P- ISSN 1991-8941 E-ISSN 2706-6703 *Journal of University of Anbar for Pure Science (JUAPS)* Open Access
2019,13 (2) :32-39

Fe_2O_3-GaSb Synthesis as coaxial Nanowires for Optical Applications

Sameer O. Nawaf

Department of Physics, College of Science, University of Anbar,Ramadi,Iraq.

ARTICLE INFO

Received: 7 / 7 /2019
Accepted: 29 / 8 /2019
Available online: 19/7/2022

DOI: 10.37652/juaps.2022.172114

Keywords:
Mie-Lorentz scattering.
Absorption coefficient.
optical transmittance spectrum.

ABSTRACT

A theoretical study shows the effect of the Gallium antimonide (GaSb) shell on several visual properties of the Iron (III) oxide (ferric oxide) Fe_2O_3 core as a nanowire using the Mie-Lorentz Scattering theory. The thickness of GaSb shell was fixed at around 20 nm with Fe_2O_3 core diameter of 20 nm. The study indicated that the nanowires of the Iron (III) oxide core have transmittance approximately 95% in the visible spectrum. Absorbance and low absorption coefficient in the Infrared (IR) are observed. Electronic transitions of the allowed direct type by the coaxial nanowire and reducing in the energy gap after adding the shell around the Fe_2O_3 to energy gap about 1.7 eV are also seen.

Introduction:

Nanowires are defined as nanostructure with a diameter approaching the nanometer [1]. The study of semiconductor has rapidly developed over the past few years where various types of nanowires have been used in modern scientific applications. In recent decades, advanced applications of nanowires have emerged as a result of their exceptional properties such as the low interaction and endurance [2].

Nano materials are a major research topic in nanotechnology because of their unique physical properties and potential applications in devices such as photovoltaic sensors [3-6]. To study the optical applications of nanowires, the optical properties of Fe_2O_3-GaSb (core-shell) are calculated.

* Corresponding author at: Department of Physics, College of Science, University of Anbar .E-mail address: Sameer@uoanbar.edu.iq

The diameter of Fe_2O_3 core and the thickness of GaSb shell are fixed at around 20 nm. In this work, a structure based on nanowires is assumed to combine the advantages of Fe_2O_3 and GaSb in order to improve the performance of the model. Optical properties play a key role in the study of the synthesis of semiconductor materials [7]. The optical properties that studied in this paper are optical absorbance spectrum, optical transmittance spectrum, absorption coefficient, and optical energy gap.

Computational part:

In this study, the optical properties of coaxial nanowire are studied using Mie Scattering Theory using online simulation program which allows to evaluate unlimited circular cylinders of basic shapes [8]. This configuration permits of the calculation of the absorption efficiency of single layers. The "Optical Properties of Single Coaxial Nanowires" online simulation program is used to calculate the un-polarized light absorption of nanowires. The coaxial nanowires are evaluated as

infinite long cylinders along the Z axis illuminated by an electromagnetic wave with the vector of the incident wave vector ($\bar{k}$) and incident angle equal to zero. The incident light is committed into two types of polarizations; *Case I*, the magnetic field is vertical to the nanowire axis direction, and *Case II* the electric field is perpendicular to the nanowire axis as shown in Figure 1[8] as well as figure 2 shows a diagram of the Fe2O3-GaSb coaxial nanowire [9].

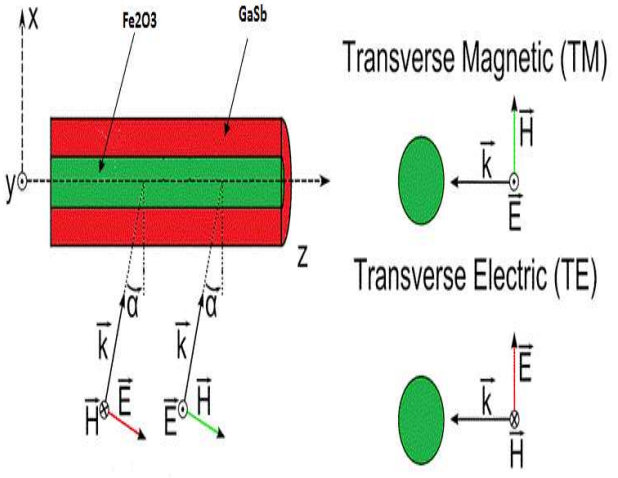

Figure 1: The Schematics of Fe2O3-GaSb coaxial nanowire with the direction of TM and TE propagation.

