

# Synthesis and Studying the Optical Parameters of Polyvinylpyrrolidone/Sic Nanoparticles

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**Abstract:-** Films (pvp-sic) were prepared on glass slides ,by adding carborundum nanoparticles (Sic) different ratios (2, 4 and 6) wt.% to the (PVP) polymer. Optical properties studied for(PVP-Sic) films, the results of experiments showed that the optical parameters (absorbance, absorption coefficient, reflectivity, refractive index, extinction coefficient and real -imaginary dielectric constant) , it generally increases with increasing weight ratio (Nano -Sic), sublimates in the ( UV -region ) and decreases in the (Vis. and Infr. Region ). The energy band gap decreases from (3.7 ev-2.8 ev) with increase weight additive of nanoparticles, which improves electron transmission, consequently improvement optical properties of the films, therefore it can be used in optical applications (LED lights, optical devices and display screens).

**Keywords:-**Carborundum · Nanoparticles · Optical Parameters · Refractive index

## 1. INTRODUCTION

In recent years, attention has shifted towards nanomaterials for obtaining new compact properties and features, they enter into optical and structural applications that are practically done. Electronic applications of Carborundum such as (LEDs) detectors and electronic devices with semiconductor content that operate on high voltages or degrees high temperatures, or both. PVP polymer is one of the important polymers due to its high stability, ease of handling, good physical and optical properties, rich in charge transport method, and it is one of the amorphous polymers has a high glass transition degree ( $T_g = 170^{\circ}\text{C}$ ) due to the presence of the solid group polyvinylpyrrolidone. When melted, it has properties that easily form in membranes, so this makes it a material that can be added to other materials which obtain optical and technological properties. It is also used in medicine for its low toxicity, as well as many other applications in electrochemical devices (screens)[1]. Polymer science is approaching a lot and combines with nanotechnology, and the dimensions of nanoparticles have not been mentioned in recent times, Carborundum or silicon carbide nanoparticles (SiC) is a semiconductor consisting of silicon and carbon. It is used in many applications, including those that need bearing capacity, such as in the automotive industry and electronic applications such as light-emitting diodes (LEDs) as well as in electronic devices that requires high heat or High voltages[2,3]. The composite materials based on nanoparticles and polymeric materials have evolved to an extent that they began to enter into several fields of their optical, electrical and chemical structural properties, which can be used to improve expand work of solar cells, sensors, electronic circuits and others. It consists of soluble polymers and the additive, whether they are metallic or Semiconductors, their ease of formation, their optical and

electrical properties, as well as they can be deposited on different substrates, And the number of scientific articles concerned with this topic became many and wide due to the decrease in cost and the researcher's obtaining of desirable properties, thus expanding the field of study for those materials[4].

## 2 . EXPERIMENTAL PROCEDURES

### a . Materials

Use the PVP polymer, a fine white powder that can dissolve in distilled water at room temperature, and other polar solvents[5]. With properties including: (melting point  $180^{\circ}\text{C}$  -density  $1.2 \text{ g/cm}^3$  - amorphous powder appearance white to light - yellow -hygroscopic ). It works in many applications including medical, technical, adhesive, film, in aqueous metal quenching and etc[6,7].

Likewise, silicon carbide (sic) nano-sized material (30n - 40n) has a gray green with characteristics: high stability, high purity, good corrosion resistance, oxidation resistance and etc. It has industrial applications such as making rubber tires, in modifying the strength of alloys and Optical properties in mirror coatings for high ultraviolet environments[8].

### b . Method and preparation

silicon carbide nanoparticles (sic) was added in different ratio (2,4,6 )% to a polymer (PVP) and prepared by casting technique on glass slides, and polyvinylpyrrolidone (PVP) was dissolved in (10ml) of distilled water, as well as using a magnetic stirrer device and left to dry at normal temperature. Optical properties were measured with a dual-beam spectrophotometer (Shi-madzu ,UV 1800A<sup>0</sup>) at wavelength (200-1000) nm. All samples with different ratios of silicon carbide nanoparticles addition were tested by optical microscope with a magnification power (x10). Various optical applications, including solar cells, microelectronic devices and optical devices and to clarify the effect of adding nan atoms (silicon carbide) to all samples in all regions of the light spectrum, as well as calculating all optical parameters.

