PHASE IDENTIFICATION,ABSORBANCE AND EMISSION SPECTRA OF Ag-PANI@CdS NANOCOMPOSITES

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Abstract:

N-type semiconducting material such as Cadmium sulfide (CdS) with a direct band gap of 2.42 eV at room temperature possess excellent physical and chemical properties, it has promising applications in many fields of technology including gas sensors, photochemical catalysis, laser and infrared radiation detectors, solar cells, nonlinear optical materials, various luminescent devices and optoelectronic devices. Polyaniline (PANI) is a conjugated polymer with extensive conjugated electronic systems, has shown promise due to its high absorption coefficients in the visible part of the spectrum, high charge-carrier mobility, and good stability. Thus we have prepared CdS nanoparticles and Ag-PANI@CdS nanocomposite in our lab and dispersed with the help of ultrasonication bath using the DI water. Phase identification of these synthesized materials was observed with the help of X-ray diffraction (XRD) technique and the absorbance and emission spectrum of the synthesized materials were observed at room temperature with the help of UV-Vis spectrophotometer. The results obtained were compared with other workers and interpretations were made.Certain technical applications were suggested to develop multifunctional materials.

Key Words:

Band gap, Nanocomposites, Conjugated polymer , Absorption peaks ,Blue shift, Microelectronics. Multifunctional materials etc.

Introduction:

Cadmium sulfide (CdS) is a n-type semiconducting material with a direct band gap of 2.42 eV at room temperature with excellent physical and chemical properties.It has promising applications in many fields of technology including gas sensors, photochemical catalysis, laser and infrared radiation detectors, solar cells, nonlinear optical materials, various luminescent devices, optoelectronic devices, etc [1-4]. Cadmium sulfide (CdS) nanoparticle is of great interest for many optoelectronic applications including solar cells, light emitting diodes, photodiodes [5], nonlinear optics [6], and heterogeneous photocatalysis [7]. Zhan et al.[8] successfully fabricated long CdS nanowires utilizing polyacrylamide. Wire like assemblies of CdS nanoparticles are fabricated within core-shell cylindrical polymer brushes [9]. Polyaniline (PANI), a conjugated polymer with extensive conjugated electronic systems, has shown promise due to its high absorption coefficients in the visible part of the spectrum, high charge-carrier mobility, and good stability[10]. The combination of nano-sized inorganic and organic components in a single material has remarkable implications in the development of multifunctional materials. These composites not only combine the beneficial properties of inorganic materials and polymers, but also exhibit many new properties that a single-phase material lacks. These compounds have become an interesting research topic in recent years due to their electrical, optical, catalytic and mechanical properties as well as possible specific applications in optics and microelectronics [11-12]. Thus we report synthesis of CdS nanoparticles and Ag-Pani@CdS nanocomposites and study its optical properties in terms of phase identification and emission spectra.

Experimental details:

To study the proposed optical properties of nanocomposites, Cadmium chloride ($CdCl_2$), Silver nitrate ($AgNO_3$), Sodium sulphide (Na_2S) powder and Polyaniline (PANI) were used.All the starting precursors were used without further purification. For the synthesis of cadmium disulphide (CdS) nanoparticles, 0.1 M solution of $CdCl_2$ and Na_2S were prepared with the help of distilled water (DI). The prepared 0.1 M solution of Na_2S was added drop by drop in the 0.1 M solution of $CdCl_2$ under the constant stirring. After completing the reaction, the pale yellow precipitate was obtained and washed several times with DI water and ethanol. Finally the washed precipitates dried in vacuum oven at 70 ^{0}C for 18h [13]. For the synthesis of Ag-PANI@CdSnanocomposite, as-prepared CdS nanoparticle, AgNO3 and PANI were dispersed with help of ultrasonication bath using the DI water. Finally the disperse solution was dried in the vacuum oven at 60 ^{0}C for 24h to produce Ag-PANI@CdS nanocomposite. Phase identification of the as-prepared materials was observed with the help of X-ray diffraction (XRD) technique and the absorbance and emission spectrum of the synthesized materials were observed at room temperature with the help of UV-Vis spectrophotometer.

Results and Discussion:

The phase composition and crystal structure of the samples are determined with the help of XRD analysis. Figure -1 presents the XRD pattern of CdS and Ag-PANI@CdS nanocomposites, which show the crystalline nature of synhesized materials. The main diffraction peaks of CdS nanoparticles are well indexed and appeared at 26.58^0, 43.92^0, 52.22^0 corresponding to (111), (220), and (311) plan [13]. In Ag-PANI@CdS. There is no extra peak of Ag and PANI and other impurity peaks are observed, which indicates that CdS, Ag and PANI form a good composite structure.

