Optical Materials 42 (2015) 335–339

Contents lists available at ScienceDirect

Optical Materials

journal homepage: www.elsevier.com/locate/optmat

Structural and optical characterization of ZnO doped PC/PS blend nanocomposites

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ARTICLE INFO

Article history:
Received 27 September 2014
Accepted 18 January 2015
Available online 11 February 2015

Keywords:
Blend nanocomposites
Ultraviolet–Visible spectroscopy
Band gap
Extinction coefficient

ABSTRACT

PC50%/PS50% polymer blend nanocomposites, undoped and doped with different concentration of ZnO nanoparticles (1, 2, 3 wt%), have been prepared using solution casting method. Structural and optical studies have been performed using X-ray Diffraction (XRD), Scanning Electron Microscope (SEM) and Ultraviolet–Visible spectroscopy (UV–Vis). ZnO nanoparticles have been synthesized by chemical route method. The nanostructure of the ZnO nanoparticles has been ascertained through X-ray Diffraction (XRD) and Transmission Electron Microscopy (TEM). Optical Absorption Spectra has been used to study optical constants of prepared blend nanocomposites. Energy band gap of PC/PS – ZnO blend nanocomposites have been calculated by using Tauc relation. The band gap of the nanocomposites decreases as ZnO wt% increases. Extinction coefficient, refractive index and real & imaginary part of dielectric constants increase with increase in ZnO nanoparticles wt%.

1. Introduction

Polymers are prevalent and dominant materials profiting from their low cost and easy processability [1,2]. However, polymer blends doped with nanoparticles have attracted great interest in the last few years because, combining the attractive functionalities of organic polymers and inorganic nanoparticles have been expected to display synergistically improved properties. The potential applications of the resultant nanocomposites are in automotive, aerospace, opto-electronics and many more [3–7]. The properties of polymer composites depend on the particles shape, size, loading, interfacial bonding and dispersion of the fillers [8–11]. Inorganic particles as fillers can improve mechanical, thermal, electronic, magnetic, redox properties, density and refractive index of polymer matrix [12]. Nanostructured zinc oxide has unique properties like high isoelectric point, biocompatibility, non-toxicity, high chemical stability and high electron transfer capability [13]. ZnO nanoparticles have been proved promising candidates for various applications such as nanogenerator, gas sensors, bio sensors, solar cells [14,15], UV photo detectors, in cosmetic industries a component of sunscreens [16], and photo catalyst in hydrogen production [17]. The study of optical absorption is a useful method for the investigation of optically-induced transitions and for the provision of information about the band structure and energy gap in both crystalline and amorphous materials [18]. Analysis of the absorption spectra in the lower energy part gives information about atomic vibrations while the higher energy part of the spectrum gives knowledge about the electronic states in the atom [19].

A plenty of work has been done on optical properties of polymer nanocomposites. Filling of nano ZnO particles in polyester have changed the microstructure of polyester and prevented the destruction of polyester banded structure during the friction process, which might be one of the anti-wear mechanisms of nano ZnO [20]. Optical properties of PVC has been studied [21] and it has been found that, absorption increase and Urbach energy values decrease as ZnO concentration increases in PVC–ZnO nanocomposites. It has been reported [22] that presence of ZnO in PEO/PVA blend sample induces a decrease of crystallinity and band tail in UV–Vis. The aim of the present work has been concerned with the study of structural and optical characterization of PC50%/PS50% blend filled with ZnO nanoparticles.

2. Experimental

2.1. Materials

The grains of polycarbonate (mw–64,000) & polystyrene (mw–280,000), zincacetatedihydrate and thioglycerol have been purchased from Sigma Aldrich (USA). Di-Methylenesulphoxide (DMSO) (density = 1.099–1.011), Potassium hydroxide (KOH) and

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http://dx.doi.org/10.1016/j.optmat.2015.01.024
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Di-chloromethane (DCM) (density = 1.325) have been purchased from Merck Pvt Ltd Mumbai (India).

2.2. Synthesis of ZnO nanoparticles

Zinc oxide nanoparticles have been synthesized by chemical route method. In this method 0.2 M zincacetatedihydrate ($(CH_3COO)_2Zn.2H_2O$) have been mixed in Di-Methylenesulphoxide (DMSO) under constant stirring. 1.2 M potassium hydroxide (KOH) solution in ethanol has also been prepared by same process. After complete dissolution of zincacetate, KOH solution has been added drop wise. After this, thioglycerol has been added and solution is stirred. When solution turns milky, the solution has been centrifuged and the precipitate has been removed. Thus, precipitated ZnO nanoparticles have been washed with ethanol and then dried in air atmosphere [23].

2.3. Preparation of blend nanocomposites

Polycarbonate (PC) and polystyrene (PS) have been used as basic polymeric material. Equal quantity of PC/PS (50/50 wt%/wt%) has been dissolved in Dichloromethane (DCM) and stirred until a homogeneous solution occurs. ZnO has been added in this solution with 1, 2 and 3 wt% and sonicated .The resulting solution has been casted on to the glass petridish and kept in a dry atmosphere. Dried film has been peeled off from petridish and used for further characterization.

