Crystalline and Absorption Studies on Cadmium Sulphide doped Polycarbonate Composite

Arunendra Kumar Patel[1,2a)], Keerti Pandey[1], Sapna Agrawal[1], Nisha Pandey[1], and Rakesh Bajpai[2]

[1]*Department of Physics, St. Aloysius College, Jabalpur.*
2Department of Physics, Rani Durgavati University, Jabalpur
[a)]Corresponding author: patelarunendra@gmail.com

Abstract. In this paper we have studied the preparation of composites of polycarbonate composite by incorporating Cadmium Sulphide(CdS) particles with different concentration. The prepared samples were characterized by the different techniques used like X-ray diffraction (XRD) techniques and UV-visspectroscopy(UV-Vis). The X-Ray diffraction technique gives the information on Crystallinity of the Sample, InterplanerDistance (d) and Crystallite Size (D). When the doping concentration is increased the crystallinity of the sample is increases and Crystallite size(D) is also increases. The UV-Vis spectroscopy technique gives information of Optical Band Gap. The energy band gap of pure polycarbonate is 4.437 eVand as we increase the concentration of cadmium sulphide the energy band gap decreases.

INTRODUCTION

Polycarbonate(PC) is an amorphous and polar thermoplastics polymer. It is used as engineering material because it has several properties such as transparency, dimensional stability, flame resistance, high heat distortion temperature and high impact strength[1]. Polycarbonate is soft in nature and the surface of polymer is easily stretched.It is used in electronic and electrical applications and has quite good insulation characteristics. Cadmium sulfide is an important II-IV group element semiconductor(at room temperature)with many excellent physical and chemical properties. This has promising application in multiple technical fields including photochemical catalysis, gas sensor, detectors for laser and infrared.

EXPERIMENTAL DETAILS

Material Used in Present Study

The polycarbonate with molecular weight 45.0Mw, from Company Acros Organics, New Jersey USA.Cadmium Sulphide(orange in colour), molecular weight 144.48 99% pure fromResearch Lab Fine Chemical Mumbai, India.

Preparation of Samples

The solvent cast technique was adopted for preparation of pure and composite samples. The specimen of pure PC, 0.2%CdS+PC, 0.4% CdS+PC, 0.6% CdS+PC, 0.8% CdS+PC, 1.0% CdS+PCin the presence of Chloroform as a solvent. The solution was constantly stirred with the help of electronics stirrer for 2hrs at room temperature and sonicated to obtained homogeneous solution. The prepared solution was poured on glass Petri disk. The film were kept at room temperature for overnight and then films were then removed from Petri disk and stored in air tight polyethylene begs for further characterization.

Characterization of Samples

X-Ray Diffraction studies has been carried out using Bruker D2 Phaser 2nd GenerationDiifractometer. X-Ray Diffraction technique is very important to determine the Degree of Crystallinity, interplanar distance d, and of the crystalline region (D). The crystallinity index is [2,3]-

$$Crystallinity = \frac{Area\ of\ Crystalline\ Peaks}{Total\ Area} \times 100\% \quad \text{i)}$$

The relationship between crystallite size and x ray line broadening was determined from Scharrer's Formula:

$$D = \frac{n\lambda}{\beta\ Cos\theta} \quad \text{ii)}$$

Where D is the crystallite size, λ is the wavelength , β is the angular line width of half maximum intensity and is the bragg's diffraction angle while k is constant 0.89 [4].

In present study the absorption studies has been carried out using ShimdzuUV-Vis Spectrometer UV-1800, and absorption coefficient can be defined as:

$$\alpha = \frac{2.303A}{d} \quad \text{iii)}$$

where A is the absorbance and d is the thickness of sample. And at given wavelength 190-1100 nm the absorbance peak determine.

The band gap energy of catalysts is calculated by the equation –

$$E_g = \frac{1239.8}{\lambda_{OS}}\, eV \quad \text{iv)}$$

Where λ is in nm and energy band gap in electron Volt(eV), the boundary starting point λ_{OS} of absorption edge zone is determined by straight line extrapolation and wavelength direction intersection from UV-Vis absorption spectra[5,6].

