

Study the Optical Properties of (PMMA-PS-TiO₂) Nanocomposite

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Abstract

In this paper, the effect of titanium oxide nanoparticles on optical properties for (PMMA-PS) composite has been studied. The titanium oxide nanoparticles was added to the (PMMA-PS) composite for different weight percentages are (4, 8, 12) wt.%. The optical properties were measured in range of wavelength (200-1100) nm. The experimental results show that the absorbance of (PMMA-PS) composite was increased with the increase of titanium oxide concentrations. The optical constants and energy gap were changed with the addition of titanium oxide nanoparticles concentrations.

Keywords : Composite, titanium oxide, Optical Properties, polymethylmethacrylate, polystyrene

1. Introduction

Polymers are an important class of materials having different applications in various fields of science and technology, particularly in optics, electronics, biotechnology, photonics and space research [1]. Polymer composites have unique properties such as light weight, high flexibility, and ability to be fabricated at low temperature and cost [2]. In early works Polymers have been used as insulators because of their high resistivity and dielectric properties and It are widely used in electrical and electronic applications [3]. PMMA is a colorless transparent plastic, i.e. transmits light almost perfectly (92%), which make them suitable to serve as a conduit for light. Chloroform, which is used as a solvent for PMMA, is considered as the greatest soluble limit for PMMA; it has the greatest evaporation rates, less viscosity and the least chemical hazard than other solvents [4]. Polystyrene has attracted the attention of scientists for its interesting features and its superior physical and chemical properties. Polystyrene (PS) is amorphous polymer with bulky side groups. Major characteristics of PS include rigidity, transparency, high refractive index, good electrical insulation characteristics, low water absorption, and ease of processing which makes important for many applications in industry [5]. In this work,

we spot light on the optical properties of (PMMA-PS) with various condensation of TiO₂ to use the final product in some technical applications.

2- Experimental Work

The polymer composite consisting of (Polymethylmethacrylate (80 wt.%), Polystyrene (20 wt.%) solution was prepared by dissolving it in chloroform by using magnetic stirrer in mixing process to get homogeneous. The nanocomposites were added with different concentrations of the titanium oxide nanoparticles are (4, 8 and 12) wt.%. The absorbance and transmittance spectra of (PMMA-PS-TiO₂) nanocomposites are recorded by using UV/1800/ Shimadzu spectrophotometer in range of wavelength (200-1100) nm.

3. Results and Discussion

3.1 Transmission Spectrum :

Transmission Spectrum (T) is computed by using formula (1) [6]:

$$T=10^{-A} \quad (1)$$

where (T) is transmittance and (A) is absorption.

Figure (1) illustrates the transmission spectrum with different concentrations of TiO₂ nanoparticle as a function of the incident wavelength for (PMMA-PS-TiO₂) nanocomposites film. From this figure we can see that the transmittance declines with increase in the wavelength for all the samples and afterwards it nearly still same at higher value wavelength .

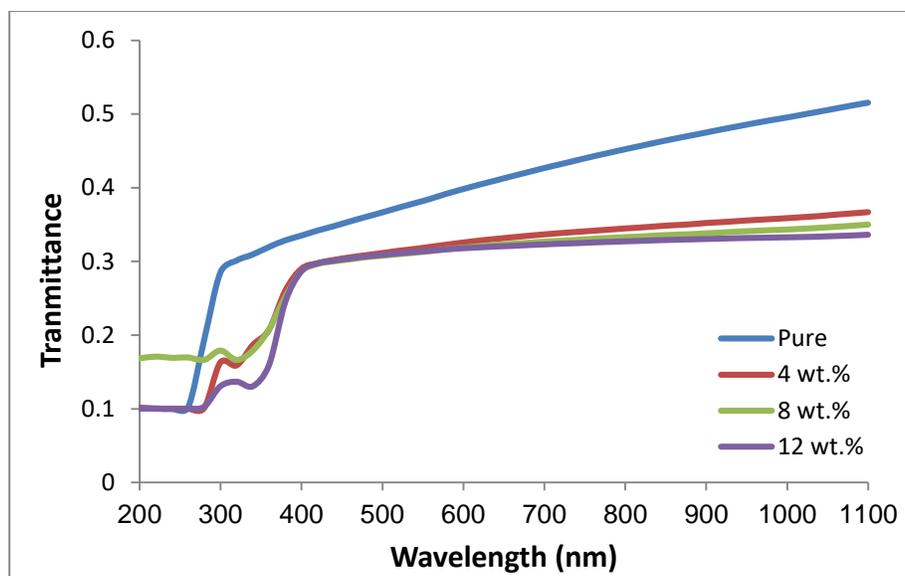


Figure (1): The transmittance versus wavelength for (PMMA-PS-TiO₂) nanocomposites.

