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REGULAR ARTICLE

Structural and Optical Properties of Polystyrene CdS Nanocomposite Prepared by a Soft Chemistry Method

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Cadmium sulfide nanocrystals were prepared by the hydrothermal method. X-ray diffraction patterns have presented a small broadening of the diffraction peaks. This broadening is due to the nanometric size of cadmium sulfide powders. The patterns also confirmed that cadmium sulfide crystallizes in the wurtzite structure (P6_3mc crystallographic group) and that crystallite sizes are nanometric. Polystyrene cadmium sulfide nanocomposite has been fabricated by soft chemistry method. This involves mixing a solution of cadmium sulfide (1 g of cadmium sulfide poured in 10 mL of chloroform) with a solution of 1 g of polystyrene dissolved in 30 mL of chloroform. After including the CdS nanopowders into the polystyrene, a decrease in size was observed, going from 20.90 nm to 16.68 nm. The SEM image revealed that the surface of the polystyrene presents pores and these pores have been filled during the fabrication of polystyrene CdS nanocrystals composite. Raman spectra show, in addition to the Raman peaks of polystyrene, the characteristic peak of the longitudinal optical phonon (LO) mode of CdS. UV-visible spectroscopy showed that the composite exhibited high transparency in the Visible region. The optical absorption spectrum at room temperature shows a shift of the absorption edge towards high energies. The energy bandgap has been obtained using second derivative curve. The value of band gap energy has been found to be 2.52 eV. The emission spectrum of polystyrene shows no luminescence, whereas the signal of the photoluminescence at room temperature of the composite polystyrene/CdS nanocrystals is formed by two bands situated respectively at 2.51 eV and 2.31 eV. The first band has been assigned to the band-to-band transition, while the second is attributed to the deep level emission.

Keywords: Polystyrene, Nanocrystals, XRD, SEM, Photoluminescence.

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1. INTRODUCTION

Recently, the nanocrystals of semiconductors embedded in various materials have been extensively studied. This investigation effort is stimulated by the interesting properties that appear when the size of the semiconductor becomes nanometric. A huge change in physical properties has been observed when the size approaches that of the molecule [1]. Indeed, a confinement of the excitations in a narrow space is then observed. Numerous investigations have been carried out in order to synthesize nanocrystals of desired size and shape [2], and to understand the influence of the preparation conditions and the nature of the host matrix on the physical properties of the nanocrystals [3].

Among II-VI semiconductors, CdS, which has a direct band gap of 2.42 eV and a Bohr exciton diameter of 3 nm, has attracted much attention due to its wide range of applications in physical devices. Consequently, CdS nanocrystals are applicable in several fields, especially in optoelectronics, white light emitting diodes, solar cells and laser devices. By improving the processing conditions, it is possible to have nanocrystals with a small size distribution. This allows a quasi-monochromatic emission in the ultraviolet if the size is small enough. On this basis, several techniques have been used to synthesize nanocrystals (NCs). These methods include embedding nanocrystals into crystal matrices by the Czochralski method, into a glass matrix by the sol-gel method, into an aqueous solution by chemical techniques and into polymer matrices by soft chemistry techniques [4]. SK Tripathi et al. [5] prepared a polystyrene composite PS/CdS NCs by chemical route (ex situ). Measurement of UV-visible absorption and fluorescence indicated that a strong confinement effect results in the PS/CdS NC composite. Dragana Sajinovi et al. [6] reported that the polystyrene matrix minimizes surface effects that promote non-radiative recombination, resulting in increased luminescence of the PS/CdS NCs composite. Vishal Mathur et al. [7]

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demonstrated the incorporation of CdS nanoparticles in the PS/PVC and PS/PMMA copolymer matrices and described the effect of the composite obtained on the effective thermal conductivity.

The choice of the host matrix is therefore very important for the specific applications envisaged since the environment of the nanocrystal strongly influences its behavior.

The aim of this work is the fabrication of luminephore devices based CdS nanocrystals embedded in a polystyrene matrix by soft chemistry method and deposited on glass matrix using the spin coating technique. The morphology was examined by SEM, where the images clearly show the filling of the pores on the surface of the polystyrene by the CdS nanocrystals.

The structural characterization was determined by DRX and Raman, whereas the optical properties were studied by UV-visible spectroscopy and photoluminescence.

