Optical and Crystalline Studies on ZnS Incorporated Polycarbonate Composite

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Abstract— In this research study, Polycarbonate (PC) was incorporated with ZnS powder and various composites were made by changing the ZnS content. The composites of polycarbonate and ZnS were prepared by solution casting technique. Incorporation of low levels of ZnS into polycarbonate matrix can often lead to an increase in the optical and crystalline properties. The developed samples were characterized using X-ray diffraction technique. The XRD study explores that the crystallinity peaks are occurring from 2θ= 10º to 40º and shows that the crystallinity factor of PC composites is influenced by the interaction occurring between the PC and the ZnS particle. The decrease in the crystallite size is observed with increase in the crystallinity index. The addition of ZnS powder in the poly vinyl alcohol can be developed as a composite with improved/enhanced crystalline properties.

Key words: Polycarbonate (PC), ZnS, UV-VIS, Energy Band Gap

I. INTRODUCTION

Polymers have actual being in natural form since life began [1]. Currently, because of organic, inorganic composite and nano-composite play an important role to improve the physical properties of conventional polymers such as mechanical, thermal, electrical and optical. The introduction of inorganic nano particles and inorganic polymers has been paid much attention [2]. To fulfil the required characterization, the development of new polymers, blends, composites and advanced materials become has become necessity for modification of electrical, mechanical, optical and thermal propertiesthat are used. For development of such films, the optical, electrical and thermal characterization of new polymeric film is essential. To improve their characteristics and to reinforcetheir structure, for particular commercial application, filters are widely used in polymer materials [3]. Polycarbonate can be used as a polymer in crystalline form [4]. A composite material is the combination of two or more materials to form a new material with enhanced properties. Composite materials such as plastics have power to control emerging materials. The application of number of composite materials has grown gradually, penetrating and conquering new markets relentlessly. There are limited applications of composite materials which are for to select the best material, and to design the part [5].

II. MATERIAL AND METHODS

A. Materials

Polycarbonate of Molecular weight of 45000 was obtained from ACROS organics New Jersey USA and imported by HFCL limited new Delhi. Zink sulphide of molecular weight of 97.44 g/mol was obtained from Research Lab Fine Chem. Industries, Mumbai, India. The Chloroform used as polycarbonate solvent was purchased from Thomas baker (chemicals) Pvt. Limited Mumbai India.

B. Preparation of Specimen

The solvent casting technique was adopted for preparation of pure polycarbonate and other composite films. The specimen of pure polycarbonate, .2%ZnS + polycarbonate, .4%ZnS + polycarbonate, .6%ZnS + polycarbonate, .8%ZnS + polycarbonate, 1%ZnS + polycarbonate in the presence of chloroforms as a solvent. The solution was constantly stirred with the help of electronic stirrer for 2hrs at room temperature to obtain homogeneous solution. The prepared solution was poured on Petri dish (glass petri dish). The films were kept at room temperature for 4 Hrs. The films were then removed from Petri dish and stored in air tight polythene bags for further characterization.

C. X-Ray Diffraction

A X-ray Diffractometer Bruker D2 Phaser Second Generation was used to obtain scanning curve for the value of 2θ ranging from 0-90º on prepared samples. The X-ray of 1.54Å wavelength was used. The degree of crystalline was record from the ratio of the areas under the crystalline peaks and total area under a peak. The degree of crystallinity can be written as [6]:

$$C_r = \frac{Areaofcrystallinefraction\ (underpeak)}{Areaofcrystallinefraction + Areaofamorphousfraction} \quad (1)$$

The interplanar distance d was calculated for the first order (n=1) using following formula:

$$d = \frac{\lambda}{2sin\theta} \quad (2)$$

The average size of the crystalline region (D) was determined from the broadening of the peaks by using Scherer's formula :

$$D = \frac{0.89\lambda}{(\beta cos\theta)} \quad (3)$$

Where β is the half width of the peak, θ is the angle and λ is the wavelength. The average inter crystalline separation (R) in the amorphous region of the sample was evaluated using following equation [7]:

$$R = \frac{5\lambda}{(8Sin\theta)} \quad (4)$$

D. UV-Vis Spectroscopy

The information about the energy gap of the Pure Polycarbonate and ZnS incorporated PC films were determined using Shimadzu UV-1800 UV-Visible spectrophotometer taken in the wavelength range 275–500 nm.

III. RESULT & DISCUSSION

A. X-Ray Diffraction

X-ray Diffraction patterns of pure PC and ZnS reinforced PC samples have been recorded. The X-ray Diffractographs of pure PC and ZnS reinforced PC samples are shown in Fig. 1 and summarized in Table 1. In all the samples, the

crystalline peak is observed between 2θ = 15º to 20º. For pure PC film, the crystalline peak is observed at 17.34º, which yields crystallinity of 57.68 %, interplanar distance, d = 1.12Å, crystallitesize D = 19.4Å and average inter crystalline separation R= 1.41Å. As a result of the addition of ZnS in PC shifts in crystalline peak are observed. For .2 % ZnS+ PC blend crystalline peak is observed at 2θ = 17.52º, which yields the crystallinity of 47.57 % with interplanar distance,d = 1.25Å, crystallite size D = 21.1Å and average inter crystalline separation R= 1.56Å. For .4, .6, .8and 1.0 wt% composites similar decrease in various properties have been observed. The crystallinity observed for .4, .6, .8and 1.0wt% composites are 47.38, 46.08, 47.58 and 69.42%, respectively, which shows the crystallinity is decreasing with concentration of ZnS except for 1.0 wt% ZnS+PC sample and developed composite having increased amorphous nature.