RESULT AND DISCUSSION

X-Ray Diffraction

X-ray diffraction pattern for pure Polycarbonate, pure Cadmium Sulphide and polycarbonate doped cadmium sulphite sample shown in Figure 1 and summarized in Table 1. In all the samples crystalline peak observed between $2\theta = 16.25^0$ to 17.69^0. For pure polycarbonate film the crystalline peak is observed $16.88^0$and there crystallinity is 33.41%, inter planer distance d= 5.245Å and crystallite size D=15.1Å. In addition of cadmium sulphide in polycarbonate shifts of crystalline peak are observed sharp in higher percentage of cadmium sulphide. For 0.2% CdS+PC polymer film, crystalline peak are observed 2θ= 17.49º, which yields the crystallinity of 40.63% with interplaner distance, d=5.066Å and crystallite size D =15.8Å. for 0.4%CdS+PC polymer film similarly increases in various properties have been observed. Crystallinity of different wt% of polymer is continuously increases 0.4%, 0.6%, 0.8% and 01% films are 45.78%, 49.50%, 51.99% and 52.47% respectively.

Table 1 Crystallinity, peaks at 2θ (º), interplanardistance 'd', crystallite size 'D' (Å) for Samples.

S. No.	Sample with wt%ofCdS	Crystallinity index CrI (%)	Peaks at 2θ (°)	Interplanar distance 'd' (Å)	Crystallite size 'D' (Å)
1	Pure PC	33.41	16.88	5.245	15.1
2	.2% CdS+PC	40.63	17.49	5.066	15.8
3	.4% CdS+PC	45.78	17.69	5.00	16.3
4	.6% CdS+PC	49.50	17.20	5.15	17.1
5	.8% CdS+PC	51.99	16.95	5.22	22.7
6	1% CdS+PC	52.47	16.25	5.44	95.6

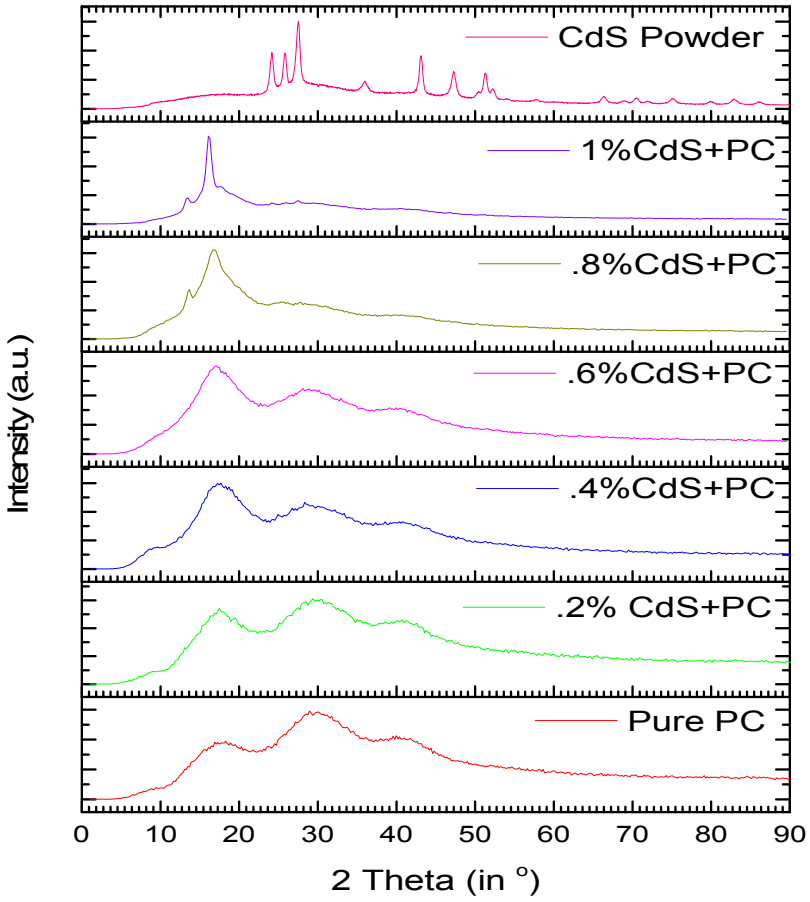
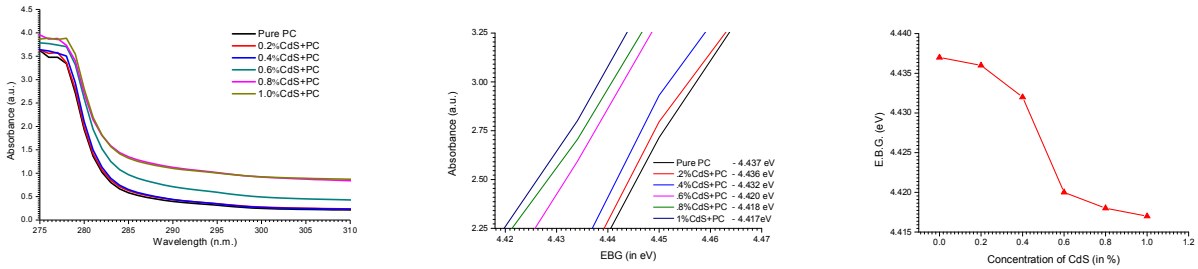