The absorbance coefficient ( $\alpha$ ) was determined for all films using the equation[7,9]:

$$\alpha t = 2.303A \quad (1)$$

where t: the sample thickness, extract the thickness of the films using the gravimetric method and A: absorbance .

The occurrence of indirect transfer of amorphous semiconductors is represented by the following equation[7,10]:

$$(h\nu - E_g^{opt.})^r = \frac{\alpha h\nu}{B} \quad (2)$$

where B: constant depended on type of material.,  $h\nu$ : is the photon energy,  $E_g^{opt.}$ : energy gap between direct transition , r: exponential constant , its value depended on type of transition , r = 2 for allowed indirect transition and r = 3 for forbidden indirect transition .

The following equation shows the refractive index[10,11]:

$$n = \sqrt{4R - \frac{k_0^2}{(R-1)^2} - \frac{(R+1)}{(R-1)}} \quad (3)$$

Where R: is the reflectance. The extinction coefficient ( $k_0$ ) is calculated by using the following equation [11]:

$$\alpha\lambda = 4\pi K_0 \quad (4)$$

Where  $\lambda$  is the wavelength of incident light.

Optical conductivity calculated from the equation:

$$\sigma_{opt} = \alpha n c / 4 \pi \quad (5)$$

### 3.RESULTS AND DISCUSSION

Figure (1) shows the microscopic images of (PVP-Sic) films with different nanoparticle concentrations(0,2,4,6) wt.% and a magnify-cation power(10X).This is clearly evident at the film with concentration (6) wt.% [19,20 ].

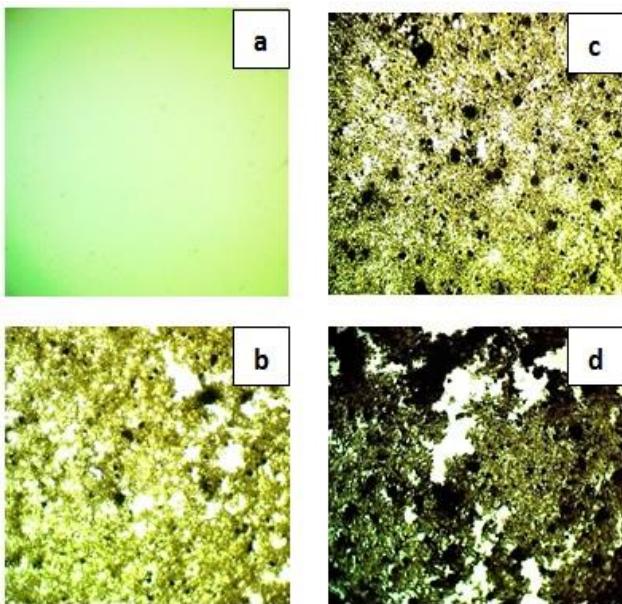


Fig. (1) :Photomicrographs (10X) for (pvp-sic) films : (a) pvp pure, (b) 2 wt.%, (c) 4 wt.%, (d) 6 wt. % .

After preparing( pvp-sic) films, figure (2) shows an increase in the absorbance spectrum when the (sic) concentration of nanoparticles increased, to increase the number of particles and atoms during the path of light. We

notice from the figure that the absorbance decreases at the wavelength (380nm) at the absorption edge, the incident photons do not have sufficient energy to interact with the atoms.

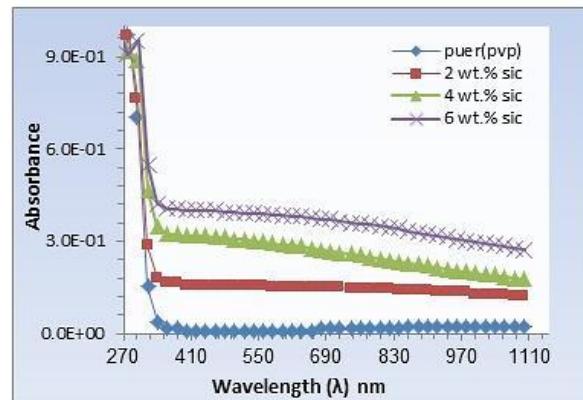


Fig. (2) :The absorbance as function of (λ) for (PVP-Sic) films.

