RESEARCH PAPER | Physics | Volume : 6 | Issue : 7 | July 2016 | ISSN - 2249-555X | IF : 3.919 | IC Value : 74.50

Structure and Optical Characterization of Polystyrene Doped With Zinc Oxide Nanoparticles

KEYWORDS: polystyrene, ZnO nanoparticles, optical properties.

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ABSTRACT *A simple and inexpensive method for preparation different concentrations of zinc oxide ZnO doped with polystyrene. Zno was prepared by precipitation method. Thin films of polystyrene (PS) with different concentrations (0, 0.5,1 and 2 wt. %) of ZnO nanoparticles (ZnO NPs) as a filler were prepared by using solution cast technique. Structural and optical studies have been performed using X- ray Diffraction (XRD), Transmission Electron Microscopy (TEM). Optical properties have been measured by using UV- Vis spectroscopy. The study has been extended to include the changes in the optical parameters including the band tail and band gap energies for the samples.*

1 Introduction:

In recent years, polymers with different optical properties have been attracted much attentions due to their application in the sensors, light-emitting diodes, and others. The optical properties of these materials can be easily tuned by controlling the filler concentrations[1-3].

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 reflective index, good electrical insulation characteristics, low water absorption, and ease of processing which makes important for many application in industry[4,5]. Moreover, PS is traditionally considered as an excellent host material for composites.

Recently much attention has been given to studies the organic/ inorganic nanocomposite materials with various compositions. By combining organic and inorganic materials, the resulting composites can posses advantages of both organic polymers (e.g., rigidity, high thermal stability, strength, hardness, high reflective index[6]. Among the many inorganic materials zinc oxide (ZnO) has been intensively studied as a promising material for optoelectronic devices such as light emitting diodes (LED) and flat display screens and as an interesting material for solar applications due to its unique combination of optical and semi conducting properties[7-9].

2 Experimental:

2.1 Materials:

Polystyrene, Toluene was used as a solvent for PS. Zinc sulfate ($ZnSO_4$), and ammonium bicarbonate (NH_4HCO_3).

2.2 Synthesis of ZnO nanoparticles:

Zinc oxide nanoparticles have been synthesis by precipitation method. In this method zinc sulfate 1.5 mol/L and ammonium bicarbonate (2.5 mol/L) were prepared in distilled water and 100 ml of $ZnSO_4$ solution was added to 126 ml NH_4HCO_3 solution while stirring at 45° C. the slurry of basic zinc carbonate (BZC) in the form of a white precipitate was obtained, filtered, washed and dried. Finally zinc oxide nanoparticle was obtained by calcining the precipitation at 500° C for 1 hour[10].

2.3 Synthesis of ZnO/ PS nanocomposite:

Thin film of ZnO/PS nanocomposite were prepared by using solution –cast technique[11]. PS was dissolved in toluene using hot plate magnetic stirrer at 50° C for I hr to obtain homogeneous solution. Then ZnO was added to the homogeneous solution of PS in different weight (0.5, 1 and 2 %). For maximum dispersion the solution was further stirrer for 2 hrs while keeping the temperature constant. By pouring the solution on optically plane glass plate thin film was obtained.

2.4 Characterization Techniques:

X-ray Diffraction patterns have been recorded using X-ray Diffratometer with Cu-Kα (1.542 A°) radiation operating at 40 KV and 25 m A, The morphology and particle size of zinc oxide were examined using JEOL GEM 3010 Transmission Electron Microscope operating at 300kv. Absorption spectra have been recorded using UV/Vis spectrophotometer in wavelength range of (190-900) nm.

3 Theoretical:

From optical absorption spectrum, absorption coefficient (α) can be determined using the following equation[12].

$$\alpha = 2.303\ A/d \qquad (1)$$

where d is the film thickness in cm and A is the defined by $\log(I_o/I)$ where I_o and I are the intensity of the incident and transmitted beams respectively.

The absorption edge for direct and non direct transition can be determined from this equation[13].

$$\alpha h\nu = C_o\,(h\nu - E_g^{opt})^n \qquad (2)$$

where, α is the absorption coefficient, ν is the frequency, h is plank constant, C_o is a constant, E_g^{opt} is the optical energy band gap between the valnce and conduction band and r is the power that characterizes the transition process. Specificially, n can take the value 1/2, 3/2, 2 or 3 for transition designated as direct allowed, direct forbidden, indirect allowed and indirect forbidden respectively[14].