2. EXPERIMENTAL DETAILS

The CdS nanocrystals were synthesized by hydrothermal method from the starting precursors cadmium nitrate ($Cd(NO_3)_2$) and thiourea (CH_4N_2S). 0.1 mol of $Cd(NO_3)_2$ and 0.1 mol of thiourea were dissolved separately in distilled water at room temperature under magnetic stirring for 30 minutes until complete dissolution. The two prepared solutions were then mixed by adding the thiourea solution drop wise into the stirred cadmium nitrate solution over a period of 1 h. The final mixture was then transferred to a 190 mL Teflon-coated stainless steel autoclave. The heat treatment was carried out in an electric oven at 180 °C for 8 hours. Once the reaction was complete, the autoclave was cooled to room temperature. The obtained powder (CdS nanocrystals) was washed several times with de-ionized water and ethanol and then dried at 80 °C for 12 h.

The composite thin film PS/CdS NCs was obtained by the soft chemistry method. This method consists in first dissolving 1 g of polystyrene in 30 mL of chloroform ($CHCl_3$). The result is kept under magnetic stirring to ensure complete dissolution of the polymer and thus to obtain a homogeneous solution. A part of this solution is kept to use for undoped films fabrication (undoped polystyrene).

0.1 g of CdS nanoparticles (previously prepared by hydrothermal method) are poured into 10 mL of chloroform. The resulting solution is kept under magnetic stirring until it becomes homogeneous.

The final solution used for the preparation of nanocomposite thin films of polystyrene (PS) doped with CdS nanoparticles with concentration of 10% (in wt) is obtained by adding the two previous solutions solvent/PS and solvent/CdS. The obtained solution is homogenized by magnetic stirring for 24 h, then left to stand so that the relatively large nanocomposites settle under the effect of gravitation at the bottom of the solution. In the last, the upper part of this solution, containing the smaller nanocomposites, is recovered for doping.

The composite films PS/ CdS NCs are obtained by the spin-coating method. Using a syringe, a drop of the solution is deposited on a glass matrix. The glass matrix is mounted on a motorized spindle rotating at a speed ranging from 300 to 3000 rpm for 60 s, the obtained film (composite thin films PS/ NCs CdS) has a yellowish color.

X-ray diffraction (XRD) was used to identify the crystal structure of the pure CdS NCs and the PS/CdS NCs composite by using the CuK_α radiation (λ_α = 1.5402 Å, voltage 45 kV, current of X-ray tube 40 mA) of a PANalytical X'Pert Pro Diffractogram in the range 2θ [10°-80°].

Raman spectra were recorded on a backscatter configuration of a Jobbin Yvon micro-Raman coupled to a DX40 Olympus microscope. The samples of the pure polystyrene film and the composite film are excited with a wavelength of 632.8 nm with an output of 20 mW.

The UV-visible spectra were recorded on a Shimadzu UVPC 3001 spectrophotometer. The photoluminescence signal was obtained by exciting the sample at room temperature with 350 nm radiation generated by an Argon laser.

3. RESULTS AND DISCUSSION

3.1 Structural Properties

Figure 1 shows the XRD diffractogram of the nanocrystalline powder of CdS. A small broadening of the diffraction peaks is observed, which is due to the nanometric size of the CdS powder.

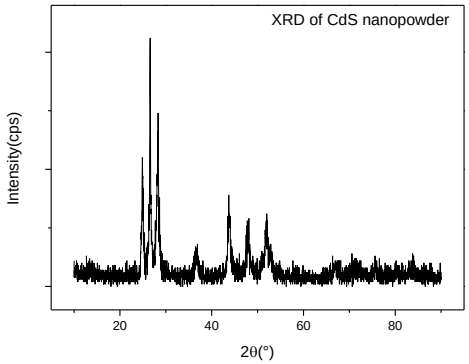


Fig. 1 – XRD pattern of CdS nanopowders

The nanocrystalline powder of CdS has a hexagonal structure (JCPDS No. 41-1049). Normally, the most intense peak of the hexagonally structured CdS powder is line (101), but it is noted that the nanocrystalline powder obtained has line (002) as the most intense peak. Consequently, the nanocrystalline powder of CdS has a texture along the plane (002). The size was estimated using the Scherer formula:

$$D = \frac{0.9\lambda}{\beta cos\theta}$$

Where D is the size of the CdS NCs, λ is the wavelength of the X-rays (1.5402 Å), β represents full half width at mi-height (FWHM), θ is the diffraction angle.