3.2 Absorption Spectrum :

Absorbance is defined as the ratio between absorbed light intensity (I_A) by material and the incident intensity of light (I_0) [7]:

$$A = I_A/I_0 \quad (2)$$

The absorption at any wavelength depends on the number of particles along the way of the incident light (concentration) and the length of the optical path passing through the form as well as the temperature [8]. Figure (2) illustrates the relationship between absorption spectrum with wavelength of (PMMA-PS-TiO₂) nanocomposites. The intensity of the absorbance for composites are decreased with the increasing of wavelength and increases with the increase of weight percentages of filler, this is according to the absorbed light by free electrons [9].

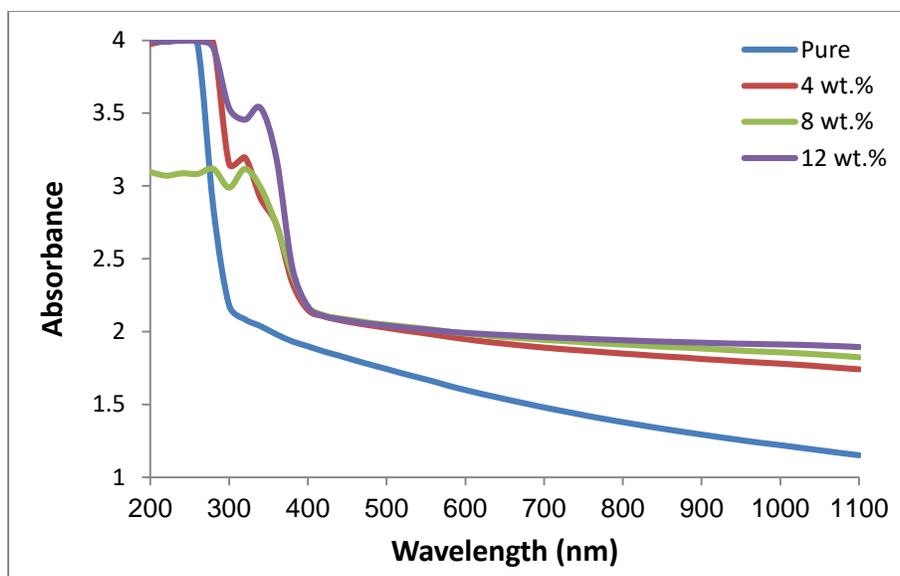


Figure (2): The absorbance versus wavelength for (PMMA-PS-TiO₂) nanocomposites.

3.3.The absorption coefficient and energy gap:

Figure (3) illustrates the link between the absorption coefficient versus the wavelength for (PMMA-PS-TiO₂) nanocomposites films. Its computed by using equation (3) [10]:

$$\alpha = 2.303A/t \quad (3)$$

where (A) absorbance and (t) is thickness.

The figure shows that the absorption coefficient increased with the increasing of the TiO₂ nanoparticle contain. The values of α are small at low energies because the probability of electrons transition are small, energy of the incident photon is not enough to move the electrons from the valence to the conduction band, whereas at high energies, the values of α are great, which lead to that probability of electrons transition are great because the energies of the incident photons are enough to move the electrons from the valence to the conduction band [11]. The absorption coefficient increased with the increasing of TiO₂ nanoparticle contain in the (PMMA-PS-TiO₂) nanocomposites.

