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Structural and Optical Properties of Novel (PS-Cr_2O_3/ $ZnCoFe_2O_4$) Nanocomposites For UV and Microwave Shielding

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THE (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanocomposites have been fabricated by solution casting method with different weight percentages of Cr_2O_3 nanoparticles and ZnCoFe2O4 are (0,2,4,6 and 8) wt.% for UV and microwave shielding applications.. The structural and optical of (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanocomposites have been studied. The structural properties include Fourier transform infrared spectroscopy (FTIR). The results of structural properties for spectroscopy (FTIR) showed shift in peak position as well as the change in shape and intensity compared with pure polystyrene. The results of optical properties for (PS-Cr_2O_3/$ZnCoFe_2O_4$) nanocomposites showed that the absorbance, absorption coefficient, dielectric constants and optical conductivity of polystyrene were increased with the increase in Cr_2O_3 nanoparticles concentrations while the transmittance and energy band gap were decreased with the increase of the Cr_2O_3 nanoparticles concentrations. The (PS-Cr_2O_3/$ZnCoFe_2O_4$) nanocomposites have high absorbance in the UV-region. The results of structural and optical properties showed that the (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanocomposites may be used for UV and microwave shielding.

Keywords: Polystyrene, Absorbance, Refractive Index, Microwave, Nanocomposites.

Introduction

The doped polymers may present useful applications in integrated optics or in real time holography. In order to tailor materials with improved properties within the doped polymer class, it is necessary to understand and control the electronic mechanisms involved in the optical behavior [1]. Polymer nanocomposites have recently attracted the great attention of scientists. The composites have been widely used in the various fields such as military equipment, safety, protective garments, automotive, aerospace, electronics, and optical devices. However, these application areas continuously demand additional properties and functions such as high mechanical properties, flame retardation, chemical resistance, UV resistance, electric conductivity, environmental stability, water repellency, magnetic field resistance, radar absorption. The nanocomposites are used in fields such as: humidity sensors, pressure sensors and piezoelectric applications, antibacterial, thermal energy storage and release and radiation shielding .Carbides have been broadly used in numerous fields, for instance composite ceramic materials, aerospace materials and wear resistance, because it has high melting temperature, high hardness, oxidation resistant, high thermal shock resistance and high abrasion resistance [2]. Polystyrene (PS) is amorphous polymer with bulky side groups. General purposes Polystyrene are hard, rigid, and transparent at room temperature and glass like thermoplastic material which can be soften and distort under heat. It is soluble in aromatic hydrocarbon solvents, cyclohexane and chlorinated hydrocarbons [3]. There has recently been a growing interest in developing antibacterial medical polymer materials. The reason for this attempt is the effort to reduce health

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complications caused by bacteria commonly found on various types of medical equipment. As the most types of the commonly applied polymers have no antibacterial action, they have to be modified to obtain polymer materials with the desired properties. The modification of virgin polymer with a bioactive agent is a possible method. In this case, the polymer is a carrier, providing transport and controlled release of bioactive substances into the environment where they are needed [4]. Transition metal oxide nanoparticles are important for both fundamental and application point of view. It can be used for the fabrication of microelectronic circuits, sensors, piezoelectric devices, fuel cells, coatings for the passivation of surfaces against corrosion, and chemical properties like reactivity, catalytic activity etc. Physical properties like electronic band gap, electrical conductivity and resistivity, color or optical transparency, nonlinear absorption or emission, fluorescence, phosphorescence were reported [5]. In general, the aims of preparation of nanocomposites or composites and studying its physical properties is improvement the properties of the matrix [6-15]. This work aims at the preparation of (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanocomposites and studying its structural and optical properties for modern applications.

Theoretical

Absorbance can be defined as the ratio between absorbed light intensity (IA) by material and the incident inten sity of light (Io)[16].

$A = I_A / I_o$ ……..(1)

Transmittance (T) is given by ratio of the intensity of the transmitting rays (IT) through the film to the intensity of the incident rays (Io) on it as follows [17].

$T = I_T / I_o$ ……..(2)

Absorption coefficient (α) is defined as the ability of a material to absorb the light of a given wavelength

$\alpha = 2.303A/t$ ……….(3)

Where A: is the absorption of the material t: the sample thickness in cm.

The absorption coefficient for this transition type is given by Taus relation [18].

$\alpha h\upsilon = B(h\upsilon - E_g^{opt})^r$ ………(4)

Where: E_g^{opt}. : energy gap between direct transition .

B: constant depended on type of material.

