTs) was studied using density functional theory (DFT). In this paper, our calculations focused on the reflectance, absorbance and transmittance. Also, the optical coefficients such as refractive index, extinction coefficient (k), absorption coefficient (α), real (εr) and imaginary (εi) dielectric constant and optical conductivity were. The optical constants are very important parameters because they describe the optical behavior of the materials. The (4,4), (5,5), and (6,6) ASWBNNTs were studied with thicknesses (d= 80.71849, 70.42897, and 64.43785) and the range of wavelength (365.01-1013.98) nm. Additionally, the energy gap was unit calculated for all ASWBNTs and it has direct band gap. The values of optical energy gap are (4.11, 4.4, 4.6) eV. We found out that the (6,6) ASBNNT is the best optical properties. Also, the best average reflection, transmittance, and absorption values for (4,4), (5,5) and (6,6) respectively. These tubes are very useful in various optical applications, such as cover for solar cell, optical window, lenses and green house because these tubes have a transmittance which is greater than other properties like absorption which is small.

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Key words: optical properties, ASWBNNTs, Transmittance, Reflectance, Absorption, DFT, Energy gap. Gaussian 09.

الخصائص البصرية للانابيب النانويه احادية الجدار لمادة نتريد البورون

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الخلاصة

تم دراسة الخصائص البصرية للانابيب النانويه احادية الجدار لمادة نتريد البورون(ASWBNNTs) باستخدام نظرية الكثافة الوظيفية (DFT). في هذه الورقة، ركزت حساباتنا على الانعكاس، الامتصاصية والنفاذية. كما أن المعاملات البصرية مثل معامل الانكسار ومعامل الانقراض (k) ومعامل الامتصاص (α) والحقيقي (εr) والخيالي العازل (εi) والتوصيل الكهربائي. الثوابت البصرية هي معاملات مهمة جدا لأنها تصف السلوك البصري للمواد. تم دراسة (4،4) و (5،5) و (6،6) ASWBNNTs (d = 80.71849، 70.42897، و 64.43785) ومدى الطول الموجي (365.01-1013.98) نانومتر. بالإضافة إلى ذلك، كانت فجوة الطاقة وحدة محسوبة لجميع ASWBNNTs ولها فجوة النطاق المباشر. قيم فجوة الطاقة البصرية هي (4.11، 4.4، 4.6) إلكتروفولت. لقد اكتشفنا أن (6،6) ASBNNT هو أفضل الخصائص البصرية. أيضا، أفضل متوسط انعكاس، نفاذية، وقيم امتصاص ل (4،4)، (5،5) و (6،6) على التوالي. هذه الأنابيب هي مفيدة جدا في مختلف التطبيقات البصرية، مثل غطاء الخلايا الشمسية، نافذة البصرية والعدسات والبيوت الخضراء لأن هذه الأنابيب لديها نفاذية التي هي أكبر من غيرها من الخصائص مثل الامتصاص الذي هو صغير.

الكلمات المفتاحية:الخصائص البصرية، ASWBNNTs ، النفاذية، الانعكاس، الامتصاص، دفت، فجوة الطاقة. غاوس 09.

1. Introduction

Boron Nitride Nanotubes (BNNTs) have the same properties of carbon nanotubes(CNTs), which have unique electrical properties, therefore they have become one of the active research fields over decades. By substituting all carbon atoms in the graphene sheet with Boron and Nitrogen atoms, scientists created Boron Nitride Nanotubes (BNNTs), BNNTs since it can be created by rolling graphene sheet as a cylinder. BNNTs play an important role in diverse applications because they have exemplary properties, such as exceptional electronic, thermal, and mechanical properties. Depending on the number of Boron Nitrogen layers, there are two types of BNNTs, single wall BNNTs (SWBNNTs) and multi-wall BNNTs (MWBNNTs). The electronic properties of BNNTs depend on the length, diameter, and chirality of the tube[1-9].