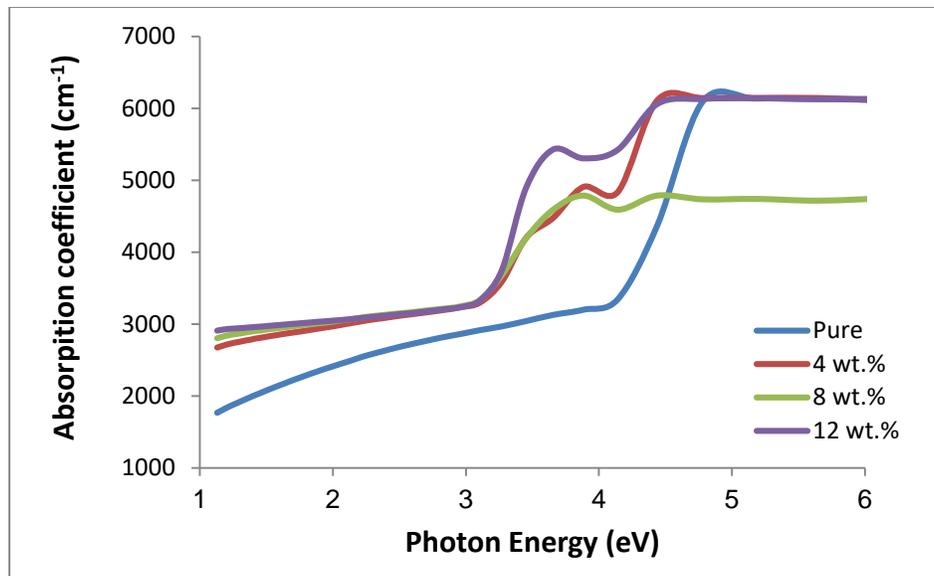


Figure 3: The absorption coefficient versus photon energy for (PMMA-PS-TiO₂) nanocomposites

The absorption coefficient help to know the nature of electron transition. If the values of the absorption coefficient are high ($\alpha > 10^4 \text{ cm}^{-1}$) lead to that transition of electrons are direct, and when the values of absorption coefficient are low ($\alpha < 10^4 \text{ cm}^{-1}$) lead to transition of electrons are indirect [12]. The obtained results showed that the absorption coefficient are lower than 10^4 cm^{-1} , which mean (PMMA-PS-TiO₂) nanocomposites have indirect energy gap.

The optical energy gap (allowed and forbidden) can be computed by using this formula [13]:

$$\alpha h\nu = B(h\nu - E_g)^r \quad (4)$$

where (E_g) is optical Energy gap, ($h\nu$) is the photon energy, (B) is a constant depending on the transition probability, and (r) is a number that characterizes the optical absorption

process, and can take the values; $r = 1/2$ for the allowed direct transition, $r = 1/3$ for the forbidden direct transition, whereas $r = 2$ for allowed indirect transition, $r = 3$ for the forbidden indirect transition. The usual method to calculate the energy band gap for indirect allowed and indirect forbidden transition is by drawing upright line from the upper part of the curve toward the x-axis at the value $(\alpha h\nu)^{1/2} = 0$. It can be seen that the values of allowed and forbidden indirect transition band optical energy gap declines with increasing the concentration of TiO₂ nanoparticle due to creation of new levels in the band gap, which lead to smooth the transition of electrons from the valence band to these local levels to the conduction band, thus the band gap declines [14,15], as shown in figures (4 and 5).