The Refractive index (n), the index of refraction of a material is the ratio of the velocity of the light in vacuum to that of the specimen:

$R = ((n-1)^2+k^2)/((n+1)^2+k^2)$

$R = (n-1)^2/(n+1)^2$ ..……(5)

$n = (1+R^{1/2})/(1-R^{1/2})$ ..……(6)

The extinction coefficient (k) was calculated using the following equation[19]:

$K=\alpha\lambda/4\pi$ ……..(7)

Dielectric constant is defined as the response of the material toward the incident electromagnetic field. The dielectric constant of compound (ǎ) is divided into two parts real(ε_1), and imaginary (ε_2).The real and imaginary parts of dielectric constant (ε_1 and ε_2) can be calculated by using equations [20]:

$$\varepsilon_1 = (n^2 - k^2) \quad ....(8)$$

$$\varepsilon = \varepsilon_1 - i\varepsilon_2 \quad ....(9)$$

$$\varepsilon_2 = (2nk) \quad ....(10)$$

The optical conductivity is defined by the following equation[21] :

$$\sigma = \frac{\alpha n c}{4\pi} \quad ………….(11)$$

Materials and Methods

The (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanocomposites were prepared from polystyrene (PS), chromium oxide (Cr_2O_3) and zinc cobalt iron oxides ($ZnCoFe_2O_4$). The nanoparticles was obtained as powder from US Research Nanomaterials, Inc, USA. The specimens were prepared using casting technique thickness ranged between (147-150)μm. The weight percentages of $ZnCoFe_2O_4$ nanoparticles which are added to (PS-Cr_2O_3) nanocomposites are (0,2,4,6 and 8) wt.%. FTIR spectra were recorded by FTIR (Bruker company, German origin, type vertex -70) Fourier transform infrared spectrometer in wavenumber range (500–4000) cm^{-1}. The UV/1800/ Shimadzu spectrophotometer device is used to measure the optical properties of (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanocomposites in the range of wavelength (260-820) nm

Results and Discussion

Figure 1 shows the FTIR spectra of pure Polystyrene taken at room temperature in the range 4000–500 cm^{-1}. The polystyrene doped by Cr_2O_3 nanoparticles. The characteristic peaks at 3260 cm^{-1} in the spectra are due to the presence of the stretching vibration of hydroxyl group OH of Polystyrene, while the spectral bands between 3500 and 3900 cm^{-1} are due to OH stretching vibration of Polystyrene, respectively and the bands around 2921 cm^{-1} correspond to the CH_2 asymmetric stretching. The C=O band at about 1705 cm^{-1} is important for further discussions, the position of this band indicates that the carboxylic acid groups form dimmers. The sharp band 1085 cm^{-1} corresponds to C-O stretching of acetyl groups present on the Polystyrene backbone which remains the same for undoped but broads for doped samples and the peak observed at about 650 cm^{-1} is due to the OH out of plane. The figures indicate the bonding nature between (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanoparticles and polymers [22].

The Absorbance and Transmittance

Figure 2 shows the spectral dependence of the absorbance of the **(**PS-$Cr_2O_{3/}$ $ZnCoFe_2O_4$) composites with different concentrations of salt. The absorbance is very large in the UV- region; this decay becomes relatively slower in the visible and near infrared regions, this attributed to the absorbance of polymers in the UV- region [23-28]**.** Figure 3 shows that transmittance spectrum as a function of wavelength for (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanocomposite. The figure shows that transmittance decreases with the increase in the concentration of $ZnCoFe_2O_4$ nanoparticles which is attributed to increase in absorption as a results increase in charges carries numbers [29-34].

The Absorption coefficient and energy gap of composite

The variation of the absorption coefficient of the nanocomposites with photon energy is shown in Fig. 4. From this figure, it can be seen that the absorption coefficient is increased with increasing of the $ZnCoFe_2O_4$ concentration which may be due to the absorption by the impurities .The absorption coefficient is smaller and stable in the low photon energy because of the scattering of the photon energy [35].

Figures 5 and 6 show the energy band gap of nanocomposites. From the values of the absorption coefficient, it can be concluded that the nanocomposites have indirect energy band gap. The energy band gap is calculated using Eq. (4) as shown in Fig. 3 and 4, it decreases with increasing the $ZnCoFe_2O_4$, this attributed to the decrease in the distant between the conduction band and valance band with the increase in $ZnCoFe_2O_4$ concentration [36].

Refractive Index and Extinction Coefficient

The extinction coefficient is calculated by using equation (7). Figure 7 shows the variation of extinction coefficient for (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanocomposites as a function of wavelength respectively. The figures shows that extinction coefficient increases with increasing the concentration of $ZnCoFe_2O_4$, this is due to the increase in optical absorption and photons dispersion in the Polystyrene polymer matrix [37]. The extinction coefficient of nanocomposites has high values at UV region, this behavior attributed to high absorbance of all samples of nanocomposites. Also, extinction coefficient of nanocomposites increases with the increasing of the wavelength at visible and near infrared regions which attributed to the absorption coefficient of nanocomposites which is approximately constant at visible and near infrared region, hence, the extinction coefficient increases with the increasing of the wavelength according to Eq. (7). The refractive index is calculated using Eq. (6). The refractive index of (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanocomposites as a function of wavelength is show, in Fig. 8. From this figure, it is noted that the refractive index decreases with increasing the weight percentages of the concentration of $ZnCoFe_2O_4$ in polystyrene, also it decreased with the increase of the wavelength. This behavior attributed to the scattering of the photons. This behavior is consistent with the results of researchers [38 ,39].