The reflective (R) can be calculated from values of transmission (T), and Absorbance (A), using the relation:

$$A+R+T=1 \quad (3)$$

For normal reflectance, the reflective index can be calculatedfrom the relation:

$$n = 1+\sqrt{R} / 1-\sqrt{R} \quad (4)$$

Where the extinction coefficient K is related to the absorption coefficient α by the relation:

$$K = \alpha\lambda / 4\pi \quad (5)$$

λ is the incident photon wavelength.

4 Results and Discussion:

4.1. X-ray Diffraction (XRD) andTransmission Electron Microscope (TEM):

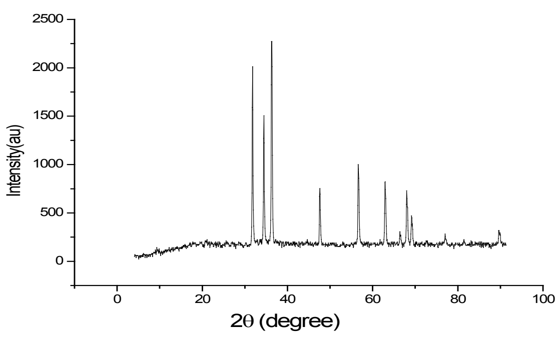


Figure (1). XRD pattern of ZnO nanoparticle.

Fig. (1) shows the XRD pattern of synthesis ZnO nanoparticles, eight apparent different peaks at 2α = 31.812°, 34.47°, 36.32°, 47.62°, 55.22°, 62.94°, 68.02° and 69.15° was observed, these peaks corresponding to the (100), (002), (101), (102), (110), (103), (112) and (001) planes of the hexagonal structured

ZnO**.** The broadening of XRD peaks indicates the formation of nanosized particles in the prepared sample the average particle size is determined from the X-ray line broadening using the scherrer equation. Fig. 1. depicts the TEM image of as synthesis ZnO nanoparticles which are in good agreement with XRD results in size estimation.

Fig. 2shows the XRD patterns of polystyrene doped with different concentrations of ZnO nanoparticles, the pattern showed a broad, noncrystalline peak of PS and more intense and crystalline diffraction peaks of ZnO. The presence of ZnO produces neither new peaks nor peak shift with respect to PS which indicates that nano ZnO filled PS composites consist of two –phase structure.

Figure (2). XRD pattern of ZnO/PS with different concentration.

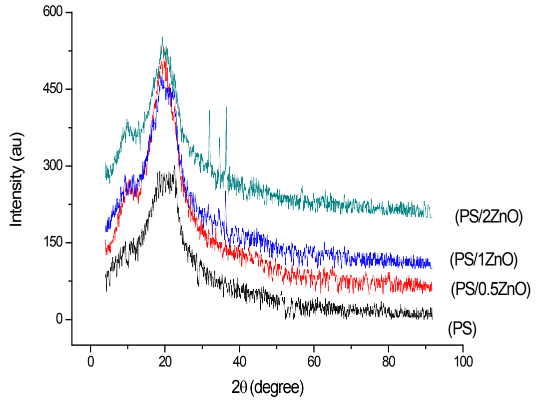
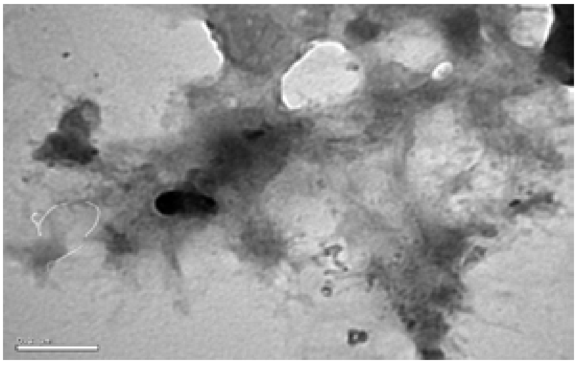
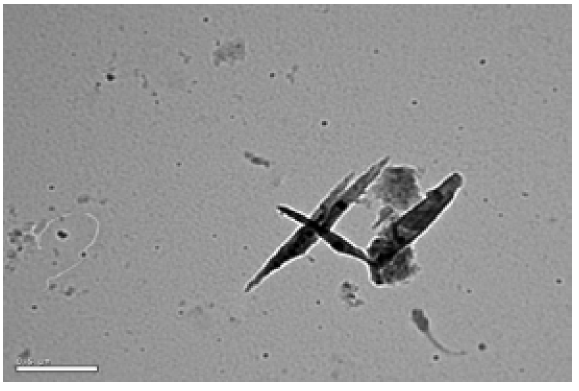