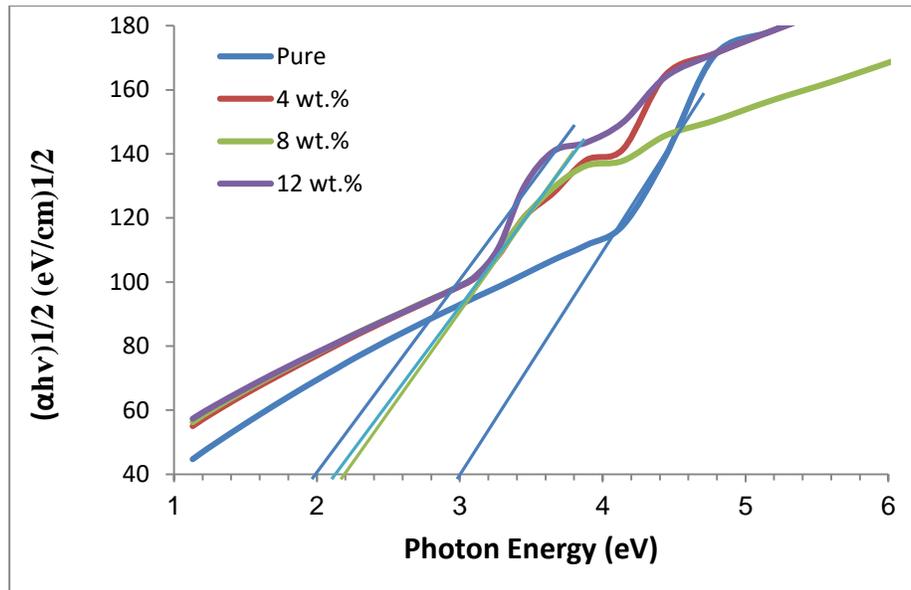


Figure (4):The plot of $(\alpha h\nu)^{1/2}$ with photon energy for (PMMA-PS-TiO₂) nanocomposites.

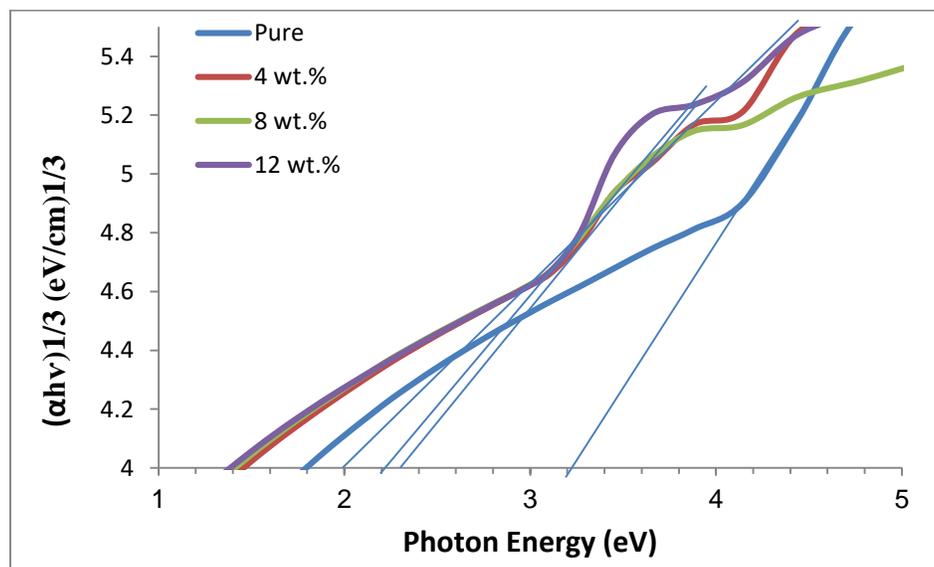


Figure (5):The plot of $(\alpha h\nu)^{1/3}$ with photon energy for (PMMA-PS-TiO₂) nanocomposites

The values of optical energy gap for indirect transition (allowed, forbidden) for the prepared films are shown in Table (1).

Table (1): The values of optical energy gap for the allowed and forbidden indirect transition for (PMMA-PS-TiO₂) nanocomposites

Samples	Optical energy gap for indirect transition	
	Allowed	Forbidden
0	3	3.2
4	2.2	2.3
8	2.1	2.2
12	2	2