The image SEM of the CdS powder shown in Fig. 2 indicates that the CdS NCs aggregate to form grains by coalescence.

The examination of the image reveals that the sizes of grains are nanometric, which confirms the XRD results.

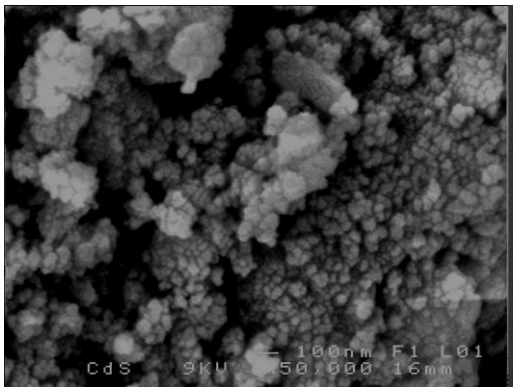
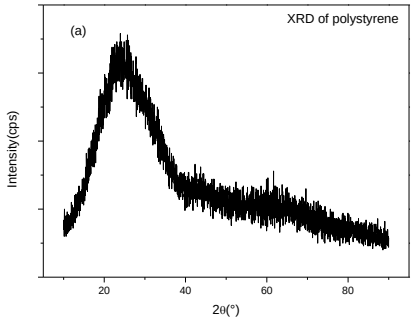
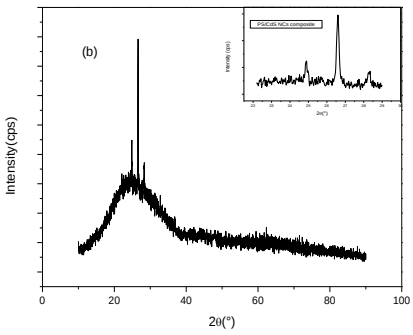


Fig. 2 – SEM image of the CdS powders

Fig. 3 displays the XRD patterns of PS/CdS NCs composite films. The undoped PS has an amorphous structure since no diffraction peak is revealed on the pattern. However, the composite PS/CdS NCs compound exhibits a crystalline behavior.



(a)



(b)

Fig. 3 – XRD pattern of (a) undoped PS (b) PS/CdS NCs composite, Figure inset magnification of 22°-29°angular domain

We observe peaks at 24.88°; 26.58° and 28.27° corresponding to the hexagonal phase of the CdS with diffraction planes (100), (002) and (101) respectively (JCPDSN° 41-1049) with a preferential orientation according to the plane (002). It can be concluded that the CdS crystallites are embedded into the polymer matrix. Moreover, it can be seen that the diffraction peaks are considerably broad indicating that the size of the CdS NCs is nanometric. In addition to nanometric size, this broadening may be due to the inhomogeneous deformation present in the films [8].

The dislocation density (δ) is calculated from the formula [9]:

$$\delta = \frac{1}{d_{002}^2}$$

Where δ represents the density of dislocations and d_{002} is the interplanar distance of the plane (002).

Finally, the deformation induced by the introduction of CdS NCs into the matrix PS is calculated by the standard relation [10]:

$$\varepsilon = \frac{0.25\beta}{tan\theta}$$

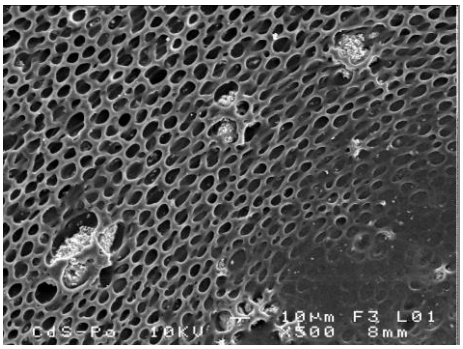
Table 1 shows the diffraction angles, sizes, dislocation density and deformations of the CdS NCs and the PS/CdS NCs composite film that correspond to the plane (002) of CdS.