Fig. (3.a) shows the micrograph of ZnO/PS nanoparticles with 0.5% concentration of ZnO nanopaticles. It can be shown that ZnO nanoparticle disperses in polymer with size 13 nm spherical nanoparticle. Fig. (3.b) shows the micrograph of ZnO/PS nanoparticles with concentration 1% ZnO nanopaticles, nanoparticle appeared in micrograph more homogenous and more distribution by increasing concentration of ZnO nanoparticle.



(a)



(b)

Figure (3) (a,b)TEM image of ZnO/PS nanoparticle with different concentration (0.5, 1) of ZnO.

4.2. The Optical Parameter:

The obtained optical parameters of PS are found to be strongly affected by ZnO NPs used as filler. Fig (4) shows the absorption spectra of the prepared samples. The absorptions increases as the ZnO percentage increases, add-

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ing different concentration of filler material to the polymer do not change the chemical structure of the polymer but new physical properties to the mixture will formed. This result agree with previous studies[15].

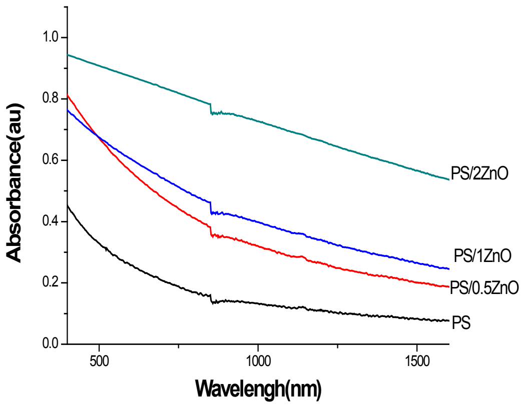

Figure (4). Variation of the absorbance against wavelength

Fig. (5) Shows an optical transmittance spectrum as a function of incident wavelength on ZnO doped PS films. The transmittance percent decrease with increasing filler concentration, this is because of layer of covalent bonds formed between polymer chains and additives which decrease the transmitting of the incident light especially at the shortest wavelengths[16].

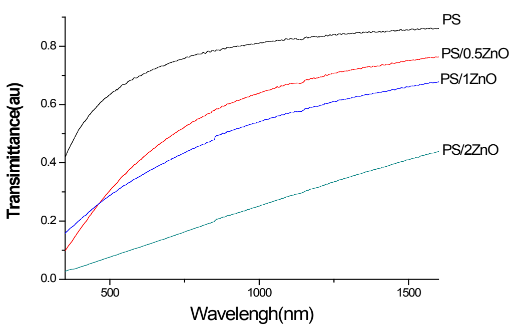

Figure (5). Variation of the transmittance against wavelength

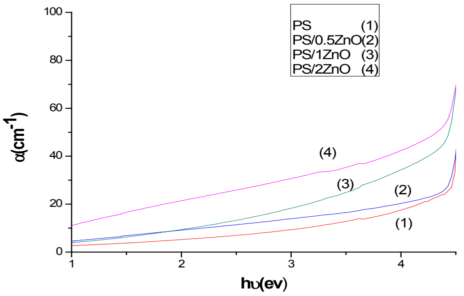

Figure (6). Variation of the absorbance coefficient against wavelength

Fig. (6) Shows the relationship between the absorption coefficient and photon energy of the PS/ZnO nanoparticles.

It was observed that at high energy, absorption is great and the forbidden energy gap is less which indicates that there is a large probability of electronic transitions.