FIGURE 1.X-ray diffraction Pattern of Pure Polycarbonate, .2%CdS+ Polycarbonate, .4% CdS+ Polycarbonate, .6%CdS+ Polycarbonate,.8% CdS+ Polycarbonate, 1%CdS+ Polycarbonate.



(a) (b) (c)

FIGURE 2.(a)UV-VIS Spectrums of Pure Polycarbonate, .2%CdS+ Polycarbonate, .4% CdS+ Polycarbonate, .6%CdS+ Polycarbonate,.8% CdS+ Polycarbonate, 1%CdS+ Polycarbonate; **(b)**Energy band gap for Pure PC and PC/CdSblend films; **(c)**Variation in Energy Band Gap with Doping Concentration of CdS.

The optical energy band gap $E_g$values for the pure as well as for doped polycarbonate filmare shown in Figure 2(a). The value of energy band gap for various dopant concentrations of the samples are presented in Figure2(b). When the dopant concentration increases the energy band gap value decreases. The decrease of optical energy band gap(E_g) due to the presence of local cross linking that occurred within the non-crystalline phase of the composite polymer.Figure 2(c) shows energy band gap for pure PC and PC/CdS blend film, here the enrgy band gap for pure polycarbonate is 4.437 eV. As the concentration of CdS is increases the energy band gap decreases. The energy band gap of 0.2%CdS+PC, 0.4%CdS+PC, 0.6%CdS+PC,0.8%CdS+PC and 01%CdS+PC is 4.436, 4.432, 4.420, 4.418, 4.417 eV respectively.

CONCLUSION

X-ray diffraction gives the crystallinity of the sample between 33.41 to 52.47. As the concentration of cadmium sulphide increases the crystallinity of the sample increases and the peak of 2θ (°), gives sharp peak and crystallite size D(Å) increases from 15.1 to 95.6 Å. Optical Absorption study of samplesreveals that, as we increase the concentration of cadmium sulphide(CdS) the energy band gap decreases. The Forenergy band gap for pure polycarbonate is 4.437 eV and it is decreasing from 4.436 to 4.417 eV with increase in concentration of CdS.

REFERENCES

1. George Wypych, *Handbook of Polymers*Second Edition (ChemTec Publishing, Published by Elsevier Inc., 2012), pp. 450–454.
2. VBF Mathot*Thermal characterization of state of matter* (Calorimetry and thermal analysis of polymer. Hanser, Munich, 1994) ,Chapter 5.
3. Statton WO *Hand book of X-ray diffraction, emission, absorption and microscopy, (*Characterization of polymer, McGraw-Hill, New York, 1967) Chapter-21.
4. Arunendrakumar Patel, R.Bajpai& J.M. Keller, Microsystem Technologies, **20**, 1 (2014).
5. H. H. Perkampus, *UV-VIS Spectroscopy and Its Applications*, (Springer-Verlag Berlin Heidelberg New York London Paris Tokyo Hong Kong Barcelona Budapest, 1992).
6. S FarjamiShayesteh. S Kolahi and Y Azizian-Kalandarragh, Indian *Journal of pure and Applied Physics*, 51, PP. 780-783(2013).