Figure (3) shows the transmittance spec-trum for different concentrations as a function of the wavelength, we notice the decrease in transmittance with increasing concentration of (Sic) nanoparticles. This is caused by the added (Sic) nanoparticles, that contain electrons which absorb electromagnetic energy and move to a higher level. As for (pvp) film, it has high transmittance due to the absence of nanoparticles. It does not have free electrons and needs high energy to transition to break the bonds.

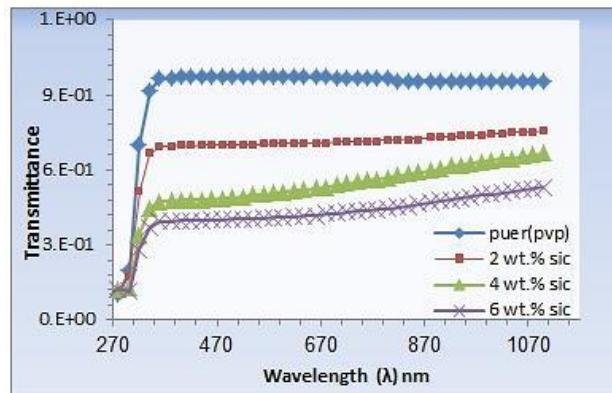


Fig.(3) :The transmittance as function of (λ) for (PVP-Sic) films.

Figure (4) shows reflectivity as a function of wavelength and we observe an increase in the reflectivity of the films with increasing the concentration of (sic) nanoparticles.

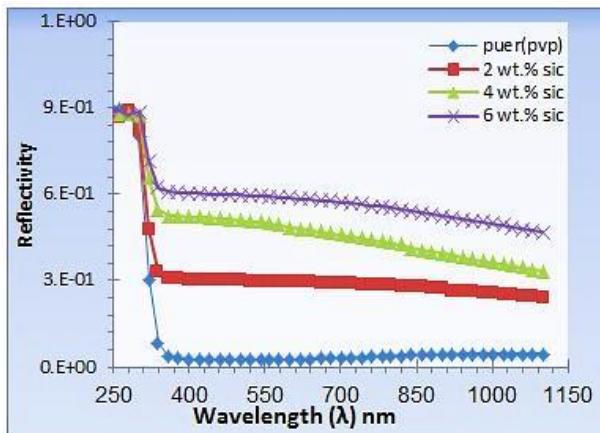


Fig.(4) :The reflectivity as function of  $(\lambda)$  for (PVP-Sic) films.

Figure (5) shows rapport between absorbance coefficient and  $(\lambda)$ , showing an increase in  $(\alpha)$  with the addition of a higher proportion of nanomaterials. This means  $(\alpha)$  is low at low energy, and electrons move slightly from the valence beam to the conduction beam. At higher energies, the absorption coefficient increases, and there is a greater electron transmission, and energy of the falling photon is greater than of  $(E_{ga})$ [12,13]. The absorption coefficient also shows two types of electronic transfers (direct, indirect) depending on the amount of the absorption coefficient.

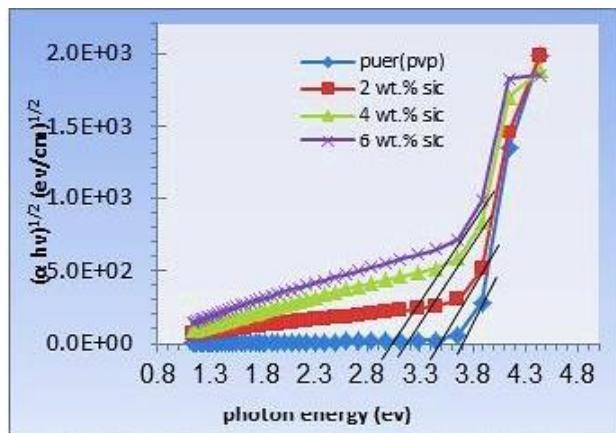


Fig. (6) : The energy gap for the allowed indirect transition  $(\alpha h\nu)^{1/2}$  as a function of photon energy of (PVP-Sic) films.

