P- ISSN 1991-8941 E-ISSN 2706-6703 *Journal of University of Anbar for Pure Science (JUAPS)* Open Access
2023,(17), (1):107– 111

Theoretical study of the optical properties for Fe2O3-(Si, Pt, Ni) Coaxial Nanowires

Qudama K. Hathal

Ministry of Education, Anbar Education Directorate, Ramadi, Anbar, Iraq

ARTICLE INFO

Received: 16 / 03 /2023
Accepted: 20 / 03/ 2023
Available online: 11 / 06 / 2023

DOI: 10.37652/juaps.2023.178871

Keywords:
Optical properties،
Mie-Lorentz scattering،
Coaxial Nanowire،
absorption coefficient،
energy gap،

ABSTRACT

In this research, a theoretical investigation of the effect of shell (Si, Pt, Ni) on some optical properties for the core of Iron oxide Fe_2O_3 as a coaxial nano wire using the scattering approximation (Mie-Lorentz Scattering theory). Thickness value of (Si, Pt, Ni) shell was limited to about (5 nm) and Fe_2O_3 core diameter of 20 nm. The work showed that the coaxial nano wires have a very high transmittance in the visible spectrum region. The values of transmittance are more than 95% for Fe_2O_3 core only and (Fe_2O_3-Si) core-shell. In construct, the compound of fe_2O_3-Pt and fe_2O_3-Ni show a low transmittance in the same region. Absorbance and low absorption coefficient of Fe2O3 and fe2O3-Si in the infrared spectrum with the appearance of two absorption edges of Fe2O3-Si. The energy gap decreases after adding (Si, Pt, Ni) shell as this in a good agreement with some experimental researches where the values of the energy gap for (fe_2O_3-Si), Fe_2O_3-Pt, and Fe_2O_3-Ni were (2.4, 2, 1.7) ev respectively.

1 Introduction

Nanowires are defined as a very small structure with a diameter close to one nanometer[1], [2]. It can also be known by the composition containing thickness Tens of nanometers and unrestricted length. During the past several years, the research of semiconductor wires has swiftly advanced, and many types of Nano-wire are already being employed in modern scientific applications [3].

Nowadays, advanced applications have emerged the nanowires due to their exceptional properties such as low reactivity and the excellent durability [4]. As a result of their exclusive physical characteristics and significant applications in devices like Photonic nano sensor devices, nanowires are a crucial study topic in nanotechnology [5]–[9].

*Corresponding author at: Ministry of Education, Anbar Education Directorate, Ramadi, Anbar, Iraq;
ORCID:https://orcid.org/0000-0000-00000;
Tel:+964000000000000000
E-mail address: qudama.khamees@gmail.com

Calculations of the optical characteristics of each Fe_2O_3 core and single Si, Pt, and Ni shell were made in order to examine the photonic applications of nanowires. Iron(III) oxide is an inorganic compound and it is one of the three main oxides of iron, the other two being FeO the rarer form, and (Fe_3O_4) which naturally as magnetite. In this work, it is expected that a structure made of nanowires will combine the benefits of Fe2O3 and (Si, Pt, and Ni) materials independently to enhance the performance of the model. In case of studying the structure of semiconductor materials, the optical characteristics clearly play a significant role [10]. The optical energy gap, optical transmittance spectrum, and absorption coefficient have all been researched as optical qualities.

2 Theoretical model

The optical characteristics of coaxial nanowires were computed in this study. Mie scattering theory's conceptual framework has been created to estimate circular cylinders with simple forms. Mie scattering theory is the general solution which defines the scattering of an electromagnetic wave by a homogeneous spherical medium. This set up makes it possible to figure out how effective a single layer's absorption is. The modelling tool

"Optical Properties of Single Coaxial Nanowires" [11] is used to determine the absorption of unpolarized light for nanowire sheets. According to estimates, coaxial nanowires are exceptionally cylinder-shaped along the Z-axis and are floodlit by electromagnetic waves in coincide with incident wave propagation vectors of (k), as seen in figure (1).