Optical properties are one of the important properties that depend on the specific future application of (4,4), (5,5) and (6,6) ASWBNNTs and depend on many calculations of optical constants such as absorption coefficient, refractive index, extinction coefficient, real and imaginary parts of dielectric constant. In our evaluation, optical properties of these ASWBNNTs were studied, which were prepared using different values of wavelength. The optical constants are very important parameters because they describe the optical behavior of the materials. The absorption coefficient of the material is a very strong function of the photon energy and band gap energy. Absorption coefficient represents the attenuation that occurs to the incident photon energy on the material per unit thickness. This attenuation is attributed to the absorption processes [10,11

1.1. Optical Energy Gap (Eg)

The semiconductor absorbs photon from the incident beam; the absorption depends on the photon energy (hν). The absorption is associated with the electronic transition between valance band (V.B.) and conduction band (C.B.) in the material starting at the absorption edge which corresponds to the minimum energy gap (E_g). The difference between the lowest value of the C.B. and the highest value of the V.B is called energy gap (E_g). If the photon energy (hν) is equal or more than energy gap (E_g), the photon interacts with a valence electron, elevates the electron into the C.B. and creates an electron–hole pair [12,13]. The process of basic absorption in semiconductors for incident rays happens when an incident photon gives its energy which is equal or larger than the forbidden energy gap (Eg) to the conduction band by absorbing that an incident photon [14].

$$h\nu \geq Eg \qquad (1)$$

Where (υ) frequency in (Hz. unit) and (h) plank's constant (6.625×10^{-34} J.s).(Eg) equal to ($Eg=h\upsilon_o$) where (υ_o) is called critical frequency. The opposite wavelength is called wavelength cut off (λc). This process happens when incident energy photon equals to width of forbidden energy gap, which can be expressed from the following equation [15]

$$\lambda c(nm) = \frac{hc}{Eg} = \frac{1240}{Eg(eV)} \qquad (2)$$

Where (c) is speed of light in vacuum.

1.2. Refractive Index (n)

The behavior of light entering a crystal is fundamentally controlled by the crystal structure. The refractive index (n) is equal to the velocity of light (c), which given wavelength in space divided by its velocity (v) in a substance, the refractive index of the ASWBNNTs can be determined by the following relation [16]

$$n = \frac{c}{v} = \frac{\lambda o}{\lambda} \quad (3)$$

Where (λ_0 and λ) are the wavelength in space and material, respectively.

1.3. ASWBNNTs thickness

ASWBNNTs are based on phenomena uniquely characteristic of the thickness, geometry, and structure of the its. The ASWBNNTs thickness measurement is conducted by optical interferometer method. This method is based on interference of light beams reflected from the surface tube of ASWBNNTs and substrate bottom. The thickness is determined using this relation [17]

$$2nd = m\lambda \quad (4)$$

Here (n, d, m, λ) are the refractive index, thickness, the interference order, and wavelength in (nm units), respectively.

1.4. Reflectance

The reflectance of a material is defined by the intensity of light (I_R), which is reflected in the surface with respect to the incident light intensity (I_o)

$$R = \frac{I_R}{I_0} \quad (5)$$

Also, the reflectance spectra can be calculated by using the following equation [18]

$$R = \left[\frac{n-1}{n+1}\right]^2 \quad (6)$$

Here (n) is the refractive index.

1.5. Transmittance (T)

The transmittance (T) is defined as the ratio of transmitted light intensity (I_T) through the material to incident light intensity (I_O)[19],

$$T = \frac{I_T}{I_O} \quad (7)$$

Also, the Transmittance spectra can be calculated by using this relation [20],

$$T = \frac{2n}{n^2+1} \quad (8)$$

1.6. Absorbance

The absorption is also called the "missing piece", which can be obtained from comparing the total reflected and transmitted energy with the incident energy [21]. The sum of these three parts should be equal to the input light. We can write the absorbance relation in the following relation if we assume the sum of input light is[22]

$$A+R+T=1 \quad (9)$$

1.7. Absorption coefficient(α)

The fraction of light absorbed per unit distance in a participating medium is called absorption coefficient. Standard unit of the absorption coefficient is fraction per meter (1 /m)[23,24].

$$\alpha = \frac{2.303}{d} A \quad (10)$$

Here (α, d, and A) are the absorption coefficient, the thickness of ASWBNNTs, and absorbance, respectively. The number (2.303) is a conversion factor from a decimal to natural log.

1.8. Extinction coefficient (K)

The extinction coefficient (K) can be defined as the amount of loss energy due to the interaction between charges of the medium and light, which calculated for all ASWBNNTs prepared from the following relationship [25]:

$$K = \frac{\alpha\lambda}{4\pi} \qquad (11)$$

1.9. Real and Imaginary part of dielectric constant (ε_r) and(ε_i)

Refractive index (n) and extinction constant (k) are related to the dielectric function (ε) by [26]

$$\sqrt{\varepsilon} = n + ik = n^* \qquad (12)$$

The dielectric constant represents the ability of material to the polarization. The dielectric constant can obtain from this relation:

$$\varepsilon = \varepsilon_r + i\varepsilon_i \qquad (13)$$

$$(n + iK)^2 = \varepsilon_r + i\varepsilon_i \qquad (14)$$

Where (ε_1)and (ε_2) are the real and imaginary parts of the dielectric function.