Table 1 – Diffraction angles, sizes, strains and dislocations density of CdS nanopowder and PS/CdS NCs composite

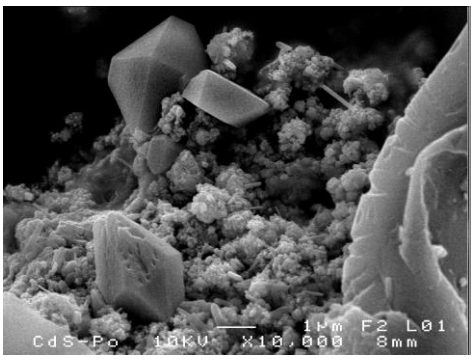
Sample	$2\theta_{002}$ **(°)**	D_{002} **(nm)**	ε_{002}	δ_{002} **(nm^{-2})**
CdS NCs	26.54	20.90	0.77	8.16
PS/CdS NCs	26.51	14.68	1.61	9.18

It is found that the average size of the crystallites decreases when the CdS NCs are embedded into the polystyrene matrix, while the stresses and the dislocation density increase. This behavior is due to the fact that when the size decreases, more stresses and dislocations appear.

The morphology of the PS/CdS NCs composite film was studied using the SEM images. Figure 4a shows that the surface of the PS contains pores and that the CdS NCs fill these pores. Figure 4b displays the SEM images of the PS/CdS NCs nanocomposite films.



(a)



(b)

Fig. 4 – SEM image of PS/CdS NCs composite: (a) CdS NCs filled PS pore; (b) magnification of a pore containing CdS NCs

A large number of CdS nanocrystals, on the PS surface, can be clearly seen. The CdS particles are agglomerated and dispersed in the PS matrix. All grains have nanometric size except a finite number whose size is micrometric. Thus, the CdS has size dispersion in the PS matrix.

Figure 5 shows the Raman spectra of pure PS (Fig. 5a) and of the PS/CdS NCs composite (Fig. 5b).

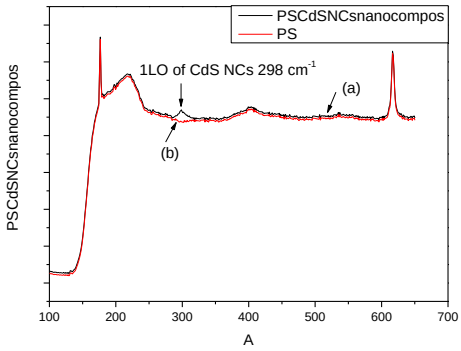
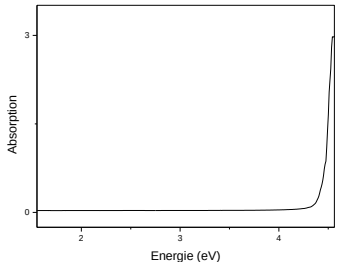
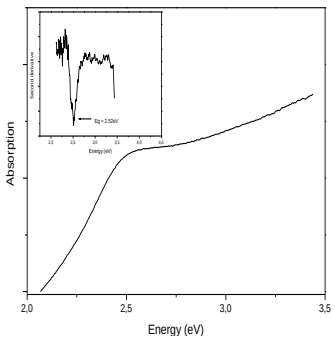


Fig. 5 – (a) Raman spectra of pure PS. (b) Raman spectra of PS/CDS NCs composite

The Raman spectrum of the composite has the characteristic peak of CdS. The peak at 298 cm^{-1} corresponds to the longitudinal optical phonons (LO); this peak has a mid-height width (FWHM) of 18 cm^{-1} and a shift of 7 cm^{-1} towards low frequencies compared to LO position of bulk CdS (305 cm^{-1}) [11]. The shift of the peak position to low frequencies in the present work is due to the quantum confinement effect that occurs when the size is small [12]. The results of Raman spectroscopy confirm results of XRD ie the embedding of CdS in PS matrix.



(a)



(b)

Fig. 6 – (a) Absorption of undoped PS. (b) Absorption of PS/CdS NCs composite. Figure inset second derivative curve

Figures 6a and 6b display the absorption of undoped and CdS NCs doped PS.

No optical absorption, in the range of 2-3.5 eV, of undoped PS is observed (Fig. 6a). This means, that the PS is transparent in the 2-3.5 eV range and all absorption in this range comes from the CdS NCs.