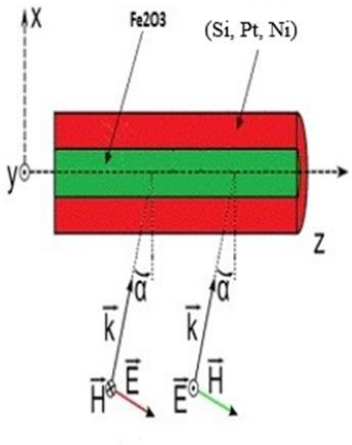

Figure (1): The Schematics of coaxial nanowire [12]

Absorption efficiency define as the geometric cross section of one thickness divided by the absorption cross section, like in the following equation:

$$Q_{abs} = \frac{C_{abs}}{C_{geom}} \qquad (1)$$

Where C_{abs} and C_{geom} are the absorption cross section and geometrical cross section respectively.

$$C_{abs} = C_{ext} - C_{scat} \qquad (2)$$

Where C_{ext} is the extinction cross section and C_{scat} is the scattering cross section

In the state of un-polarized light for example sunlight, the absorption cross section can be represented by the following equation:

$$C_{abs} = \frac{(C_{ext}^{TE} + C_{ext}^{TM})}{2} - \frac{(C_{scat}^{TE} + C_{scat}^{TM})}{2} \qquad (3)$$

To evaluate the Mie coefficients of a system, the following steps should be followed:

- Calculating the solutions of the 2D wave equation in different ranges to express the electromagnetic fields.

-Replacing the magnetic field with the electric field in Maxwell's equations.

-These solutions can be written in the form of a Bessel function, whose coefficients have been computed by calculating the boundary conditions.

-Application of boundary conditions for continuity in state of interference

-Displaying the results in the form of matrix.

-Calculating unknown Mie coefficients of a system [11].

3. Results and discussion

3.1. Optical transmittance

The optical transmittance spectrum is directly associated to the thickness of the material and the crystal structure. The transmittance spectrum for an iron oxide (Fe_2O_3) core with a diameter of 20 nm, and a shell of (Si, Pt, and Ni) individually as coaxial nanowires NWs, is shown in Figure 2 as a function of wavelength. For both Fe_2O_3 and Fe_2O_3-Si, the considered model displayed that a low diffusion spectrum in the low wavelength region (300–400 nm), followed by an abrupt increase in transmittance spectrum in the visible spectrum which in a good agreement with the experimental results of P. A. K. Elttayef [13] . This increase is due to the electronic transitions in the energy groups inside the optical absorption region. In addition, it is clear that the compounds of Fe_2O_3-Pt and Fe_2O_3-Ni have a stable value of transmittance for wavelength range under the study. This may be due to an increase in the surface roughness of the nanoparticles which leads to increase the scattering due to the increase in the thickness of the nanowires.

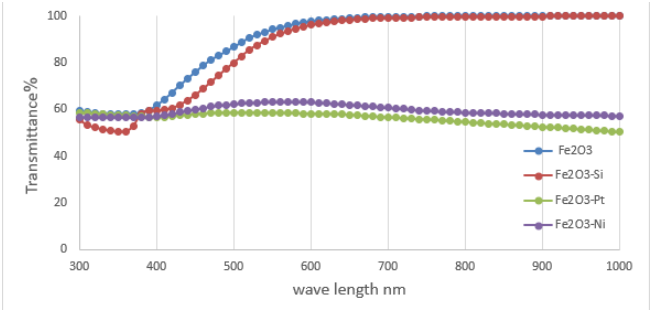

Figure (2): the transmittance% as a function of the wavelength nm

3.2. Absorption Coefficient

One of the essential variables which gives a number of characteristics of the materials used to make semiconductors is the study of the absorption

coefficient. Studying the behavior of electron transitions between energy groups is particularly important because it indicates how many photons will be absorbed by matter per unit length, which is highly dependent on the energy of the input photons. Figure (3) depicts the change in the absorption coefficient of iron oxide nanowires as a function of wavelength by using the following relation [14].

$$\propto = 2.303\ \frac{A}{t} \qquad (4)$$

Where t denotes the nanowire's thickness and A denotes absorbance. For values more than $1.5 \times 10^4 cm^{-1}$for both Fe2O3 and Fe2O3-Si, Figure (3) illustrates a progressive decline in the absorption coefficient values with the direction of the high wavelengths, indicating that there is an optical energy gap from the direct form.

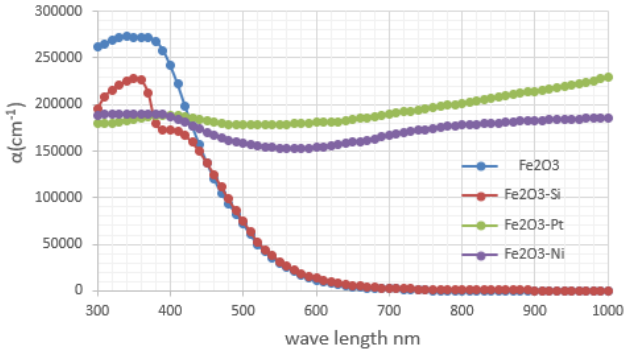

Figure (3): the absorption coefficient as a function of wave length for coaxial nanowire.