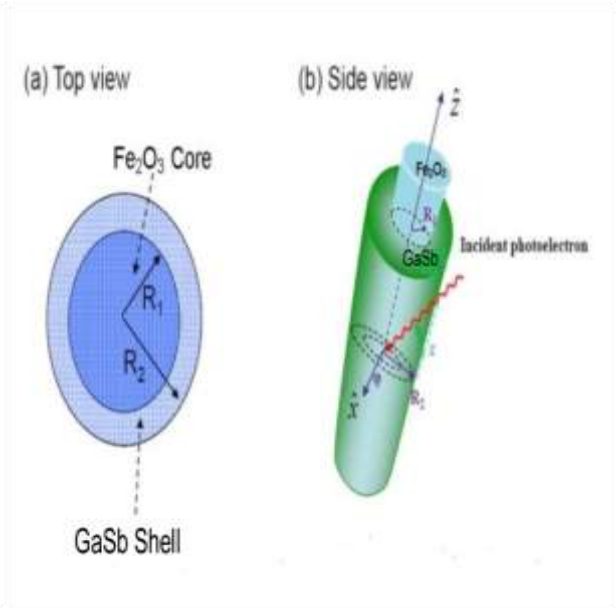

Figure 2: Diagram of the Fe2O3-GaSb coaxial nanowire

The efficiency of absorption $Q_{abs}$is the ratio of the cross-section of the absorption to the geometric cross-section of a single wire:

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

Where $C_{abs}$and$C_{geom}$are the cross sections of absorption and the cross sections of geometry 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 case of un-polarized light similar to sunlight, we can represent the cross-section of the absorption C_{abs} as following:

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

The absorption efficiency of individual layers can also be calculated. The total absorption and scattering efficiencies can be determined from the coefficients as follows [8]:

$$Q_{sca}^{(I)} = \frac{2}{k_0 c}\{\sum_{n=-\infty}^{+\infty}(\left|a_n^{(I)}\right|^2 + \left|b_n^{(I)}\right|^2)\} \quad (4)$$

$$Q_{ext}^{(I)} = \frac{2}{k_0 c}\{\sum_{n=-\infty}^{+\infty} Re(b_n^{(I)})\} \quad (5)$$

$$Q_{abs}^{(I)} = Q_{ext}^{(I)} - Q_{sca}^{(I)} \qquad (6)$$

$$Q_{sca}^{(II)} = \frac{2}{k_0 c}\{\sum_{n=-\infty}^{+\infty}(\left|a_n^{(II)}\right|^2 + \left|b_n^{(II)}\right|^2)\} \quad (7)$$

$$Q_{ext}^{(II)} = \frac{2}{k_0 c}\{\sum_{n=-\infty}^{+\infty} Re(b_n^{(II)})\} \quad (8)$$

$$Q_{abs}^{(II)} = Q_{ext}^{(II)} - Q_{sca}^{(II)}$$

Absorption efficiencies for non-polarized light can be calculated by:

$$Q_{abs} = \frac{1}{2}\left\{Q_{abs}^{(I)} - Q_{abs}^{(II)}\right\} \qquad (9)$$

Where $Q_{abs}^{(I)}$ *and* $Q_{abs}^{(II)}$ indicate the absorption efficiencies of individual layers.

Results and discussion:

Optical absorbance spectrum:

Absorbance spectrum is an important factor to determine many optical properties of Nano-materials. Figure (3) shows the change of absorbance with the change of wavelength within spectrum range between 300-1000 nm for the iron oxide core before and after it was wrapped with Gallium antimonide as nanowire at room temperature. Figure 3 revealed three absorbance edges (a, b and c) that refers to three optical band gaps will appear. The appearance of these three absorption zones indicates the occurrence of effective electronic transitions within this range of spectrum [10]. It is clear as shown in the figure that absorption is significantly reduced by increasing the wavelength within the visible spectrum to the basic absorption threshold (the boundary between the high absorption area and the low absorption area at 565 nm of the visible spectrum. This result is consistent with the results of reference [11].

This is followed by a regular decrease and relative stability within the infrared spectrum. The physical explanation of this situation is that the energy needed to transfer the electrons from the valence band to the conduction band is limited and less than the optical energy gap. Therefore, the absorbance values are low within this range of the electromagnetic spectrum under study. The absorbance values are increased in case of coaxial nanowire compared with the iron oxide core individually, which may be due to increased attenuation of the photovoltaic light by increasing the number of atoms exposed to the radiation and thus increasing the absorbance values in general.