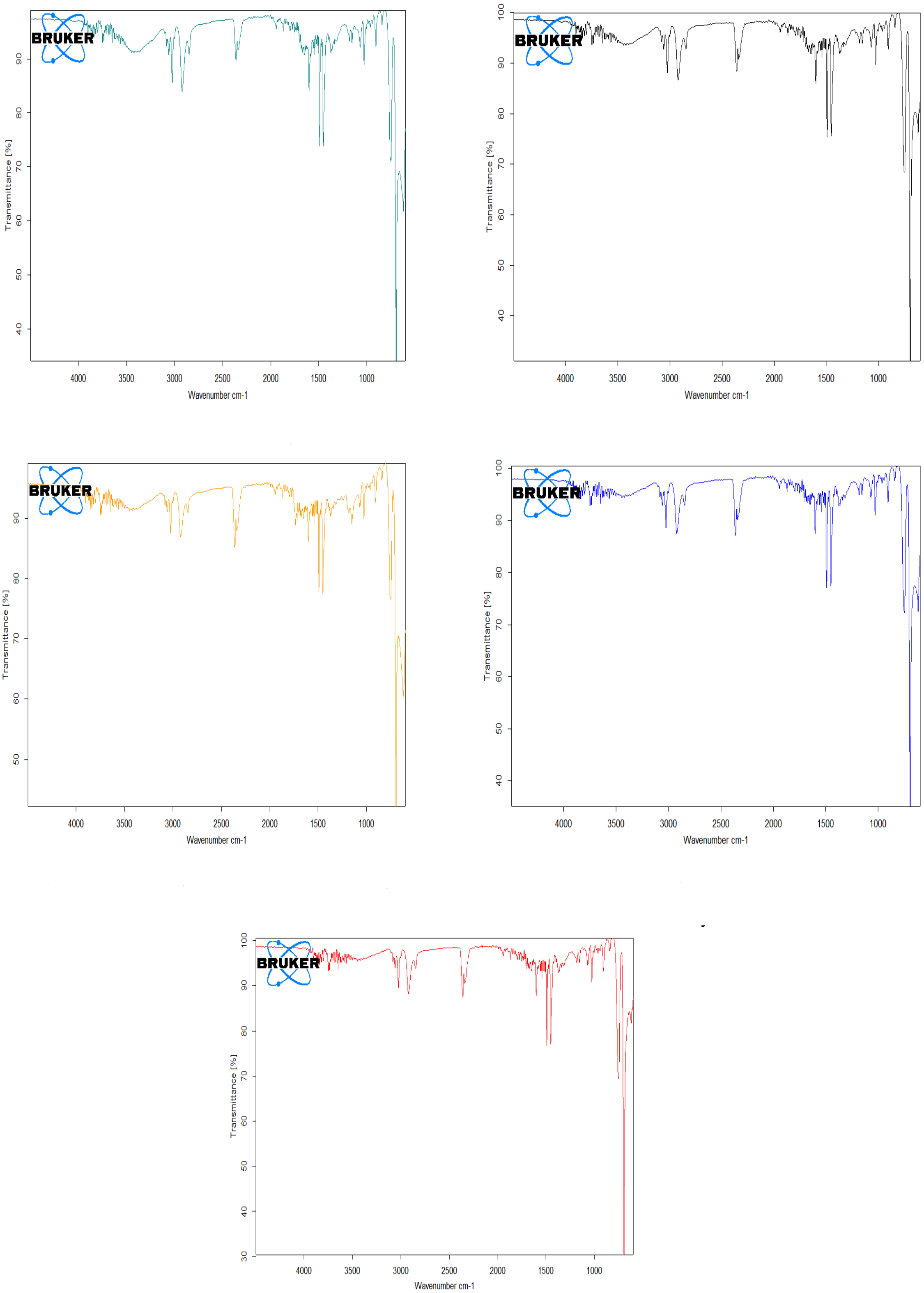

Fig. 1. FTIR spectra for (PS-Cr_2O_3/$ZnCoFe_2O_4$) nanocomposites A-for (PS-Cr_2O_3), B- 2 wt.% $ZnCoFe_2O_4$, C- 4 wt.% $ZnCoFe_2O_4$, D- 6 wt.%$ZnCoFe_2O_4$, E-8 wt.% $ZnCoFe_2O_4$