The findings demonstrated that the absorption coefficients for Fe2O3 and Fe2O3-Si peaked in the visible spectrum area, then steadily declined to achieve their lowest values in the infrared spectrum. The relative stability in transmittance values for Fe2O3-Pt and Fe2O3-Ni is correlated with the stability of the absorption coefficient values for these two compounds.

3.3. Optical Energy gap

Depending on the Tauc formula, which is presented in the following format [15], the optical energy gap was calculated:

$$\propto = \frac{B(h\upsilon - E_g)^n}{h\upsilon} \qquad (5)$$

Using the absorbance that was calculated using the software and mentioned in the theoretical section, where stands for the absorption coefficient, B is a constant that depends on the type of material used, h is the energy of the incident photons, n is a constant whose value be determined by the type of electronic transition that occurs between the two energy bands, and E_g is the optical energy gap [16]. The optical energy gap values were calculated by first sketching the connection between (h) and (1/n) as a function of the incident photon energy (h), and then by tangentially intersecting the right segment of the curve with the h axis. When hν=0, it reflects the material's optical energy gap values as shown in Figure.

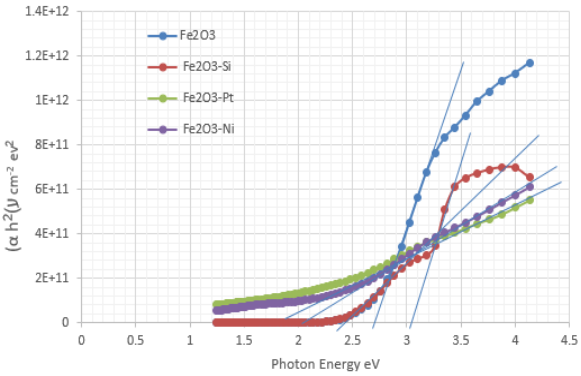

Figure (4): $(\alpha h\upsilon)^2$ as a function of photons energy.

In general, it is shown that the optical energy gap value reduces as the thickness of Fe_2O_3 nanowires increases by encasing them in (Si, Pt, Ni) shells which is in a good agreement with the researcher[17]. This may be because certain local levels in the optical energy gap area have been removed, lowering the optical energy gap's value. There are several mechanisms that have been developed to explain the variation in the energy gap values, including changes in quantitative confinement, the height of the well barrier as a result of crystalline dimension changes, and differences in the proportions of combined impurities that affect pressure or tensile strength as well as improvement or deformation in the crystal structure[18].

4 Summery and Conclusions

The optical properties of Fe2O3-(Si, Pt, Ni) nanowires were considered. It was shown by theoretical simulation by Scattering Mie theory that the combination of Fe2O3-Si leads to an increase in the values of each absorption spectrum and the absorption coefficient, while there was a decrease in the transmittance values. Increasing the nanowire

thickness produced by the addition of the (Si, Pt, Ni) shell led to decline in the value of the optical energy gap. By studying the optical properties discussed of Fe2O3-(Si, Pt, Ni) nanowires show that nanowires can extremely work an significant role in the field of manufacturing optoelectronic device.

Acknowledgements

The author would like to thank theoretical physics group in the department of physics, college of science, university of Anbar for their support.

Conflict of interest

There is no conflict of interest.

References

[1] B. Wang, S. Yin, G. Wang, A. Buldum, and J. Zhao.(2001). Novel structures and properties of gold nanowires. Phys Rev Lett, vol. 86, no. 10: p. 2046

[2] K. Gall, J. Diao, and M. L. Dunn. (2004).The strength of gold nanowires. Nano Lett, vol. 4, no. 12: pp. 2431–2436.

[3] S. Nawaf, A. K. Ibrahim, and A. A. Al-Jobory. (2023).Electronic structure and optical properties of Fe-doped TiO2 by ab initio calculations. International Journal of Modern Physics C (IJMPC), vol. 34, no. 02: pp. 1–9,.

[4] S. Ju et al., "Proton radiation hardness of single-nanowire transistors using robust organic gate nanodielectrics. (2010). Appl Phys Lett, vol. 89, no. 7: p. 073510, 2006.

[5] P. Yang, R. Yan, and M. Fardy, "Semiconductor nanowire: what's next?," Nano Lett, vol. 10, no. 5, pp. 1529–1536,

[6] C. Soci, A. Zhang, X.-Y. Bao, H. Kim, Y. Lo, and D. Wang. (2010). Nanowire photodetectors. J Nanosci Nanotechnol, vol. 10, no. 3: pp. 1430–1449,

[7] X. Chen, C. K. Y. Wong, C. A. Yuan, and G. Zhang. (2013). Nanowire-based gas sensors. Sens Actuators B Chem, vol. 177: pp. 178–195,

[8] M. Motlak, A. Hamza, and S. Nawaf. (2019). Synthesis and application of Co/TiO2 nanoparticles incorporated carbon nanofibers for direct fuel cell. in Journal of Physics: Conference Series, , vol. 1178, no. 1. doi: 10.1088/1742-6596/1178/1/012006.

