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Synthesis and Surface Studies of CdS / PVK Nanocomposites

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Cadmium sulfide (CdS) is excellent materials for optoelectronic applications. It is interesting to investigate their optical properties at nanometer regime where the properties become size dependent. The nanocomposites have been successfully prepared by chemical method. The samples have been characterized by AFM, SEM and XRD. The XRD study shows formation of CdS nanocrystals with cubic zinc blend crystal structure, having three peaks corresponding to (111), (220) and (311) planes. The crystal size computed by Debye Scherrer's formula is in the range of 3 to 12 nm. The AFM and SEM studies show the clusters of particles in the range of a few tens of nm. The results obtained from XRD, SEM and AFM studies show increase in particle size, by increasing the CdS concentration in PVK.

Keywords: CdS / PVK nanocomposites, XRD, AFM, SEM

Introduction

Nanocomposites consisting of organic polymers and inorganic nanoparticles frequently exhibit a host of electrical, mechanical, magnetic and optical properties, which are far greater compared with those of the individual components[1-4]. These attractive properties are derived from a complex interplay among the building blocks and the interfaces separating the building blocks. The hole transport organic semiconducting polymer is Poly N-vinyl carbazole (PVK). It has been generally used as an optical and electronic material[4]. The CdS is an inorganic semiconductor and excellent materials for optoelectronic applications[5-10]. Hybrids of CdS nanoclusters and PVK show the excellent carrier generation efficiency and mobility of the inorganic semiconductor and processability of the organic polymer[11-14]. When CdS nanoclusters were finely dispersed in the PVK matrix then the photoconductivity enhancement of PVK has been observed.

The CdS nanoclusters, in this case acts as a sensitizer for the photogeneration of charges and the PVK polymer serves as the carrier transporting medium[11]. Previously, the nanocomposite of CdS/PVK was prepared by mixing PVK and CdS nano cluster or their precursors were prepared by mixing the synthesized nanoparticles with polymer. The effect of the inevitably caused due to introduction of precursor molecules or the synthesized semiconductor nanoparticles is not clear to date, further more the conventionally synthesized semiconductor nanoparticles have a tendency to accumulate into larger clusters and their fine dispersion in the polymer is not very easy. Wang *et al*.[15-17] have made a new approach for the preparation of truly two components CdS / PVK nanocomposites. Khanna *et al*.[18] have reported that the careful preparation of CdS nanoparticles in DMF with the metal-rich surface can be considered responsible for stable light emission.

CdS particles could be synthesized in the polymers such that the film can be cast directly, thus avoiding and reducing the loading of the particles via multistage processes. This desire has encouraged us to extend the synthetic methodology to functionalized and non-functionalized polymers. Polymers are considered a good choice as matrix materials for such purpose due to their long-time stability and because they possess flexible reprocess ability[19]. The electrical and optical properties of nanocomposites can be controlled by their particle size and attracted much interest for their fundamental aspects. Recent studies have been undertaken to synthesize CdS/PVK nanocomposite with various concentration of CdS in PVK characterize them by XRD, AFM, SEM and studies their property.

Experimental

For the preparation of CdS/PVK nanocomposites films, 400 mg of poly N-vinyl carbazole (PVK) was dissolved in 10 mL dimethylformaldehide (DMF) through constant stirring and heating at 80 ºC temperature. Cadmium acetate was then added to the

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solution as 10, 20, 30 40 and 50% weight of PVK, so that CdS concentration in polymer equivalent weight.

The resulting solution was stirred for 30 min. The solution was refluxed by applying nitrogen and then H_2S gases for a 30 s. The solution immediately turned turnip yellow. Now again the solution was stirred for a few seconds. The chemical reaction as follows:

$$PVK + Cd(CH_3COO)_2 + H_2S \rightarrow CdS/PVK + 2CH_3COOH$$

Then the solutions were caste over glass slides and conducting glass plates and were dried in an oven for several hours to obtain uniform film of CdS / PVK nanocomposite. These films were characterized by XRD, SEM, AFM and their optical properties like absorption spectra, photoluminescence are studied.

Results and Discussion

Atomic force micrographs

The AFM images were obtained by using DIAFM- 4 at UGC DAE CSR Indore. The 2-dimensional and 3-dimensional AFM images of CdS/PVK nanocomposites with different concentration of CdS in PVK are shown in Fig. 1. these have shown a typical morphology of CdS/PVK nanocomposite films. The cluster size and roughness obtained are given in Table 1. The results indicate that with increasing the concentration of CdS in PVK, the roughness decreases and particle size increases.