$$\varepsilon_r = n^2 - k^2 \qquad (15)$$

$$\varepsilon_i = 2nk \qquad (16)$$

The optical conductivity (σ) depends directly on the wavelength and absorption coefficient [27]

$$\sigma = \frac{\alpha n c}{4\pi} \qquad (17)$$

2. Result and discussion

Our systems (4,4), (5,5) and (6,6) ASWBNNTs created by using DFT as it is implemented in the Gaussian 09 program package [28-29] at the level of B3LYP/6–31G basis set as shown in fig. 1. The optical band gap of the structures was evaluated from the difference between HOMO and LUMO. We found out the (E_g) value for our structures (4,4), (5,5), and (6,6) as follow (4.111, 4.4, 4.6) eV respectively. Also, the behaviors of our systems are found to be as insulator.

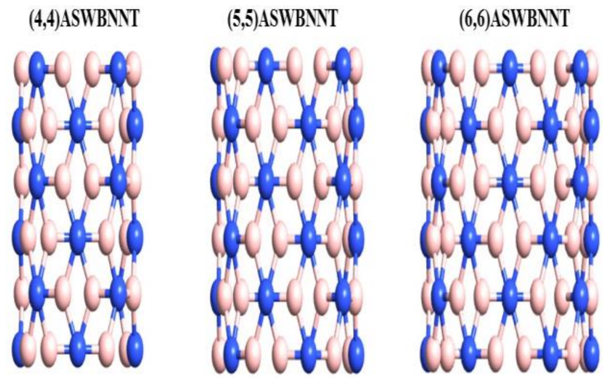

Fig.1. The atomic configuration of the (n,m) ASWBNNTs

As we know that the refractive index dispersion has an important role in the research for optical materials because it is a major factor in optical communication and in designing devices for spectral dispersion. Table.1 represents that the refractive index (for our structures) versus wavelength. We calculated the wavelength from optical band gap by using equation (2), which represented the value critical frequency. Then, we calculated the refractive index at UV-vis and NIR regions by using equation (3). Also, the wavelength cutoff for our structures was calculated and we got that it's (301.7032, 281.8182 and 269.5652) nm for (4,4), (5,5), (6,6), respectively. Additionally, the refractive index values computed by dividing the wavelengths of UV-Vis-NIR by wavelength cutoff for all our structures. Found out a higher value of the refractive index, which has to be expected at least at a high wavelength [26].

By optical interferometer method, the ASWBNNTs thickness measurements were determined. This method is based on interference of the light beam reflection from thin film surface and substrate bottom. Wavelengths cutoff were used to calculate values of thickness, and the thickness was determined using the formula in equation (4) and we get table.1. Obviously, the minimum thickness for the first interference order (m=1). The average thickness for (4,4), (5,5) and (6,6) ASWBNNTs are (80.71849, 70.42897, and 64.43785) nm, respectively.

The optical reflectance spectra was calculated from the refractive index data by using equation (6) which refers to relationship between reflectance and refractive index. The reflectance increased with the increase the wavelength in the structure Fig. 2 shows the transmittance spectra at UV-Vis- NIR of wavelength of sample thin film. By using equation (8), we computed the optical transmittance spectra as seen in Fig. 4. We found out that the optical transmissions of three structures were decreased by increasing in wavelength attributable to enhance the energy of photon. The photon in short wavelength at UV region has a high energy, then the photon will pass through the sample. The region of strong transparency is located in (365.01) nm. It is opposite transmittance more than (95%). In the visible region, the value of the average transmission is (79%) for (4,4) and (5,5) ASWBNNTs. While it is (75%)for (6,6) ASWBBNNTs.

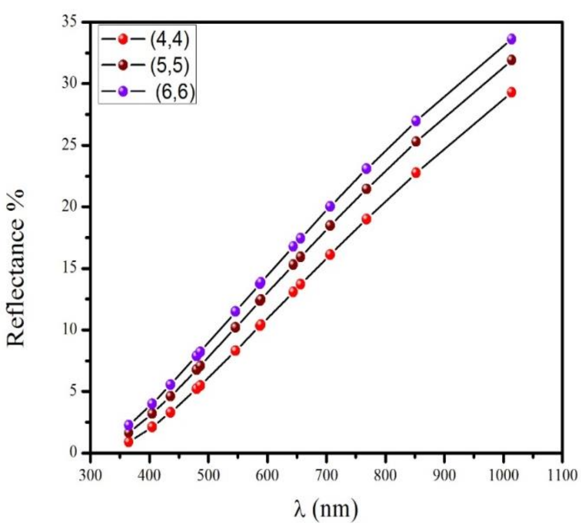

Fig.2 The wavelengths versus Reflectance R%.