Figure (6) shows the energy gap for all films for different addition ratios of silicon carbide nanoparticles.

The indirect energy gap can be seen to decrease by adding a higher concentration of (Nano-Sic), this behavior is due to the formation of energy levels subsets of the  $(E_{ga})$  [13,14]. As shown in the table (1).

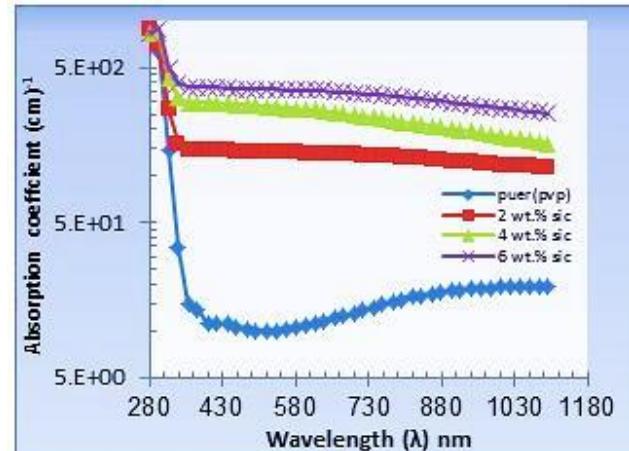


Fig. (5) :The absorption coefficient as function of  $(\lambda)$  for (PVP-Sic) film

Figure (7) shows the energy gap with respect to forbidden indirect transmission as a function of  $(E_{ph})$ , a decrease in  $(E_{ga})$  is observed with an increase to concentration of (Sic) nanoparticles[14,15].

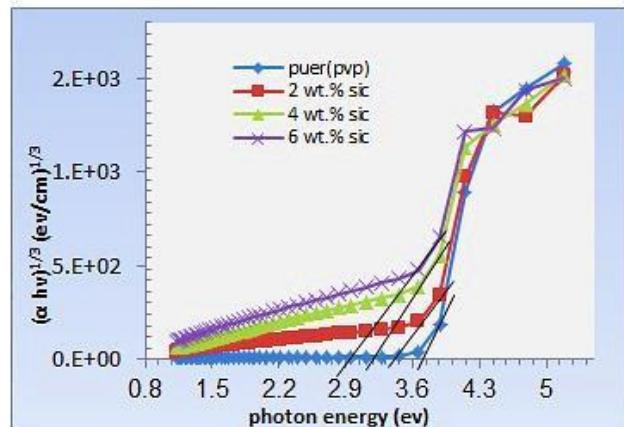


Fig. (7) :The energy gap for the forbidden indirect transition  $(\alpha h\nu)^{1/3}$  as a function of photon energy of (PVP-Sic) films.

Table (1) values of energy gap for the (forbidden and allowed) indirect transition for (PVP-Sic) films.

Silicon carbide nanoparticles wt. %	The values of $(E_{gap})$ indirect transition (eV)	
	allowed	forbidden
0	3.7	3.7
2	3.35	3.3
4	3.1	3
6	2.9	2.8

Figure (8) shows the extinction coefficient with respect to the wavelength of all (PVP-Sic) films. We see a rise in ( $K_0$ ) with an increase in the concentration of nanomaterials. These results demonstrate a change in the host polymer structure (PVP) [16].

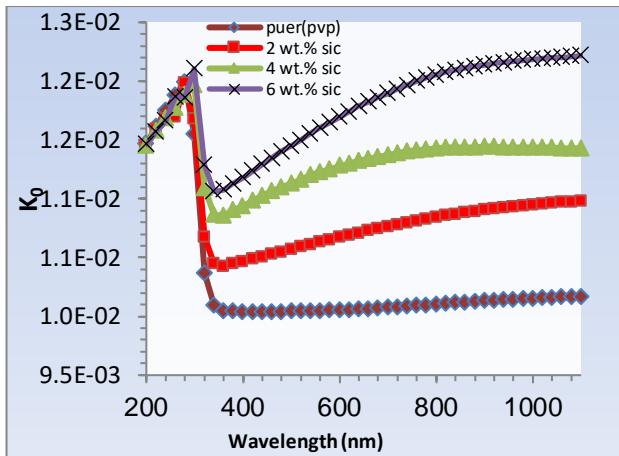


Fig. (8):The Extinction coefficient( $K_0$ ) as a function of wavelength for (PVP-Sic) films.