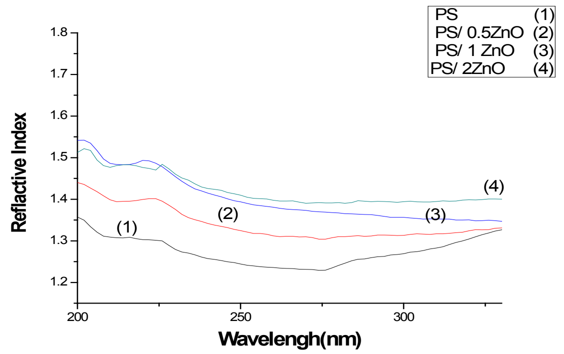

Figure (7). Variation of the reflective index against wavelength

The variation of reflective index with respect to wavelength has been shown in fig. (7), it has been observed that reflective index increases with increasing ZnO wt%. Polymers have reflective index up to1.3. Result reveals that reflective index of PS/ZnO polymer blend nanocomposite have been exceeded that limit. This type of polymer nanocomposite can be used in wave guide technology (e.g. planar waveguide and optical fiber), anti reflective coating, photonic devices, solar cells and image sensor[17,18].

The variation of extinction coefficient (k) with wavelength for PS/ZnO is shown in figure (8). The extinction coefficient increase with increasing ZnO wt%. This behavior of extinction coefficient is high at the longest wavelengths and high concentration.

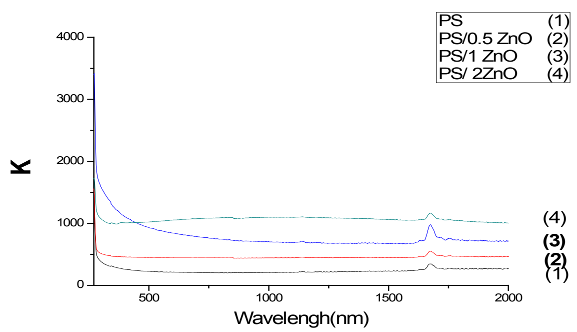

Figure (8). Variation of extinction coefficient against wavelength

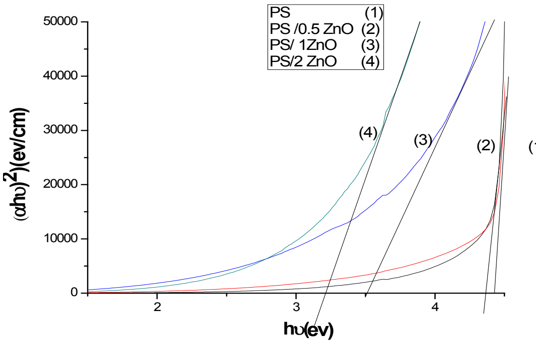

Figure (9). Variation of $(\alpha h\nu)^2$ against $(h\nu)$

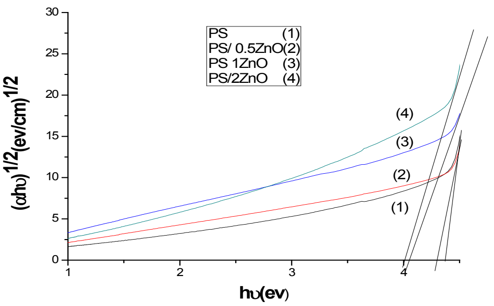

Figure (10). Variation $(\alpha h\nu)^{1/2}$ of the against ($h\nu$)

Figs. (9, 10) show the variation of the optical energy gap for PS/ZnO against the photon energy for direct and indirect allowed transitions. It was observed that at law photon energy the curve is characterized by the presence of an exponentially decaying tail, and the optical energy gap decreased with increasing dopant concentration.

5. Conclusion:

Polystyrene undoped and doped with ZnO nanoparticles(0.5, 1 and 2 wt%) have been prepared by using solution casting method and structural characterization have been done using XRD and TEM. The average particle size of nanoparticles has been calculated by Debyr- Scherrer Equation, which comes out at 19 nm. Results reveal that is a strong adhesion between the surface of ZnO nanoparticles and polymer. Optical absorption spectra have been used to study optical constant of prepared blend nanocomposites films. The absorbance, absorption coefficient and reflective index of ZnO doped PS films increase with increase of doping percentages, except the transmittance. The optical energy band gap was evaluated, the decreasing trend of optical band gap with ZnO NPs concentration, which may be attributed to formation of charge transfer complexes, suggests the presence of deeps localized state in the band gaps.

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