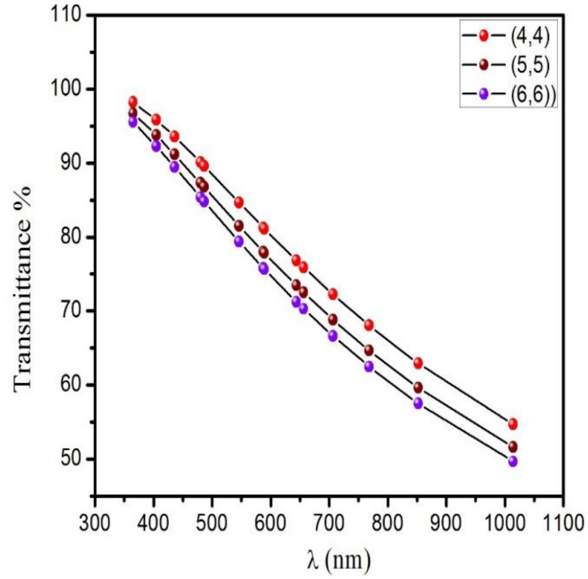

Fig. 3 The wavelength versus Transmittance T%.

The light from the source is transferred by optics in the instrument and strikes the surface of the sample, where the light is divided into three parts: transmission (T), reflection (R) and absorption (A). The sum of the three parts should be equal to the input light. Therefore, a formula can be written, as equation (9). Then by using equation (9), the absorption is calculated. Fig. 4 illustrated the optical absorbance increased rather quickly when the wavelength increased. Further, observation shows the prepared nanomaterials show low absorption at UV spectrum, and high absorption at NIR spectrum approximately 16%.

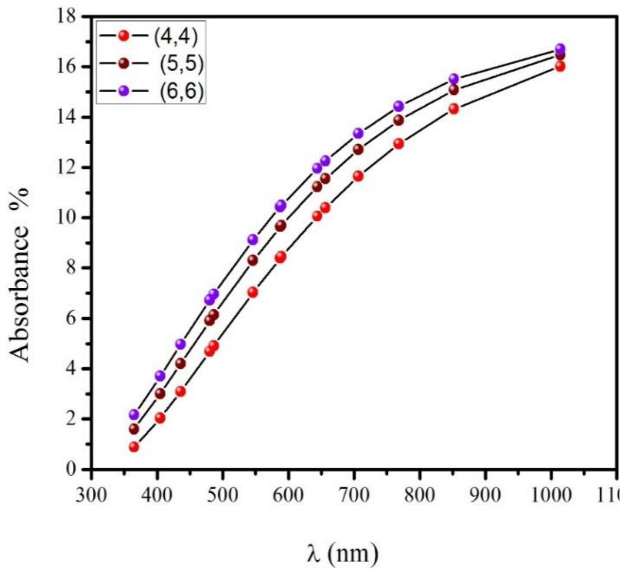

Fig.4 The wavelength versus absorbance %.

The absorption coefficient was also calculated using equation (10). Table1 shows that the absorption coefficient at UV region of wavelength having values less than (10^4 cm^{-1}), while at Vis and NIR it becomes large (10^4 cm^{-1}). This result demonstrates that in first case ultraviolet wavelength leads to increase probability of occurrence indirect transition, while in second case visible and near infrared wavelength will be direct transition.

Table (1): Refractive index (n), Thickness (d nm), Absorption Coefficient (α cm^{-1})