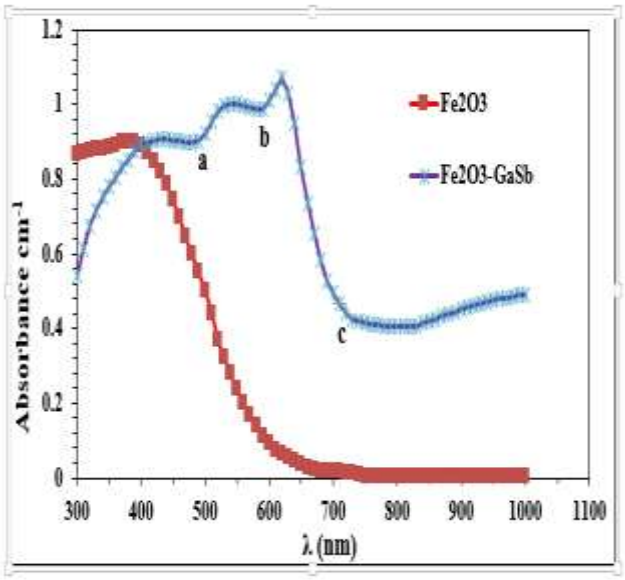

Figure 3: Absorbance as a function of the wavelength

Optical transmittance spectrum:

The spectrum of optical transmittance is directly related to the thickness and crystalline composition of the material as well as the surface distribution of their atoms. Figure (4) shows the transmittance spectrum as a function of the wavelength for Fe2O3 core within diameter of 20 nm before and after covering with the shell of 20 nm of GaSb (Coaxial NWs). The studied model shows a low transmittance range within the low wavelength area (300-450 nm) followed by a rapid and quick increase of spectrum within the visible spectrum as a result of electronic transitions in the energy bands within the optical absorption region [12], and relative stability to reach the highest value (98.8) %) After the wavelength (760 nm), a result similar to that reached by the researcher Abdulhussein K. Elttayef[13] which may

be attributed to a significant decrease of the influence of scattering [14].

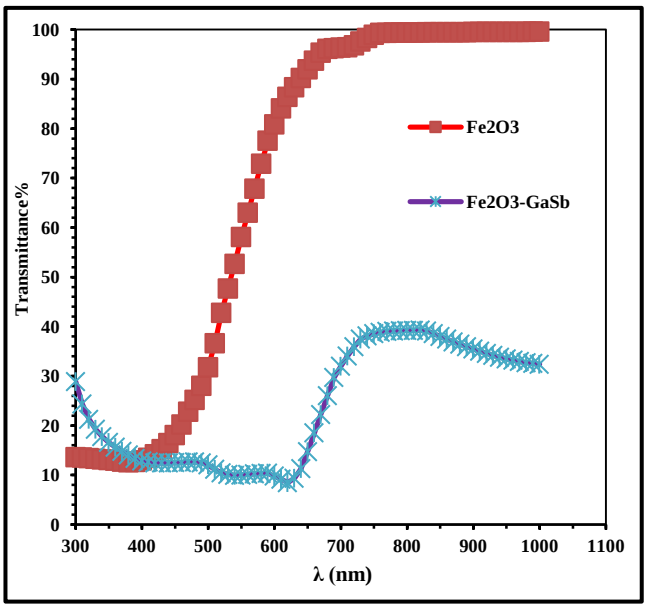

Figure 4: Optical transmittance as a function of the wavelength

In general, a significant decrease in transmittance values when GaSb is present as a shell with Fe3O2 core, which may have increased the roughness of the surface of the nanowire and thus increasing of scattering due to increasing thickness of nanowires when the shell is present with the core. The spectral behavior is similar within the confined area between (380 and 620) nm when the core is rotated with GaSb followed by gradually increasing the transmittance values to make a peak at 750nm and gradually decreasing to 32% at the end of the spectral range under study. This variation in transmittance values is due to the difference in the absorption of nanowires of the electromagnetic spectrum within the specified wavelengths.

Absorption coefficient:

Optical absorption coefficient is one of the important parameters that explains some of the properties of semiconductor materials in addition to studying the behavior of electronic transitions between the energy bands, as it represents the ratio of photons that may be absorbed by matter to the distance unit and deeply depends on the energy of incident photons.