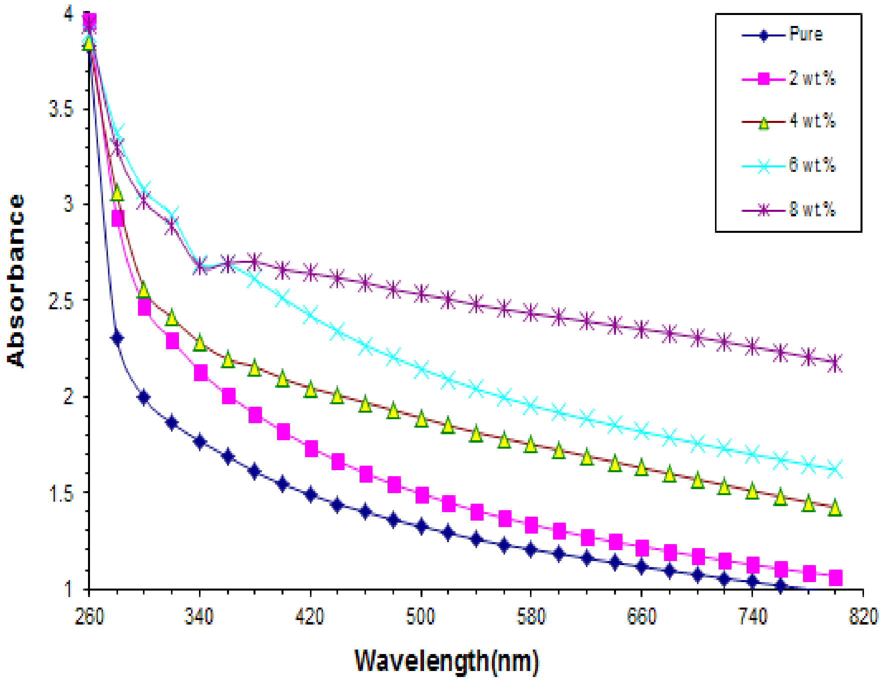

Fig. 2 . Variation of absorbance for (PS-Cr_2O_3/$ZnCoFe_2O_4$) nanocomposites with wavelength.

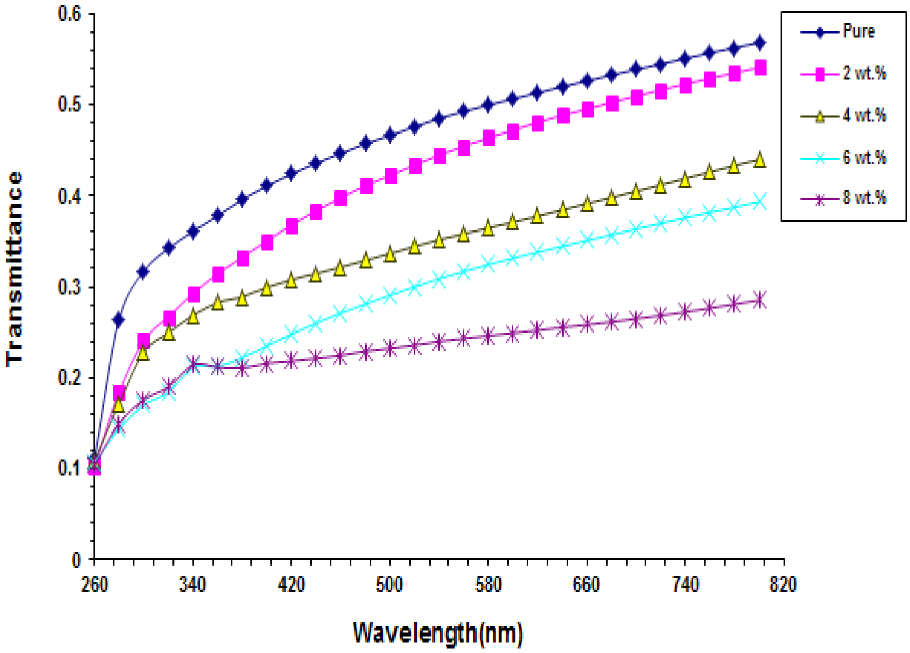

Fig. 3. Variation of transmittance for (PS-Cr_2O_3/$ZnCoFe_2O_4$) nanocomposites with wavelength.