The absorption edge appears around 450 nm. Furthermore, the precise values of the band gap for the PS/CdS NCs composites can be obtained from the second derivative of the absorption spectrum [13]. The curve of the second derivative is illustrated in the insert of Figure 6. The value of the band gap of the PS/CdS NCs composite is estimated to be 2.52 eV. Comparison of this value with that of the CdS bulk crystal (E_g = 2.42 eV) indicates a blue shift of the optical absorption edge (ΔE = 0.10 eV). This blue shift is caused by the nanometric size of the CdS NCs.

Another important optical property of CdS NCs, which can provide information on the various defects of the CdS structure, is emission. The photoluminescence (PL) spectrum at room temperature of the PS/CdS NCs composite is displayed in Figure 7. No PS emission is recorded in the UV-visible region. The measured emission signal of the PS/CdS NCs composite is thus assigned to the CdS. Two PL bands are observed: a net centered at 493 nm (2.51 eV) attributed to the band-to-band transition (near band emission) and a broad centered at 536 nm (2.31 eV) (green luminescence) which can be attributed to the deep level emission (DLE). This peak emission of green photoluminescence (DLE) is explained by the emission of intrinsic defects of interstitial cadmium I_{Cd}, sulfur deficiencies V_s and cadmium deficiencies V_{Cd} [14, 15].

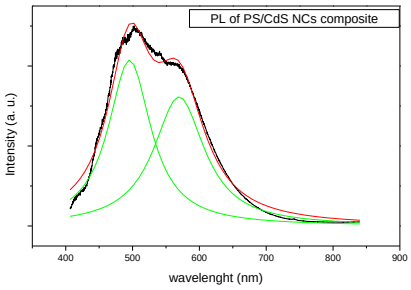


Fig. 7 – PL signal of PS/CdS NCs composite. The signal is deconvolved into 2 curves centered at 493 nm (2.51 eV) and 536 nm (2.31eV) respectively

4. CONCLUSIONS

X-ray diffraction and Raman spectroscopy confirmed the formation of the PS/CdS NCs composite film. The SEM images show that the CdS NCS fill the pores on the surface of the polystyrene.

UV-visible spectroscopy shows a shift of the band gap towards high energies. The energy band gap was found to be 2.52 eV (i.e., 0.1 eV blue shift). The photoluminescence spectrum consists of two bands located respectively at 2.51 eV and 2.31 eV. These bands are assigned to band-to-band transitions and deep level emission, respectively.

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Структурні та оптичні властивості нанокомпозиту полістиролу CdS, отриманого методом м'якої хімії

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Нанокристали сульфіду кадмію були отримані гідротермальним методом. Рентгенівські дифрактограми показали невелике розширення дифракційних піків. Це розширення зумовлене нанометричним розміром порошків сульфіду кадмію. Дифрактограми також підтвердили, що сульфід кадмію кристалізується у структурі вюрциту (кристалографічна група P6_3mc) і що розміри кристалітів є нанометричними. Нанокомпозит полістирол-сульфід кадмію був виготовлений методом м'якої хімії. Він включає змішування розчину сульфіду кадмію (1 г сульфіду кадмію, залитого в 10 мл хлороформу) з розчином 1 г полістиролу, розчиненого в 30 мл хлороформу. Після додавання нанопорошків CdS до полістиролу спостерігалося зменшення розміру з 20,90 нм до 16,68 нм. Зображення SEM показало, що поверхня полістиролу має пори, і ці пори були заповнені під час виготовлення композиту з нанокристалів полістиролу CdS. Спектри комбінаційного розсіювання, окрім піків комбінаційного розсіювання полістиролу, показують характерний пік поздовжньої оптичної фононної (LO) моди CdS. УФ-видима спектроскопія показала, що композит продемонстрував високу прозорість у видимій області. Спектр оптичного поглинання за кімнатної температури демонструє зсув краю поглинання в бік високих енергій. Ширина забороненої зони була отримана за допомогою кривої другої похідної. Значення енергії ширини забороненої зони становило 2,52 еВ. Спектр випромінювання полістиролу не демонструє люмінесценції, тоді як сигнал фотолюмінесценції композиту полістирол/нанокристалів CdS за кімнатної температури утворений двома смугами, розташованими відповідно при 2,51 еВ та 2,31 еВ. Перша смуга була віднесена до міжзонного переходу, тоді як друга – до глибокого рівня випромінювання.

Ключові слова: Полістирол, Нанокристали, Рентгенівська дифракція, РЕМ, Фотолюмінесценція.