Changing absorption coefficient (α) as a function of the wavelength of nanowires of iron oxide is shown in figure (5) by drawing the relationship between the values of the absorption coefficient and the wavelength under study using the following relationship[15]:

$$\alpha = 2.303\frac{A}{t} \dots\dots\dots\dots\dots\dots (10)$$

Where A is the absorbance and t thickness of the nanowire.

Figure 5 shows a slow decrease in the values of the absorption coefficient towards the high wavelengths and that they have values close to 104 cm-1 indicating that the optical energy gap is from direct type, ie the value of (n) in equation (11) will be equal to (1/2). The results show that the highest value of the absorption coefficient is within the visible spectrum and then the values of (α) gradually decreased to the lowest values within the infrared region. The relative stability of α values within the confined spectrum area between 700-1000 nm is due to the relative stability of the transmittance values within that region, which is also due to the fact that the electronic transitions within that region are very low and then begin to be increased when reaching the optical absorption edge .

Returning to Fig. 4, the edge of the optical absorption towards the red wavelengths when the core of the iron oxide is folded up, because there is an absorption thresholds within the specified spectrum regions. In general, the values of the absorption coefficient after the core is folded up by the shell, the nanowire has higher

values for the absorption coefficient when compared to those of the core before adding GaSb shell. This may be because the presence of the shell has created donor levels near the conduction bands that will absorb the energy of photons with low values and thus increase the absorption coefficient values [16].

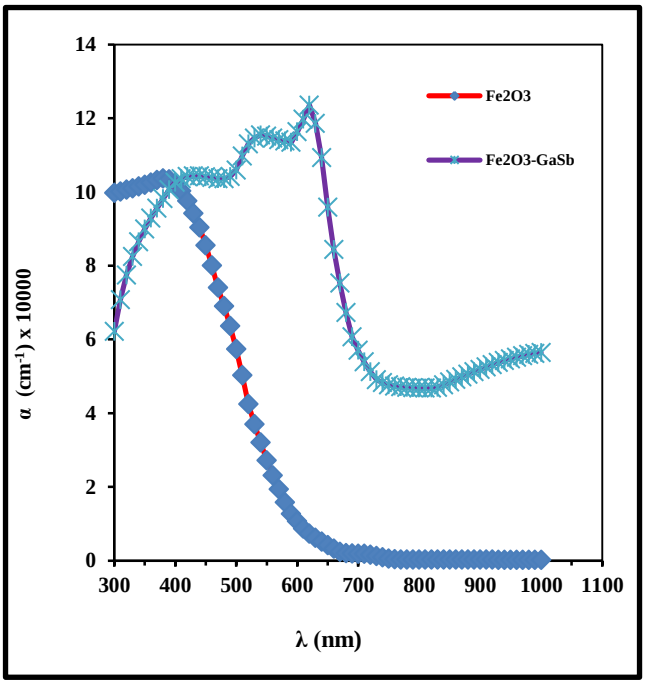

Figure 5: Absorption coefficient as a function of the wavelength

Optical energy gap:

The optical energy gap is calculated based on the Tauc formula given as [17]:

$$\alpha = \frac{B(h\nu - E_g)^n}{h\nu} \dots\dots\dots\dots\dots\dots (11)$$

Whereαrepresents the absorption coefficient and$B$is a constant depends on the material type and $h\nu$is the incident photon energy while$E_g$represents the optical energy gap and n is a constant whose value depends on the nature of the electronic transmission between the two energy bands [18].

The values of the optical energy gap are calculated by drawing the relationship between $(\alpha h\nu)^{\frac{1}{n}}$as a function of the incident photon energy ($h\nu$) and by drawing the tangent of the straight part of the curve and its intersection with the $h\nu$ axis, ie αhν = 0, Evaluate the optical energy gap of the material, as shown in Figure (6). Some reports indicate that the iron oxide compound have an optical energy gap of the allowed direct type [13] [19] while the researcher [20] indicates that Fe2O3 possessed an indirect type of optical energy gap, while the researcher [21] shows that Fe2O3 has both types. As shown in Fig. 6, the Fe_2O_3 core has a direct-type optical energy gap equal to 2.3eV, a result very similar to that of the researcher [15].