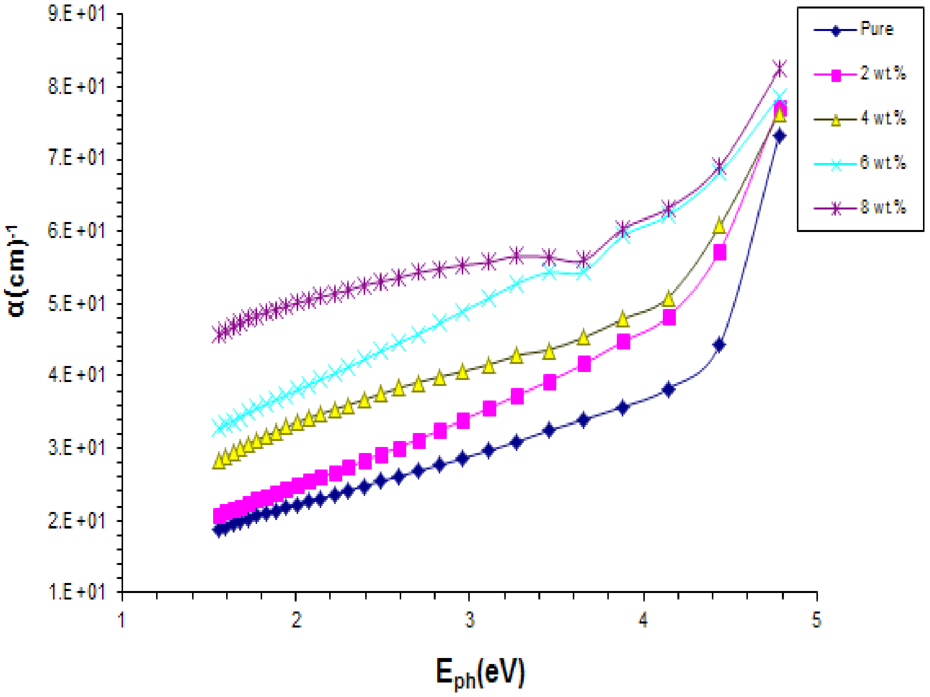

Fig. 4. Variation of absorption coefficient (α) for (PS-Cr_2O_3/$ZnCoFe_2O_4$) nanocomposites with photon energy

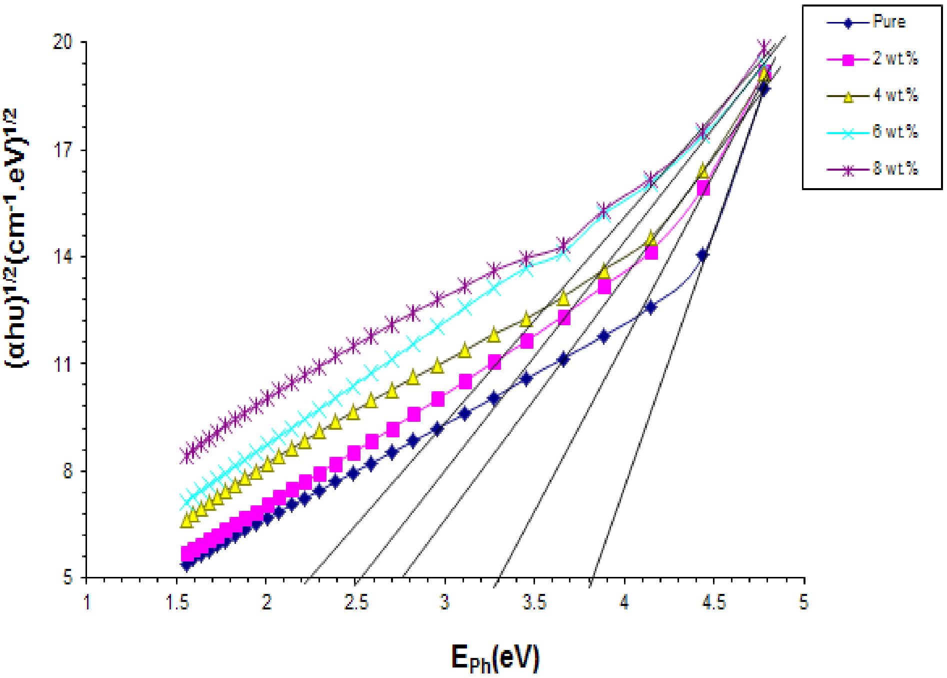

Fig. 5. Variation of $(\alpha h\upsilon)^{1/2}$ for (PS-Cr_2O_3/$ZnCoFe_2O_4$) nanocomposites with photon energy.