It is evident in figure (9) that the refractive index ( $n$ ) increases with the increase in the addition of nanoparticles, as well as the refractive index is high in the UV region, due to the lack of transmittance in it, as for visible region, the refractive index is low because the high transmittance, and this behavior has been shown in many previous studies.

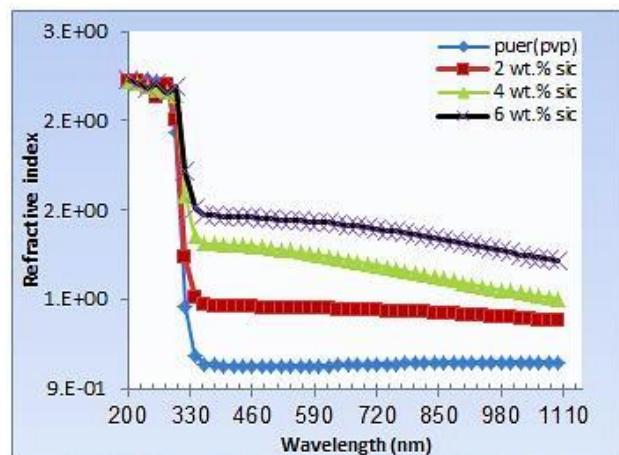


Fig. (9):The refractive index( $n$ )as a function of wavelength for (PVP-Sic) films.

Figures (10) and (11) show the real and imaginary dielectric constant as a function of the wavelength, as well as the shape can be understood from ( $E_{photon}$ ), where the imaginary and real parts of the dielectric constant decrease with increasing photon energy, and so do the isolation constants increase with increasing the concentration of nanoparticles. The data for dielectric constants ( $\epsilon_1, \epsilon_2$ ) provides knowledge of the loss factor, which is the ratio between real and imaginary dielectric constant [18,21].

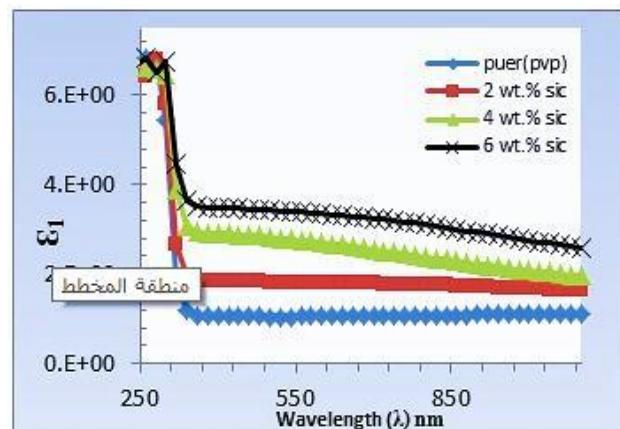


Fig. (10):The real dielectric constant( $\epsilon_1$ ) as a function of incident wavelength for(PVP-Sic) films.

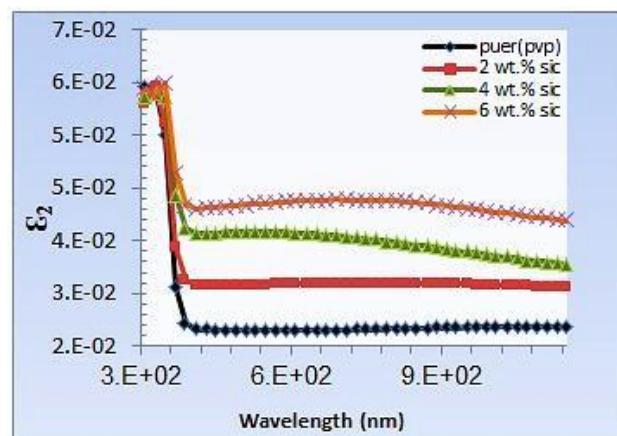


Fig. (11): The imaginary dielectric constant ( $\epsilon_2$ ) as a function of wavelength for (PVP-Sic) films.