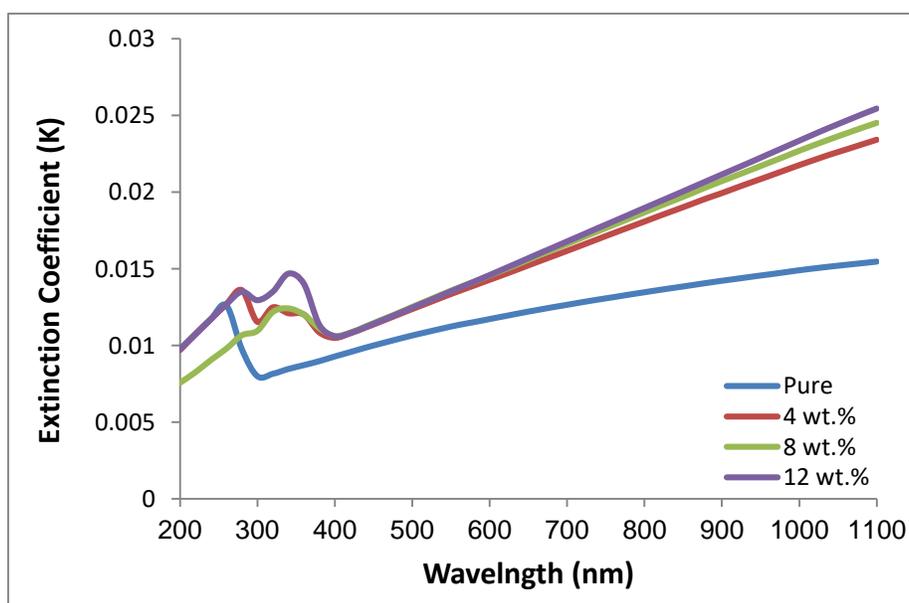
3.4 Extinction Coefficient

Figure (6) illustrates the diversity of extinction coefficient with photon energy for (PMMA-PS-TiO₂) nanocomposites. The extinction coefficient (k_o) is directly proportional to the absorption coefficient (α) and its computed by using formula (6) [16]:

$$k_o = \frac{\alpha\lambda}{4\pi} \quad (6)$$

where λ is wavelength of light.

From this figure, It can be noticed that k_o is increase with the increasing of TiO₂ nanoparticle concentration which related to the increase of absorb part of the incident light.



Figure(6):The Extinction coefficient versus wavelength for (PMMA-PS-TiO₂) nanocomposites.

3.5 Refractive Index

The figure (7) illustrates the link between refractive index and photon energy of the (PMMA-PS-TiO₂) nanocomposites composites with various content of TiO₂ nanoparticle. The refractive index (n) can be computed from the formula [17]:

$$n = (1+R^{1/2}) / (1-R^{1/2}) \quad (7)$$

where (R) is the reflectance.

From this figure, it can be noticed that the refractive index is increase with the increasing of the TiO₂ content according to the increase of packing density as a result of neodymium oxide content [18]

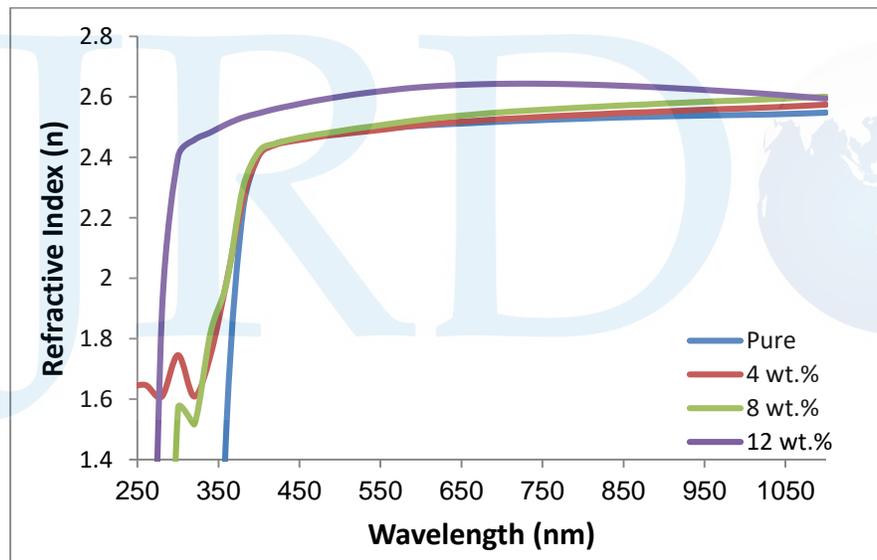


Figure (7): The refractive index versus wavelength for (PMMA-PS-TiO₂) nanocomposites.

3.6 The real and imaginary dielectric constants (ϵ_1 , ϵ_2)

Figures (7 and 8) illustrates the variation of real and imaginary parts of dielectric constant with wavelength for (PMMA-PS-TiO₂) nanocomposites. The real dielectric constant (ϵ_1) and imaginary dielectric constant (ϵ_2) are determined by using the formulas [19]:

$$\epsilon_1 = n^2 - k^2 \quad (8)$$

$$\epsilon_2 = 2nk \quad (9)$$

The variation of ϵ_1 mainly depends on (n^2) because of small values of the (k^2) , but the ϵ_2 mainly depends on the (k) values which are related to the variation of absorption coefficients. It can be seen that ϵ_1 and ϵ_2 increased with the increasing of NdO content which attributed to increase the absorption of incident light.