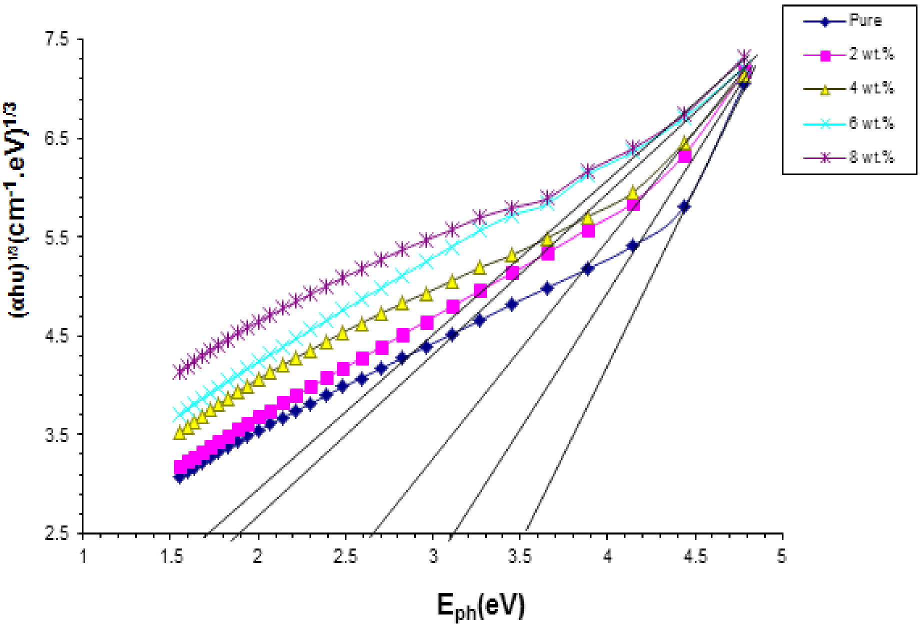

Fig. 6. Variation of $(\alpha h\upsilon)^{1/3}$ for (PS-Cr_2O_3/$ZnCoFe_2O_4$) nanocomposites with photon energy.

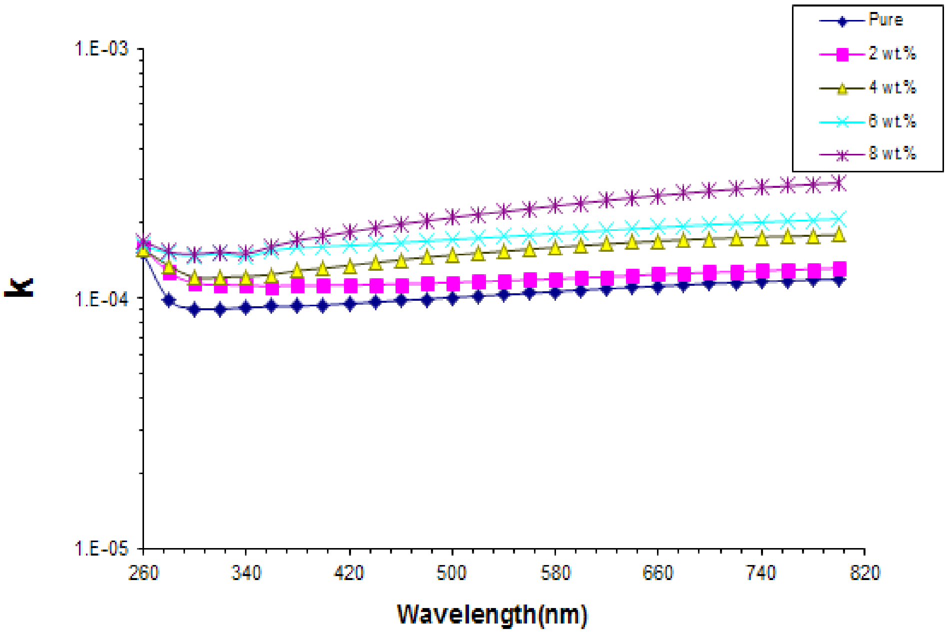

Fig. 7. Variation of extinction coefficient for (PS-$Cr_2O_{3/}ZnCoFe_2O_4$) nanocomposites with wavelength.

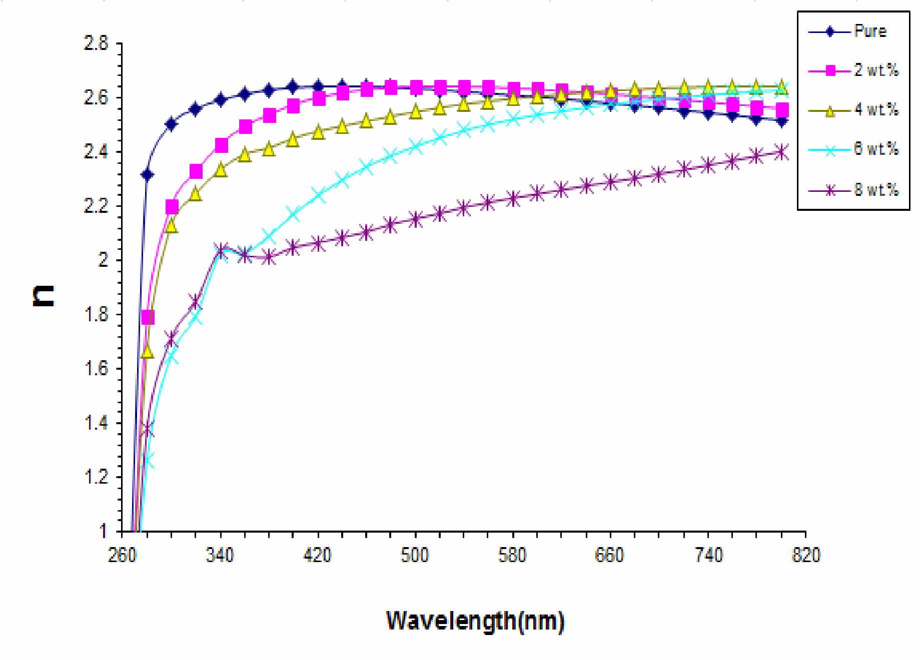

Fig. 8. Variation of refractive index for (PS-Cr_2O_3/$ZnCoFe_2O_4$) nanocomposites with wavelength.