Figure (12) shows the optical conductivity of (pvp-sic) films. An increase in optical conductivity is observed when increasing the nano-particle additive, especially in the ultraviolet region.

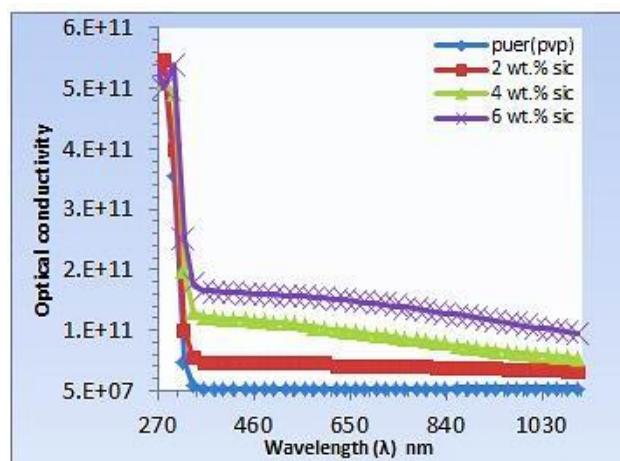


Fig.(12): Optical conductivity ( $\sigma_{opt}$ ) as a function of wavelength for (PVP-Sic) films.

#### 4.CONCLUSIONS

**1-**Absorbance increases for all (pvp-sic) films with increasing concentration of (sic) nanomaterial's, as well as increasing absorbance in ( UV ) region and decreasing in the (vis. and infr.) region.

**2-** energy gap of each (PVP-Sic) films decreases with increasing concentration of (sic) nanoparticles and allowing electrons to move from the valence beam to the conduction beam.

**3-**Optical parameters (absorption coefficient( $\alpha$ ), refractive index( $n$ ), extinction coefficient( $k_0$ ), real and imaginary dielectric constants(  $\epsilon_1$  ,  $\epsilon_2$ )) behave identically: their values increase by increasing the concentration of nano-materials and vary depending on the spectrum region.