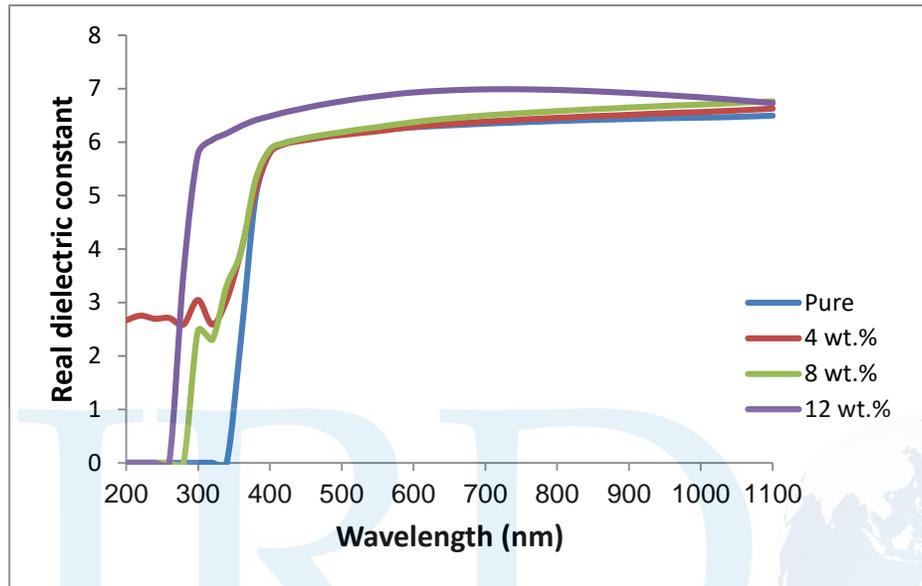


Figure (8): The real part of dielectric constant versus wavelength for (PMMA-PS-TiO₂) nanocomposites

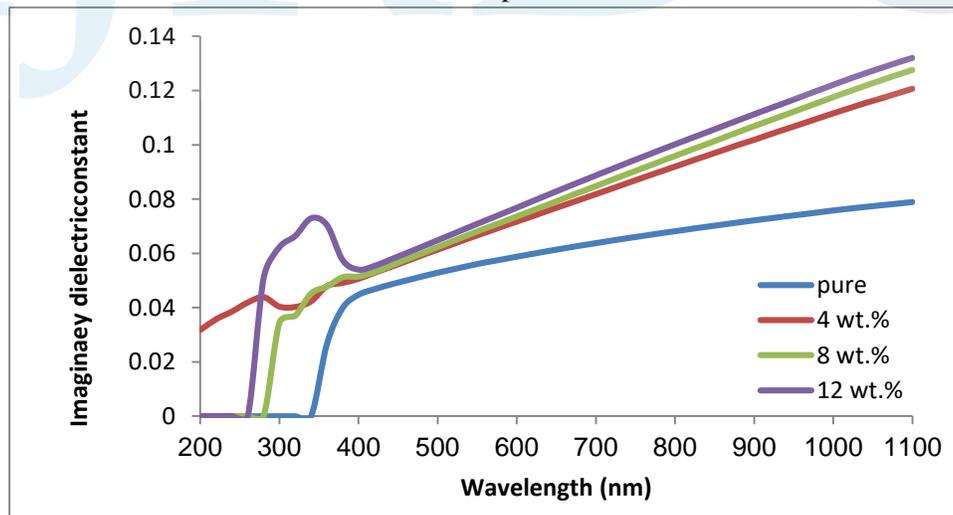


Figure (9): The imaginary part of dielectric constant versus wavelength for (PMMA-PS-TiO₂) nanocomposites

4 .Conclusions

The absorbance and the absorption coefficient for all (PMMA-PS-TiO₂) nanocomposites samples increases trend as the increasing of TiO₂.wt% concentration as well as the absorption coefficient is less than (10^4 cm^{-1}), this indicates to forbidden and allowed indirect electronic transitions., while the transmittance decreased. The energy band gap declines trend as the increasing of TiO₂.wt% concentration, while extinction coefficient, refractive index and real and imaginary parts of dielectric constant values are increased as a result of increasing of TiO₂.wt% concentration.