The Real and Imaginary Parts of Dielectric Constant

The real and imaginary parts of dielectric constant are calculated using Eq (8) and (10), respectively. Figure 9 shows the variation of the real dielectric constant with the wavelength for (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanocomposites as a function of wavelength respectively. The effect of Cr_2O_3 nanoparticles on the imaginary part of dielectric constant is shows in Fig. 10 for (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanocomposites . The figures show that the real part increase while imaginary part decreases with the increase of $ZnCoFe_2O_4$ concentration; this behavior due to the decrease in refractive index values and increases in extinction coefficient values. As shown in the figures, the real and imaginary parts of dielectric constant of polystyrene are changed with the wavelength, this is due to the real part of dielectric constant depending on refractive index because the effect of extinction coefficient is very small and the imaginary part of dielectric constant depends on extinction coefficient especially in the visible and near infrared regions of wavelength where the refractive index is approximately constant while extinction coefficient increases with the increase of the wavelength. This behavior is consistent with the results of researchers [40,41].

The Optical Conductivity

Figure 11 shows the variation of optical conductivity with the wavelength for (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanocomposites. The figure shows that the optical conductivity of all samples of nanocomposites are decreased with the increasing of the wavelength, this behavior which is attributed to the optical conductivity depending strongly on the wavelength of the radiation incident on the samples of nanocomposites; the increase of optical conductivity at low wavelength of photon is due to high absorbance of all samples of nanocomposites in this region, hence, increase of the charge transfers excitations. The optical conductivity spectra indicated that the samples are transmittance within the visible and near infrared regions. Also, the optical conductivity of nanocomposites is increased with the increase of $ZnCoFe_2O_4$ concentrations, this behavior is related to the creation of localized levels in the energy gap; the increase of $ZnCoFe_2O_4$ concentrations increasing the density of localized stages in the band structure, hence, an increase in the absorption coefficient consequently increasing the optical conductivity of (PS-Cr_2O_3/$ZnCoFe_2O_4$) nanocomposites. This result is similar to the results of the researcher [42,43].

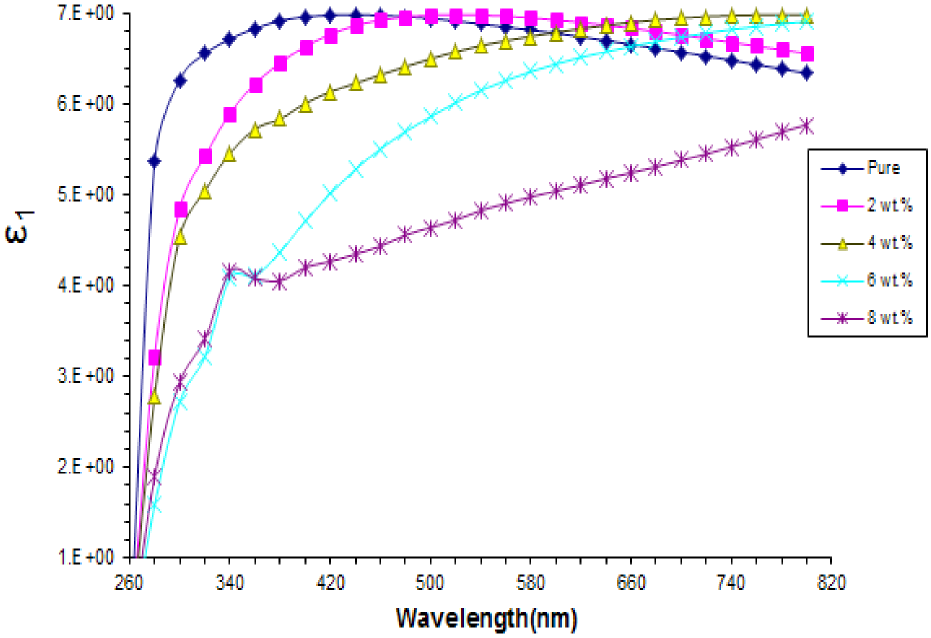

Fig. 9. Variation of real part of dielectric constant for (PS-Cr_2O_3/$ZnCoFe_2O_4$) nanocomposites with wavelength.