λ (nm)	Refractive index for (4,4) ASWBN NTs	Refractive index for (5,5) ASWBN NTs	Refractive index for (6,6) ASWBNN Ts	Thickness for (4,4) ASWBN NTs (d)nm	Thickness for (5,5) ASWBNNT s (d)nm	Thickness for (6,6) ASWBN NTs (d)nm	Absorbance Coefficient for (4,4) ASWBNN Ts (1/cm)	Absorbance Coefficient for (5,5) ASWBN NTs (1/cm)	Absorbance Coefficient for (6,6) ASWBN NTs (1/cm)
365.01	1.209832	1.295197	1.354069	124.6881	108.7936	99.53893	2526.46	5233.071	7727.485
404.66	1.341252	1.43589	1.501158	112.4707	98.1336	89.78575	5809.241	9821.068	13241.25
435.84	1.444599	1.546529	1.616826	104.4246	91.11312	83.36248	8832.867	13735.23	17767.17
479.99	1.590935	1.70319	1.780608	94.81947	82.73244	75.69471	13374.04	19322.72	24051.54
486.13	1.611286	1.724977	1.803385	93.62187	81.6875	74.73866	14010.52	20085.48	24896.61
546.07	1.809958	1.937668	2.025744	83.34536	72.72098	66.53488	20068.38	27154.04	32606.26
587.56	1.947477	2.08489	2.179658	77.46	67.58585	61.83658	23959.77	31539.64	37289.47
589.3	1.953244	2.091065	2.186113	77.23129	67.3863	61.654	24116.05	31713.5	37473.63
643.85	2.134051	2.284629	2.388476	70.68789	61.67701	56.43038	28707.1	36746.29	42754.78
656.27	2.175218	2.3287	2.43455	69.35011	60.50977	55.36243	29666.71	37780.12	43827.43
706.52	2.341772	2.507006	2.620961	64.41771	56.20611	51.42488	33224.87	41557.63	47708.67
768.2	2.546211	2.725871	2.849774	59.24551	51.69324	47.29589	36911.94	45372.44	51559.38
852.11	2.824332	3.023616	3.161053	53.41141	46.60284	42.63851	40854.44	49316.01	55443.7
1013.98	3.360853	3.597994	3.761539	44.88491	39.16324	35.83177	45714.62	53868.7	59699.01

The extinction coefficient could be calculated by using the relation (11). Fig.5 shows the extinction coefficient of the our ASWBNNTs. It is clear that the extinction coefficient has the same behavior. The increasing of the extinction coefficient values is increased wavelength due to increase in the absorption.

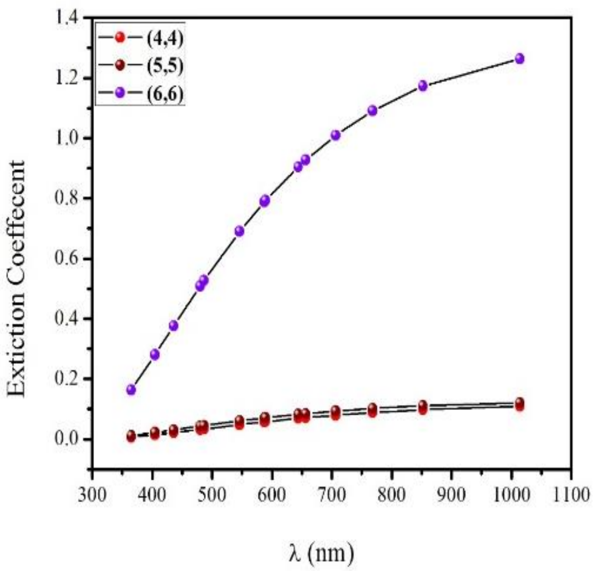

Fig.5 The wavelength versus Extinction coefficient.

Real and imaginary parts of dielectric constants were determined using equations (15) and (16) respectively. The plots of (ε_r and ε_i) parts for ASWBNNTs structures at various wavelength are shown in figs. 6 and 7. The figures show that the real part behaves like the refractive index because of the smaller value of (K^2) as compared to (n^2), while ε_2 depends mainly on the (K) values, which is related to the variation of the absorption coefficient. This means that the real and the imaginary parts are increased when the wavelength is increased. Fig. 8 shows that the variation of optical conductivity as a function of wavelength for three different nanomaterials, and it's evaluated by using equation (17). It is clear form this figure that the optical conductivity for our structures is increased by increasing wavelength, where the (6,6) ASWBNNT has maximum optical conductivity, while the (4,4) ASWBNNT has minimum optical conductivity. Also, high absorption of our structures behavior may be due to the photon-atom interaction leading to higher carrier concentration. This effect increase the optical conductivity