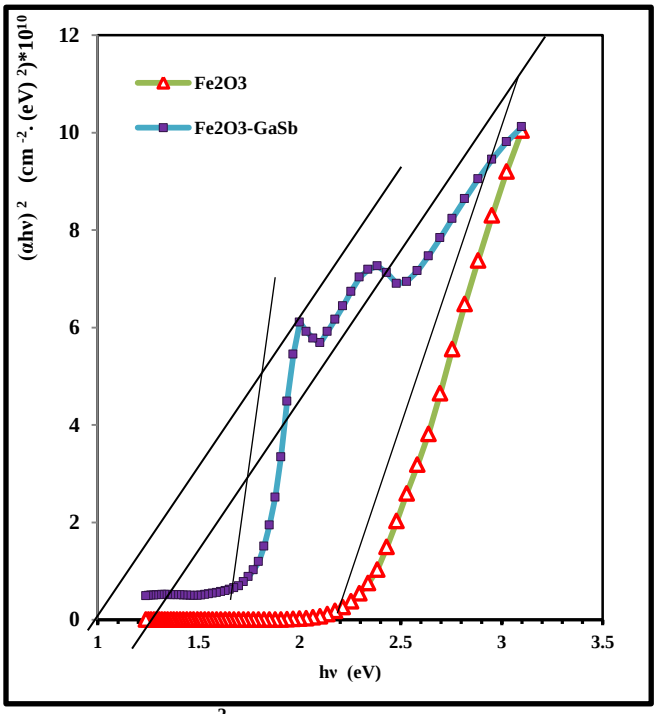

Figure 6: $(\alpha h\nu)^2$ as a function of photon energy

In general, when increasing the thickness of the nanowire by adding the GaSb shell, the value of the optical energy gap decreased. Three amounts for energy gap (1.2, 1.45 and 1.7) eV revealed from figure 6 returns to the sample Fe_2O_3-GaSb core-shell. This may be due to

the increase in the spot levels in the optical band gap area and hence decreased. There are several mechanisms that have been used to explain the change (increase or decrease) in the optical energy gap values, due to the change in quantum volume, changes in the height of the voltage barrier caused by the change in crystalline dimensions, differences in the added impurities that result in stress or tensile stresses of the crystalline surface and also improves or deforms the crystalline structure[22].

Conclusions:

The optical properties of the basic Fe_2O_3-GaSb nanowire are studied using Mie scattering theory. It is shown in the Fe_2O_3-GaSb structure led to increase the values of both the optical absorption spectra and absorption coefficient. This gives the possibility of using such samples in the processes of absorbent coatings, which are used in the coating of high-rise windows to absorb sunlight in low-temperature areas, in addition to use as effective surfaces in the manufacture of solar cells within this range of electromagnetic spectrum. Increasing the thickness of the nanowire caused by the adding of the GaSb shell leads to a decrease in the value of the energy gap and obtain three edge of optical absorption, illustrate the importance of these samples in the field of use as electronic gates in the field of light-emitting diodes. Through the study of the optical properties discussed in the Fe_2O_3-GaSbnanowires, it can play a key role in the manufacturing of optical electronic devices.

References:

[1] L. J. Lauhon, M. S. Gudiksen, D. Wang, and C. M. Lieber, "Epitaxial core–shell and core–multishell nanowire heterostructures," *Nature*, vol. 420, no. 6911, p. 57, 2002.

[2] S. Ju *et al.*, "Proton radiation hardness of single-nanowire transistors using robust organic gate nanodielectrics," *Appl. Phys. Lett.*, vol. 89, no. 7, p. 73510, 2006.

[3] U. Cvelbar, Z. Chen, M. K. Sunkara, and M. Mozetič, "Spontaneous Growth of Superstructure α-Fe2O3 Nanowire and Nanobelt Arrays in Reactive Oxygen Plasma," *Small*, vol. 4, no. 10, pp. 1610–1614, 2008.

[4] O. Lupan *et al.*, "Localized synthesis of iron oxide nanowires and fabrication of high performance nanosensors based on a single Fe2O3 nanowire," *Small*, vol. 13, no. 16, p. 1602868, 2017.

[5] Y. Fu, J. Chen, and H. Zhang, "Synthesis of Fe2O3 nanowires by oxidation of iron," *Chem. Phys. Lett.*, vol. 350, no. 5–6, pp. 491–494, 2001.

[6] Q. Yang, K. Tang, C. Wang, Y. Qian, and S. Zhang, "PVA-assisted synthesis and characterization of CdSe and CdTe nanowires," *J. Phys. Chem. B*, vol. 106, no. 36, pp. 9227–9230, 2002.