#### REFERENCES

- [1] A.M. Abdelghany, E.M. Abdelrazek, D.S. Rashad, "Impact of in situ preparation of CdS filled PVP nano-composite", *J. Spectrochim. Acta A Mol. Biomol. Spectrosc.* ,130, PP.302-308 ,(2014).
- [2] Chen Z., Ahyi A.C., Zhu X., Li M., Isaacs-Smith T., Williams J.R. and Feldman L.C. ,"*MOS Characteristics of C-Face 4H-SiC*", *J. Of Elec. Mat.* , 39 , 5 ,PP. 526–529, (2010).
- [3] Márton Vörös ,Péter Deák , Thomas Frauenheim , and Adam Gali , "The absorption of oxygenated silicon carbide nanoparticles ",*J. of Chemical Physics* , 133, 6 ,(2010).
- [4] Qayssar M. Jebur , Ahmed Hashim and Majeed A. Habeeb , "Fabrication, Structural and Optical Properties for (PolyvinylAlcohol-Polyethylene Oxide- Iron Oxide) Nanocomposites",*Egypt.J.Chem.* , 63, 2 , pp. 611-623, (2020).
- [5] Haaf F., Sanner A. and Straub F. ,"*Polymers of N-Vinylpyrrolidone: Synthesis, Characterization and Uses*", *Polymer Journal*, 17,10,PP. 143–152, (1985).
- [6] Song G., Lin Y., Zhu Z., Zheng H., Qiao J., He C. and Wang H., "Strong Fluorescence of Poly(N-vinylpyrrolidone) and Its Oxidized Hydrolyzate", *J.Macromolecular Rapid Communications*, 36 , 3 .pp. 278–85,(2015).
- [7] A. Hashim and M. Ali Habeeb ,"*Synthesis and Characterization of Polymer Blend-CoFe2O4 Nanoparticles as a Humidity Sensors for Different Temperatures*",*J. Transactions on Electrical and Electronic Materials*, 20 , 2 , PP.107-112 , ( 2019).
- [8] H. Abderrazak , M. Abdellaoui ,"*Synthesis and Characterization of Nanostructured Silicon Carbide*",*J. Materials Letters* , 62,23,PP.3839-3841 , (2008).
- [9] N.K. Abbas, M.A. Habeeb, A.J.K. Algidsawi," Preparation of chloro penta amine cobalt(III) chloride and study of its influence on the structural and some optical properties of polyvinyl acetate", *Int. J. Polym. Sci.* , 10 (2015). (Article ID 926789)
- [10] W. Khalid Kadhim ,"*Preparation and Studying the Optical Properties of (Sb2o3) Thin Films*", *Journal of University of Babylon for Pure and Applied Sciences* ,26 , 10, PP. 249 – 256 ,(2018).
- [11] M. Ali Habeeb and W. Khalid Kadhim, "Study the optical properties of (PVA-PVAC-Ti) Nanocomposites ", *Journal of Engineering and Applied Sciences*,9,4,pp. 109-113,(2014).
- [12] A. Mohd Meftah ,E. Gharibshahi ,N. Soltani ,W. Mahmood Mat Yunus and Elias Saion ,"*Structural, Optical and Electrical Properties of PVA/PANI/Nickel Nanocomposites Synthesized by Gamma Radiolytic Method* ",*Polymers* , 6, 9 , pp.2435-2450, (2014).
- [13] K. Sivaiah, B. Hemalatha Rudramadevi , S. Buddhudu, G. Bhaskar Kumara and Varadarajulu," Structural, thermal and optical properties of Cu<sup>2+</sup> and Co<sup>2+</sup>: PVP polymer films ",*Indian Journal of Pure and Applied Physics* ,48, 9,pp.658-662, (2010).
- [14] N.Hayder, M.Ali Habeeb and A.Hashim," Structural, Optical and Dielectric Properties of (PS- In<sub>2</sub>O<sub>3</sub> /ZnCoFe<sub>2</sub>O<sub>4</sub>) Nanocomposites ", *Egypt.J.Chem.* , 62, pp. 577 - 592 (2019).
- [15] F.L.Rashid, A.Hashim, M.A.Habeeb, S.R.Salman and H. Ahmed ,"*Preparation of PS-PMMA copolymer and study the effect of sodium fluoride on its optical properties*", *Journal of Engineering and Applied Sciences*, 8 , 5 ,(2013).
- [16] N.S.Wadathkar and S.A.Waghuley," Complex optical studiesnon conducting polyindoleas-synthesized through chemical route", *Egypt. J. Basic Appl. Sci.* , 2, 1,pp. 19-24, (2015).
- [17] R. Mahmood Mohammed, M. Ali Habeeb and A. Hashim ,"*Effect of Antimony Oxide Nanoparticles on Structural, Optical and AC Electrical Properties of (PEO-PVA) Blend for Antibacterial Applications* ", *International Journal of Emerging Trends in Engineering Research*, 8 , 8 ,pp. 4726 – 4738, (2020).
- [18] Vlaeva, T. Yovcheva, S. Sainov, V. Dragostinova and S. Stavrev, "Optical properties of PVA films with diamond and titania nanoparticles", *J. of Phys. Conf. Ser.* , 253 , 1 ,pp.1-6, (2010).
- [19] H.M. Ragab," Spectroscopic investigations and electrical properties of PVA/PVP blend filled with different concentrations of nickel chloride", *J. Physica B* , 406, 20, pp.3759–3767, (2011).
- [20] W. Khalid Kadhim, M. Khalid Alshmmari , M. Adnan Al-Ethary ,"*Synthesis and Characteristics of (PAV-PAVC-Ti) Nanocomposites* ", *Iraqi Journal of Nanotechnology, synthesis and application* , 1 ,pp.21-26 ,(2020).
- [21] S. B. Aziz ,M. A. Brza ,Muaffaq M. Nofal ,Rebar T. Abdulwahid ,Sarkawt A. Hussen ,Ahang M. Hussein and Wrya O. Karim," A Comprehensive Review on Optical Properties of Polymer Electrolytes and Composites ",*Materials* , 13, 17, pp.3675-3729,(2020).