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References

- 1- Khalid Haneen Abass, Akeel Shakir Alkelaby, Musaab Khudhr M."Effect of Neodymium Oxide on Optical Properties of (PVA-PEG) Composites", Sun International Journal of Pharma, Medical and Allied Sciences, Vol.1, NO.1, pp.6–10.,(2017).
- 2- Asogwa p. u., Band gap shift and optical characterization of PVA- Capped PbO thin films : Effect of thermal annealing, Chalcogenide Letters, 8 (2011) 163-170.
- 3- Alias A. N., Zabidi Z. M., Ali A. M., Harun M. K., Optical Characterization and Properties of Polymeric Materials for Optoelectronic and Photonic Applications, Intern.J. of Applied Science and Technology, 3(2013) 11-38.
- [4] Y.F., Qian, Y. Su, X.G. Li, H.S. Wang and C.L.He,2010. Electrospinning of Polymethyl Methacrylate Nanofibres in Different Solvents, Iranian Polymer Journal,19(2): 123-129.
- 5- J P Walker and S A Asher , Analytical Chemical 77 (6), 2005, p. 1596
- 6- Musaab Khudhur Mohammed, Khalid Haneen Abass, Duha M.A. Latif., "Improvement in Optical Properties of (PVA-PEG) Composites By the Addition of Antimony Trioxide (Sb₂O₃)", Sun Journal of Chemical and Pharmaceutical Sciences, Vol. 1, No.1, pp. 6-9,(2017).
- 7- Mott F. N., Davis E. A., Electronic Processes in Non- crystalline Material, Oxford University press, Oxford, (1979).
- 8- Omed G., Abdullah, Dlear R. S., Luqman O. H., Complexion Formation in PVA/PEO/CuCl₂ Solid Polymer Electrolyte, Universal J. of Materials Sci., 1(2015) 1-5.
- 9- Mwolfe C., Holouyak N., Stillman G. N., Physical properties of Semiconductor, prentice Hall, New York, 8(2011) 163-170.
- 10- Hussein Hahim, Abdulameer Khalaf, Jameel Habeeb Ghazi, Ahmed Hashim, Musaab Khudhur," Optical Properties of Polyvinylpyrrolidone (PVP) Films Doped with Nickel Nitrate (NiNO₃)", International Journal of Science and Research., Vol.3, No.10, pp.1869-1870,(2014).
- 11- Kramadhathi S., Thyagarajan K., Optical properties of pure and doped (KNO₃ & MgCl₂) polyvinyl alcohol polymer thin films, Intern. J. of engineering research and development, 6(2013)15-18.

- 12- Kasap S. O., Principle of electronic materials and devices, 2nd edition, Mc Graw-Hill, New York, (2002).
- 13- Musaab Khudhr M. and Khalid Haneen Abass, "Effect of Al-doping on the Optical Properties of ZnO Thin Film Prepared by Thermal Evaporation Technique", International Journal of Engineering and Technologies, Vol. 7, pp. 25-31, (2016).
- 14- Sabah A. S., Asaad A. K., Maysam A. R., Preparation and Study of Some Optical Properties of (PVA-FeCl₃) Composites Films, J. of Chemical, Biological and Physical Sci., 6 (2016)1270-1280.
- 15-Khalid H. A. and Duha M. A., The Urbach Energy and Dispersion Parameters dependence of Substrate Temperature of CdO Thin Films Prepared by Chemical Spray Pyrolysis, Intern. J. of ChemTech Research, 9(2016) 332-338.
- 16- Frohlich H., Theory of Dielectrics, Oxford Uni. Press, (1958).
- 17- Zaky A., Hawley R., Dielectric solid, Routledge and kegan paul Ltd, London, Newyerk, (1970).
- 18- Adnan K., Influence of AlCl₃ on the optical properties of new synthesized 3-armed poly(methyl methacrylate) films, Turk J. of Chemistry, 34(2010) 67 – 79.
- 19-Khalid H. A., Spray pyrolysis deposition and effect of annealing temperature on urbach energy and dispersion parameters of Cu:NiO film, Material Sci. of An Indian J., 13(2015)145-150.