[7] P. Yang *et al.*, "Controlled growth of ZnO nanowires and their optical properties," *Adv. Funct. Mater.*, vol. 12, no. 5, pp. 323–331, 2002.

[8] Sarath Ramadurgam, Katherine Elizabeth Hansen, Tzu-ging Lin, Amartya Dutta, sulaiman Abdul-Hadi, Chen Yang (2018), "Optical Properties of Single Coaxial Nanowires,".(DOI: 10.4231/D3ZP3W30Z).

[9] S. Y. Wu, "Self-Assembly of Copper Oxide Core-Shell Nanowires Through Ethyl Alcohol," in *Nanowires-Recent Advances*, IntechOpen, 2012.

[10] H. I. Abdulah, A. M. Farhan, and A. J. Ali, "Photo-synthesis of nanosized α – Fe2 O3," *J. Chem. Pharm. Res.*, vol. 7, no. 6, pp. 588–591, 2015.

[11] A. S. Ibraheam, Jamal M. Rzaij, and M. A. Fakhri, "Structural, optical and electrical investigations of Al:ZnO nanostructures as UV photodetector synthesized by spray pyrolysis technique," 2019.

[12] Jamal M. Rzaij, "Characterization of CuO thin films for gas sensing applications," *Iraqi J. Phys.*, vol. 14, no. 31, pp. 1–12, 2016.

[13] P. A. K. Elttayef, A. Prof, M. H. Jaduaa, and M. A. Muhammed, "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, 2015.

[14] B. A. Hasan, Jamal M. Rzaij, and I. M. Ali, "Sensing Properties of (In2O3:Eu) Thin Films," *Aust. J. Basic Appl. Sci.*, vol. 10, no. 8, pp. 143–150, 2016.

[15] Bushra K.H.Al-Maiyaly, "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, 2014.

[16] Jubair A. Najeem and Jamal M. Rzaij, "Study the Effect of Thickness on Structural and Optical Properties of ZnO Thin Films Doped with 7% Cadimium Prepared by Chemical Spray Pyrolysisi Method," *J. Univ. Anbar Pure Sci.*, vol. 6, no. 3, pp. 138–145, 2012.

[17] N. F. Mott and Edward Arthur Davis, *Electronic processes in non-crystalline materials*. Oxford: Clarendon Pr., 1979.

[18] D. Depla and S. Mahieu, *Reactive sputter deposition*. Berlin: Springer, 2008.

[19] A. Tanushevski and D. Sokolovski, "Structural and optical properties of CdTe thin films obtained by electrodeposition," *RAD Conf. Proc.*, vol. 2, pp. 149–154, 2017.

[20] G. Zotti, G. Schiavon, S. Zecchin, and U. Casellato, "Electrodeposition of Amorphous Fe2O3 Films by Reduction of Iron Perchlorate in Acetonitrile," *JOURNAL- Electrochem. Soc.*, vol. 145, no. 2, pp. 385–388, 1998.

[21] M. F. Al-Kuhaili, M. Saleem, and S.M.A. Durrani, "Optical properties of iron oxide (α-Fe2O3) thin films deposited by the reactive evaporation of iron," *J. Alloys Compd.*, vol. 521, pp. 178–182, 2012.

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

P- ISSN 1991-8941 E-ISSN 2706-6703 *Journal of University of Anbar for Pure Science (JUAPS)* Open Access
2019,13 (2) :32-39

تصميم Fe_2O_3-GaSb كاسلاك نانوية للتطبيقات البصرية

سمير عبيد نواف

جامعة الانبار، كلية العلوم، قسم الفيزياء،الرمادي ،العراق

الملخص:

في هذا البحث تمت الدراسة النظرية لأسلاك نانوية من غلاف غاليوم انتيموند (GaSb) كقشرة ذات السمك 20 نانومتر وتأثيرها على الخواص البصرية لقلب حديدي من اوكسيد الحديد الثلاثي (Fe2O3) بسمك 20 نانومتر أيضا باستخدام نظرية الانتشار (Mie–Lorentz). اظهرت الدراسة ان اسلاك اوكسيد الحديد النانوية تمتلك نفاذية 95% ضمن مدى الطيف المرئي ومعامل امتصاص واطئ في منطقة الاشعة تحت الحمراء من الطيف الكهرومغناطيسي. كما اوضحت الدراسة انخفاض فجوة الطاقة من 2.3الى 1.7 الكترون فولت بوجود القشرة مع القلب الحديدي.