Scanning electron micrographs

The SEM images were obtained by using FEI Quanta 200F environmental SEM, in BHU Banaras. In order to investigate the surface morphology of the samples were analyzed by scanning electron microscope. Figure 2 shows the SEM images of CdS/PVK nanocomposites. In these images it is seen that the particles shapes are spherical. It is also observed that from SEM micrograph, which the small nanoparticles of CdS are coupled together and form large clusters. From Fig. 2, it can observe that cluster size increases with increasing CdS concentration in the composite.

X- ray diffraction analysis

The CdS/PVK nanocomposites were characterized by X-ray powder diffraction which showed on perfect match with the diffraction pattern in the literature[20].

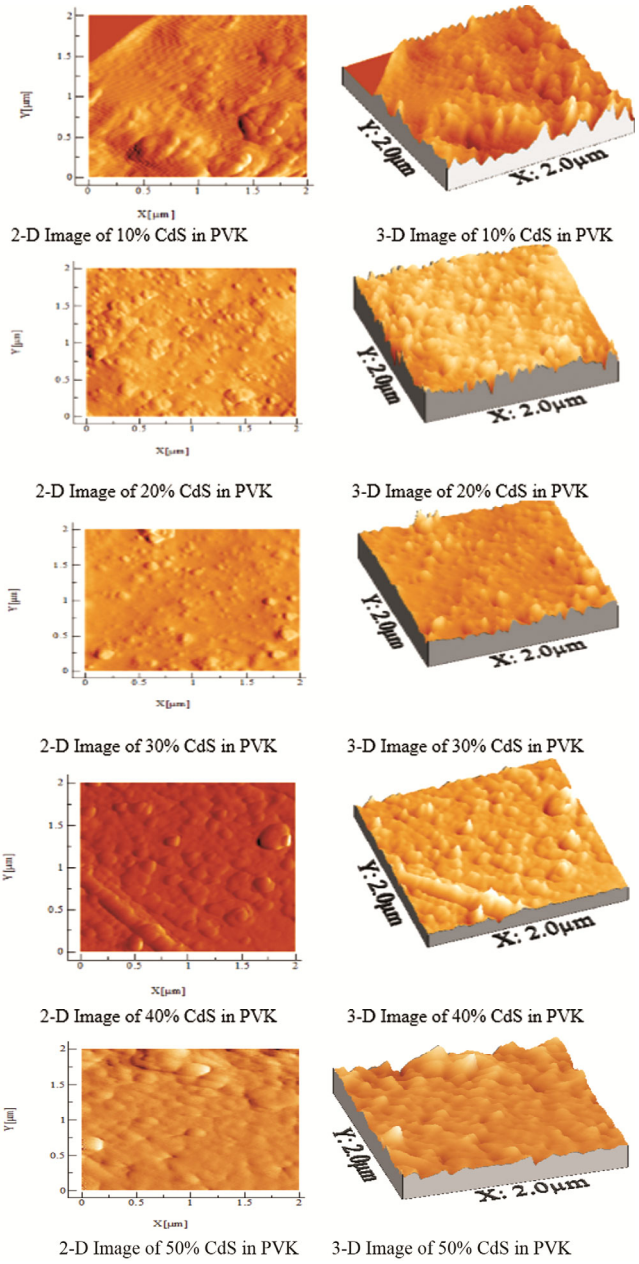

Fig. 1 — AFM images of CdS/PVK nanocomposites for area (2×2) µA.

Table 1 — Surface roughness of CdS/PVK nanocomposites for different concentration of CdS in PVK.

Sample name	CdS concentration in PVK in (%)	Area in µm (2×2)	Surface roughness Rms (in nm)	Average particle size (in nm)
CdS/PVK - I	10	2×2	144	20
CdS/PVK – II	20	2×2	99	25
CdS/PVK – III	30	2×2	69	35
CdS/PVK – IV	40	2×2	57	38
CdS/PVK – V	50	2×2	46	40