S. No.	Sample with wt% of PVP	Crystallinity Index CrI (%)	Peaks at 2θ (°)	Interplanar Distance 'd' (Å)	Crystallite size 'D' (Å)	Average inter Crystalline Separation R (Å)
1	Pure PC	57.68	17.34	1.129	19.4	1.410
2	.2% ZnS+PC	47.57	19.34	1.252	21.1	1.564
3	.4% ZnS+PC	47.38	19.93	1.324	22.1	1.653
4	.6% ZnS+PC	46.08	19.81	1.309	21.75	1.634
5	.8% ZnS+PC	47.58	20.07	1.045	22.3	1.304
6	1% ZnS+PC	69.42	15.68	0.771	6.85	0.962

Table 1: Crystallinity, peaks at 2θ (º), interplanar distance 'd', crystallite size 'D' (Å), and average inter Crystalline Separation R (Å)

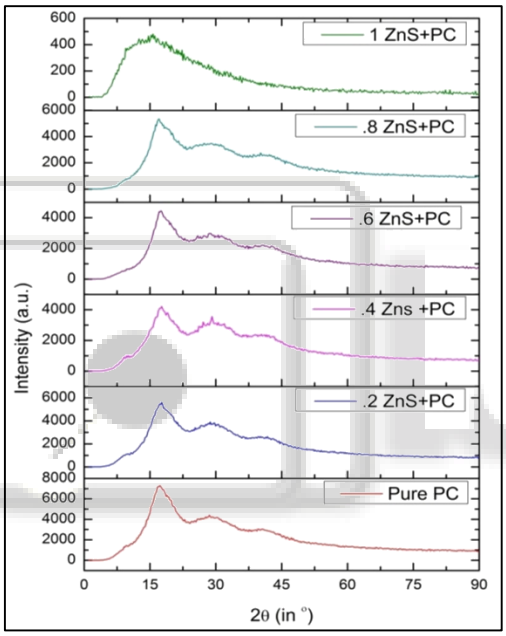

Fig. 1: X-ray diffraction Pattern of Pure Polycarbonate, .2%ZnS+ Polycarbonate, .4% ZnS+ Polycarbonate, .6%ZnS+ Polycarbonate,.8% ZnS+ Polycarbonate, 1%ZnS+ Polycarbonate.

A. UV-Vis Spectroscopy

Fig. 2 shows UV–vis absorption spectra of Pure PC and ZnS powders incorporated PC composite films. The boundaries starting point λ_{os} of absorption edge zone is determined by straight-line extrapolation and wavelength direction intersection from UV–vis absorption spectra. The band gap energy of catalysts is calculated by following equations [8]:

$$E_g = \frac{1239.8}{\lambda_{OS}}\ eV \qquad 5$$

Where λ is in nm and energy band gap is in eV.

The calculation results are listed in Table 1. The energy band gap for Pure PC is 4.39eV and for ZnS incorporated samples, it is also approximately same. It is clear that the addition of ZnS in to the polycarbonate does not play any major role in energy band gap.

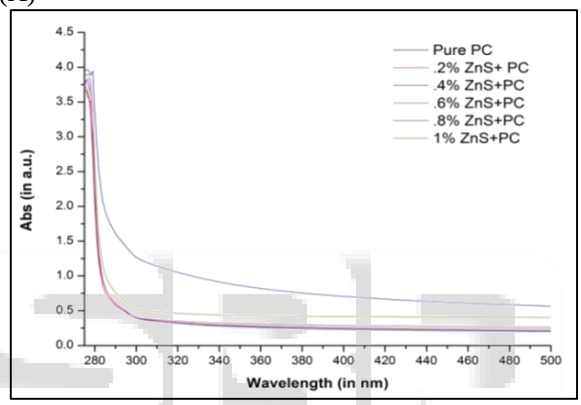

Fig. 2: UV-VIS Spectrums of Pure Polycarbonate, .2%ZnS+ Polycarbonate, .4% ZnS+ Polycarbonate, .6%ZnS+ Polycarbonate, .8% ZnS+ Polycarbonate, 1%ZnS+ Polycarbonate.

S. No.	Sample	Band Gap (in eV)
1	Pure PC	4.39
2	.2% ZnS+PC	4.40
3	.4% ZnS+PC	4.35
4	.6% ZnS+PC	4.40
5	.8% ZnS+PC	4.40
6	1% ZnS+PC	4.39

Table 2: Energy band gap of Pure Polycarbonate, .2%ZnS+ Polycarbonate, .4% ZnS+ Polycarbonate, .6%ZnS+ Polycarbonate,.8% ZnS+ Polycarbonate, 1%ZnS+ Polycarbonate.

IV. CONCLUSION

The PC/ZnS composites were synthesized by a simple and convenient sol–gel method. The above study reveals that the addition of ZnS in to the polycarbonate matrix does not play any major role. The crystalline properties are decreasing, which shows the developed material is going towards the amorphous in nature. Similarly the energy band gap is also not changing very much.

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