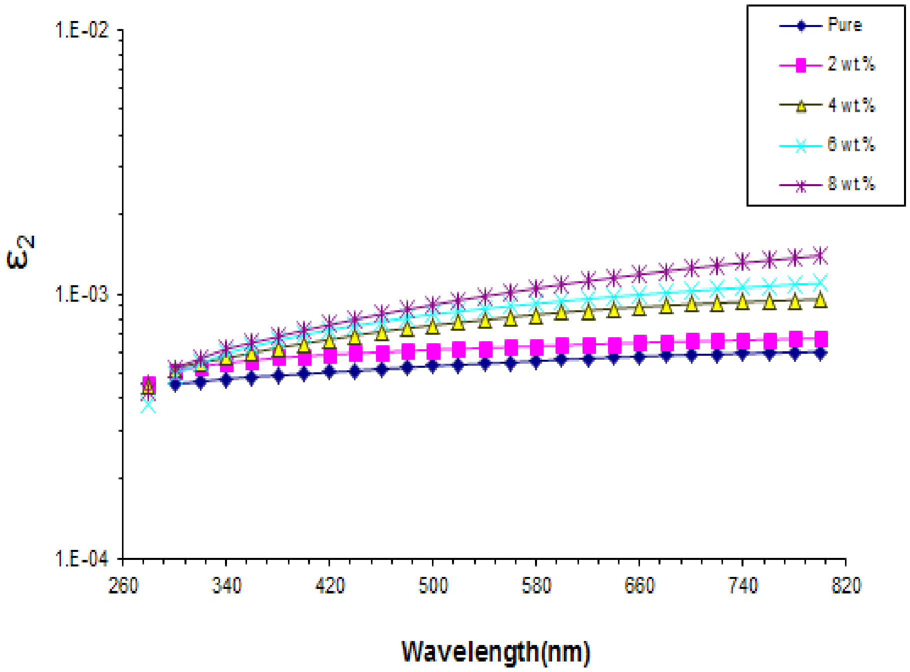

Fig. 10. Variation of imaginary part of dielectric constant for (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanocomposites with wavelength.

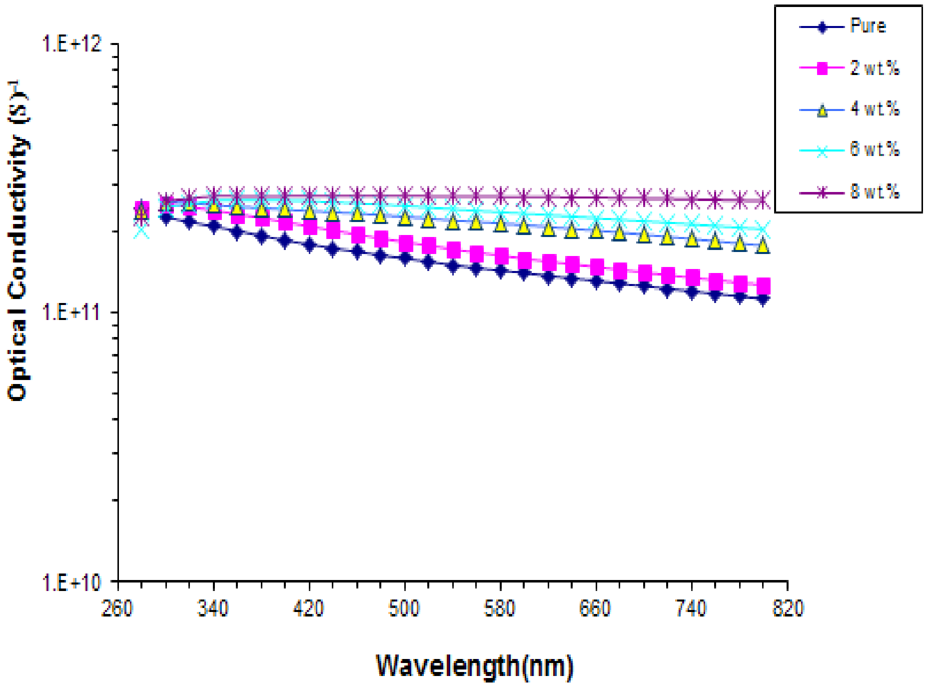

Fig. 11. Variation of optical conductivity for (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanocomposites with wavelength.

Conclusion

1. The absorbance, absorption coefficient and optical conductivity of (PS-Cr_2O_3) are increased with the increase in $ZnCoFe_2O_4$ nanoparticles concentrations.
2. The transmittance and energy band gap for allowed and forbidden indirect transitions are decreased with the increase in weight percentages of $ZnCoFe_2O_4$ nanoparticles.
3. The refractive index , extinction coefficient, real and imaginary parts of dielectric constant of (PS-Cr_2O_3) are increased with the increase in $ZnCoFe_2O_4$ nanoparticles concentrations.
4. The optical results showed that the (PS-Cr_2O_3/ $ZnCoFe_2O_4$) nanocomposites can be used for good UV-shield with low cost, low weight and high mechanical properties.

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