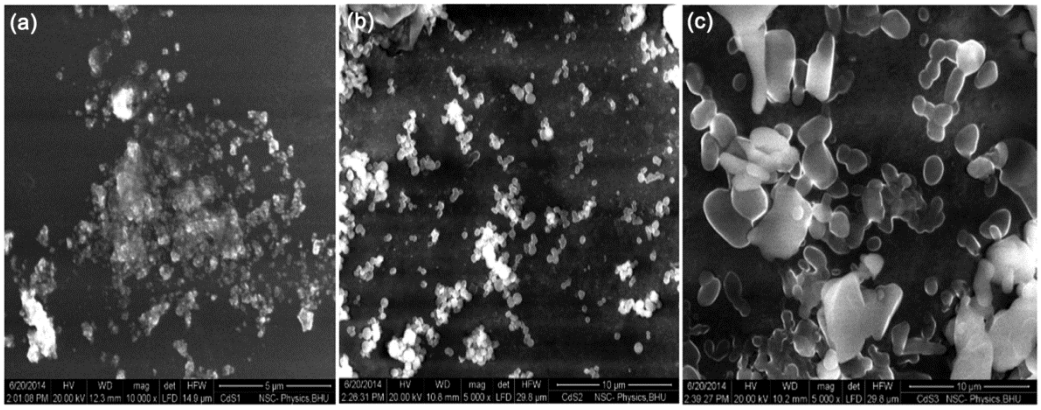

Fig. 2 — SEM images of CdS/PVK nanocomposite at various concentration of CdS in PVK (a) SEM images of CdS/PVK nanocomposites, (b) SEM images of CdS/PVK nanocomposites with 10% CdS concentration in PVK with 20% CdS concentration in PVK and (c) SEM images of CdS/PVK nanocomposites with 30% CdS concentration in PVK.

The X-ray diffraction patterns of CdS/PVK nanocomposites of different CdS concentration are shown in Fig. 3. The CdS/PVK nanocomposite shows considerable broadening in the X-ray pattern. This broadening of the diffraction peak is primarily due to the finite size of the nanocrystallites. The diffraction peaks are found at 2θ values approximately 17.46º, 26º, 44º and 52º. The diffraction peak at 2θ = 17.46º corresponds to PVK as seen from Fig. 3. The other peaks at 2θ value 26º, 44º and 52º, matching the (111), (220) and (311) crystalline planes of cubic CdS, indicated the formation of CdS[21].

The broad nature of the XRD peaks could be attributed to the nano-crystalline nature of the CdS particle. The lattice spacing is calculated from the Bragg's formula[22]. The size of the particles has been computed from the broadening of XRD peaks using Debye Scherrer formula[22].

$$D = \frac{K\lambda}{\beta \cos\theta} \quad \ldots (1)$$

Where D is crystal size, λ is wavelength of X-rays used. β is the full width at half maxima (FWHM) of the XRD peak, θ is Bragg angle and K is the shape factor, which has the value close to unity. The crystal size was computed from the broadening of peak using Eq. (1) and it is obtained in the range of 3 to 12 nm. The lattice parameter has been computed as 5.8 Å, which is very close to the standard value (5.83 Å).

Conclusions

The CdS/PVK nanocomposites were prepared using chemical technique for different concentration s such as 10, 20, 30, 40 and 50% of CdS concentration in PVK. CdS/PVK nanocomposite films have been characterized by XRD, AFM and SEM. The size of the nanoparticle is found to increase with increasing concentration of CdS in PVK. AFM and SEM images show the clustering with the size in the range of a few tens of nm. The increasing concentration of CdS causes decrease in the roughness of CdS/PVK nanocomposites significantly. SEM shows clusters of particles in a spherical shape, which increase with increasing concentration of CdS in PVK. XRD studies show that the CdS/PVK, CdS crystals have a structure like cubic zinc blende, crystalline sizes obtained by XRD using Scherrer's formula are of the order of 3 to 12 nm and found to increase by increasing CdS concentration.

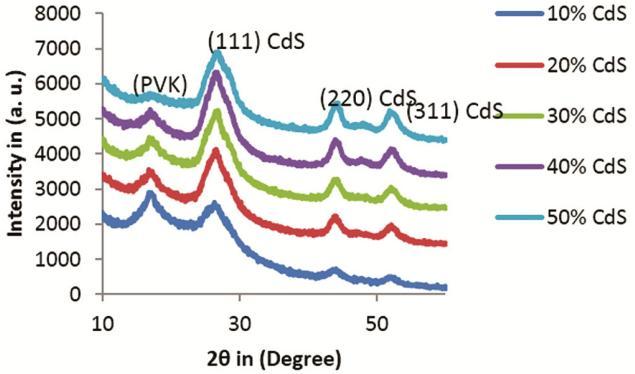

Fig. 3 — XRD pattern of the CdS/PVK nanocomposites.

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