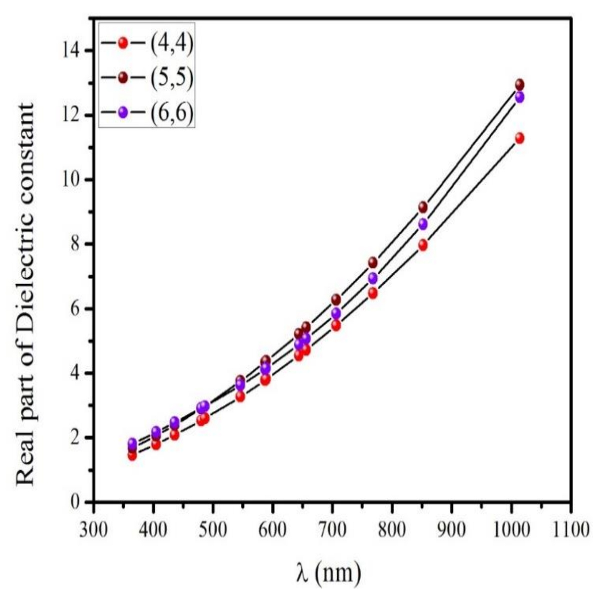

Fig.6 The wavelength versus Real dielectric constant

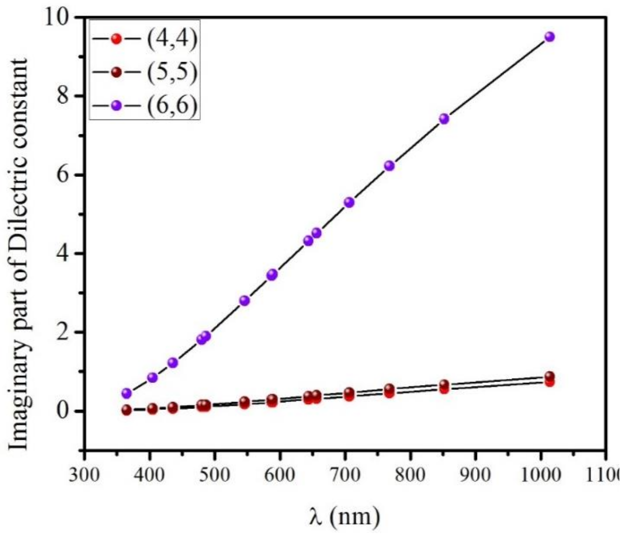

Fig.7 The wavelength versus Imaginary dielectric constant

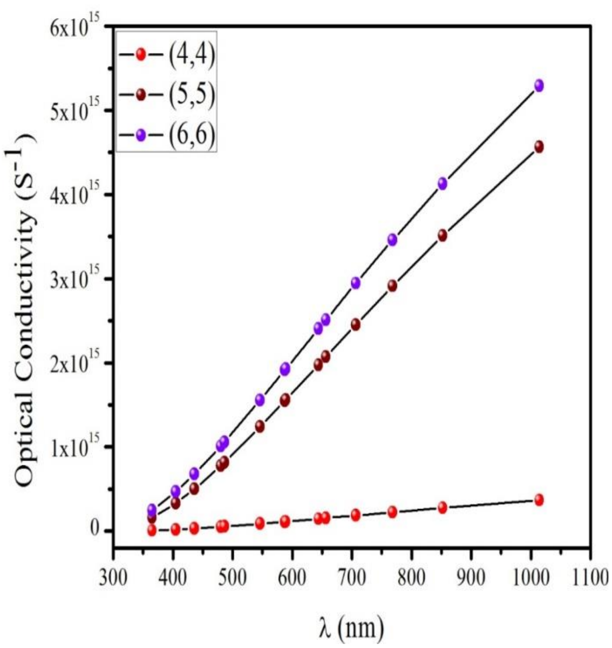

Fig.8 The wavelength versus Optical conductivity

3. Conclusion

ASWBNNTs is a wide band-gap semiconductor and the optical energy gap for (4,4), (5,5) and (6,6) ASWBNNTs are (4.11, 4.4, 4.6) eV respectively. These types of ASWBNNTs have an insulator behavior. The refractive index of ASWBNNTs have shown variation values with different parameters such as wavelength and film thickness. By increasing the wavelength, the reflectance is increased and the transmittance decrease. The maximum value of the transmittance is greater than (95%), and minimum value for transmittance is approximately (50%).

Absorption coefficient in UV region of wavelength having values less than $10^4 cm^{-1}$. While at Vis and NIR become larger 10^4 cm^{-1}. This means that absorption coefficient in first case (UV) will be indirect transition while in second case (Vis-NIR) will be direct transition. The average transmittance in the visible region greater than (75%), and absorption increases with increase the wavelengths. Optical constants (n, k, ϵ_r, ϵ_i, and σ) are increased with the wavelengths. This means that our types of ASWBNNTs suitable for using as solar cell applications.

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