2.4. Characterization techniques

X-ray Diffraction patterns have been recorded using X-ray Diffractometer Bruker D8 Advance with Cu (Kα) radiation (λ = 1.54 Å) in the range of 2θ = 15°–70°.

Absorption spectra have been recorded using Perkin Elmer LAMBDA-750 UV/Vis/NIR spectrophotometer at room temperature in the wavelength range of 250–800 nm.

3. Theory

The optical absorption coefficient (α), which is a function of wavelength; have been calculated from the optical absorbance spectra by using the relation [24,25].

$$\log\left(\frac{I_\circ}{I_t}\right) = 2.303A = \alpha t \tag{1}$$

where $I_\circ$ and I_t are the intensities of the incident and transmitted beams respectively, (A) is the optical absorbance, and (t) is the film thickness.

The transmission coefficient (T) has been calculated using the formula [25];

$$T = 10^{(-A)} \tag{2}$$

While, the reflection have been obtained from the value of absorbance and transmission coefficient from the relation;

$$R = 1 - (A + T) \tag{3}$$

The absorption edge for transitions can be obtained in view of the model proposed by Tauc [26,27] as;

$$\alpha h\nu = C_\circ (h\nu - E_g^{opt})^n \tag{4}$$

where C_0 is energy-independent constant related to the properties of the valance and conduction bands, ($h\nu$) is the photon energy, (α) is the absorption coefficient, E_g^{opt} is the optical energy band gap of the material. The value of parameter 'n' for allowed direct transition is ½ [27]. The variation of $(\alpha h\nu)^2$ against ($h\nu$) yields a good straight line fit to the absorption edge and the extrapolated ($h\nu$) at which $(\alpha h\nu)^2 = 0$ provides the optical band gap E_g^{opt}.

The extinction coefficient (k) is directly proportional to absorption coefficient (α), k can be obtained from the relation [28] as;

$$k = \frac{\alpha\lambda}{4\pi} \tag{5}$$

where λ is the wavelength of light.

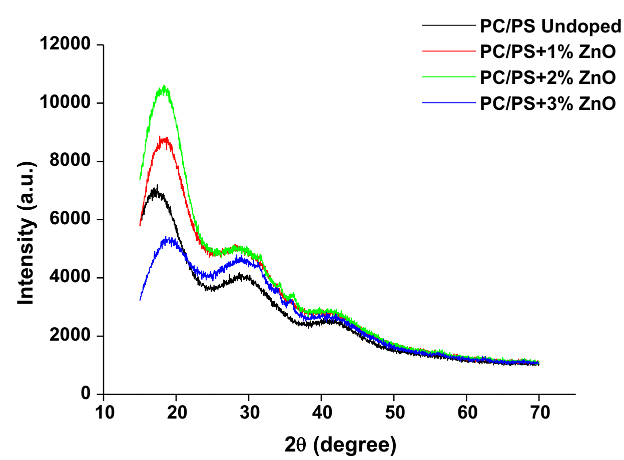

Fig. 2. XRD of undoped and doped PC50%/PS50% with ZnO 1, 2, 3 wt%.

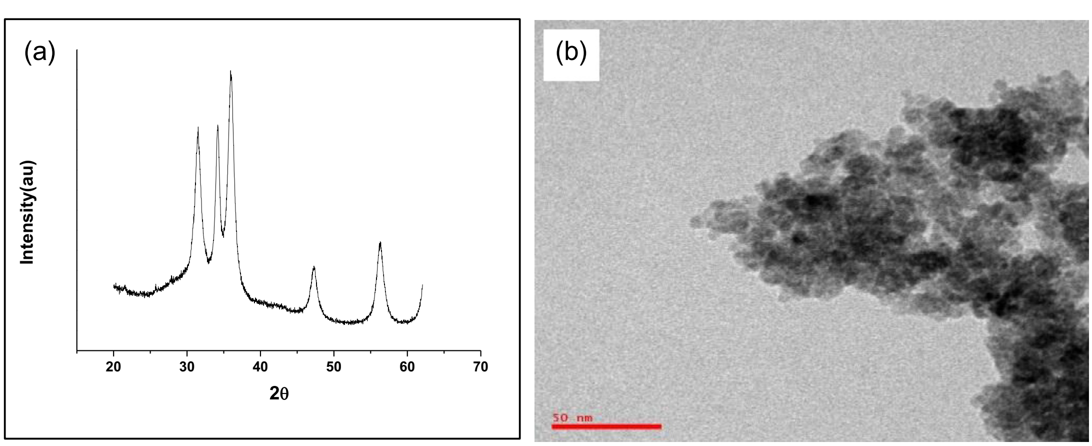

Fig. 1. (a) XRD pattern and (b) TEM image of ZnO nanoparticles.