[9] J. M. Rzaij, S. O. Nawaf, and A. S. M. Khalaf. (2019) . A study on the scattering and absorption efficiencies of Si-Ag coaxial nanowire. Iraqi Journal of Science, vol. 60, no. 9, pp. 2003–2008, 2019, doi: 10.24996/ijs.2019.60.9.13.

[10] W. Chen, J. Z. Zhang, and A. G. Joly. (2004). Optical properties and potential applications of doped semiconductor nanoparticles. J Nanosci Nanotechnol, vol. 4, no. 8: pp. 919–947,.

[11] Ramadurgam, S., Hansen, K. E., Lin, T. G., Dutta, A., Abdul-Hadi, S., & Yang, C. (2018). Optical properties of single coaxial nanowires.

[12] Nawaf, S. O. (2019). Fe2O3-GaSb synthesis as coaxial nanowires for optical applications. J. Univ. Anbar Pure Sci., 13(2), 32.

[13] P. A. K. Elttayef, A. Prof, M. H. Jaduaa, and M. A. Muhammed. (2015). Study the structural and optical properties of Fe2O3 thin films prepared by RF magnetron. Int. J. Appl. or Innov. Eng. Manag., vol. 4, no. September, pp. 99–105,

[14] B. K. H. Al-Maiyaly. (2017) . The Effect of Thickness on Electrical Conductivity and Optical Constant of Fe2O3 Thin Films. Ibn AL-Haitham Journal For Pure and Applied Science, vol. 27, no. 3, pp. 237–246,.

[15] N. F. Mott and E. A. Davis. (2012). Electronic processes in non-crystalline materials. Oxford university press.

[16] D. Depla and S. Mahieu, Reactive sputter deposition, vol. 109. Springer, 2008.

[17] Bushra K.H.Al-Maiyaly. (2014). The Effect of Thickness on Electrical Conductivity and Optical Constant of Fe2O3 Thin Films. Ibn Al-Haitham Jour. Pure Appl. Sci, vol. 27. no. 3, pp. 237–246.

[18] R. Mariappan, V. Ponnuswamy, P. Suresh, N. Ashok, P. Jayamurugan, and A. C. Bose. (2014). Influence of film thickness on the properties of sprayed ZnO thin films for gas sensor applications. Superlattices Microstruct, vol. 71, pp. 238–249.

P- ISSN 1991-8941 E-ISSN 2706-6703 *Journal of University of Anbar for Pure Science (JUAPS)* Open Access
2023,(17), (1):107– 111

دراسة نظرية للخصائص البصرية لأسلاك Fe_2O_3-(Si, Pt, Ni) النانوية متحدة المحور

قدامة خميس هذال

وزارة التربية العراقية، مديرية تربية الانبار، الرمادي، الانبار، العراق

الخلاصة

في هذا البحث تم الدراسة نظريا تأثير القشرة للعناصر التالية (Si، Pt، Ni) على بعض الخواص البصرية في لب أوكسيد الحديد الثلاثي Fe2O3 (III) كسلك نانوي متحد المحور باستخدام برنامج تقريب التشتت (مي–لورينز). تم استخدام نموذج المحاكاة " Optical Properties of Single Coaxial Nanowires" لحساب قيم معاملات الخواص البصرية مثل النفاذية البصرية ومعامل الامتصاص وفجوة الطاقة البصرية .تم تحديد سمك الغلاف للعناصر (Si، Pt، Ni) على حوالي 5 نانومتر وقطر لب Fe2O3 يبلغ 20 نانومتر. أظهرت الدراسة أن الأسلاك النانوية المحورية لها نفاذية عالية جدًا في منطقة الطيف المرئي. قيم النفاذية هي أكثر من 95٪ في لب Fe2O3 فقط و (Fe2O3-Si). يُظهر مركب fe2O3-Pt و fe2O3-Ni نفاذية منخفضة في نفس المنطقة. أظهرت النتائج ان معامل الامتصاص منخفض لـ Fe2O3 و fe2O3-Si في طيف الأشعة تحت الحمراء مع ظهور حافتي امتصاص من Fe2O3-Si. تقل فجوة الطاقة بعد إضافة الغلاف حيث كانت قيم فجوة الطاقة لكل من (Fe2O3-Si) و Fe2O3-Pt و 2.4) Fe2O3-Ni، 2.4, 2, 1.7)) على التوالي.