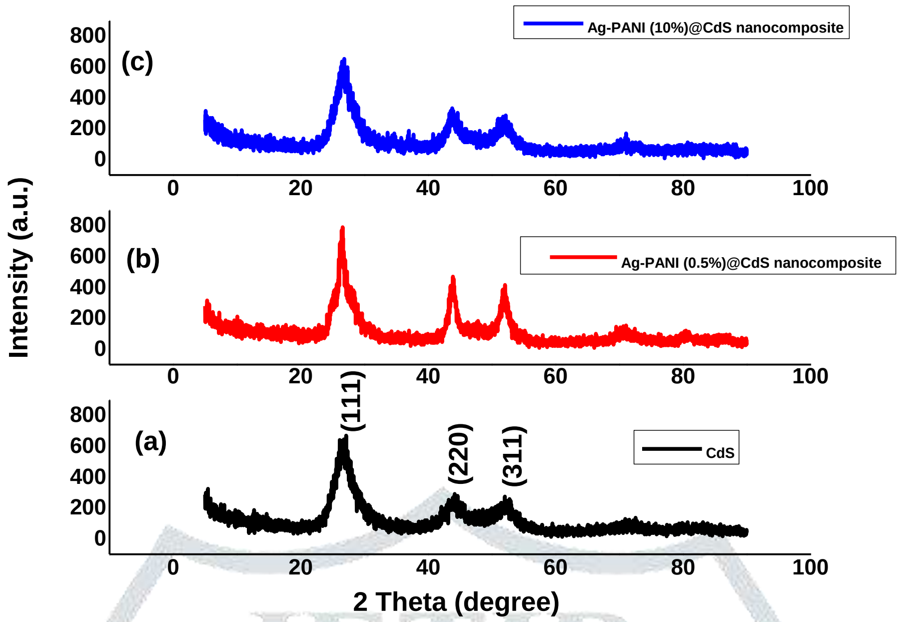

Fig. 1. XRD spectra of CdS nanoparticles and Ag-PANI@CdS nanocomposite. (**a**) CdS nanoparticle, (**b**) Ag-PANI(0.5%)@CdS nanocomposite, (**c**)Ag-PANI(0.5%)@CdS nanocomposites

The absorption spectra of prepared CdS nanoparticles and Ag-PANI@CdS nanocomposite are presented as Fig. 2. Fig. 2 (a), clearly shows that CdS nanoparticle have a broad absorption peak at 477 nm which was assigned to the optical transition of the first excitonic state, which is in agreement with the previous reported result [14]. In case of Ag-PANI@CdS nanocomposite , the absorbance of CdS nanoparticles decreased after the adding of Ag and PANI in CdS nanoparticles i.e. there is a blue shift.

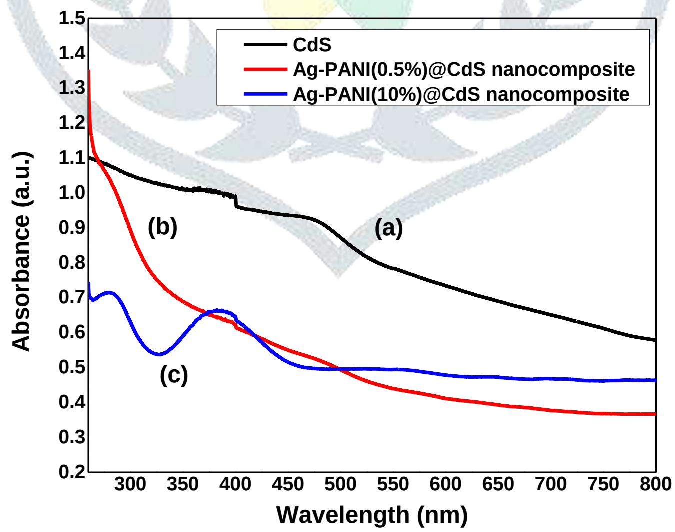

Fig. 2. UV-visible spectra of CdS nanoparticle and Ag-PANI@CdS nanocomposite. (**a**) CdS nanoparticle, (**b**) Ag-PANI(0.5%)@CdS nanocomposite, (**c**)Ag-PANI(0.5%)@CdS nanocomposite.

The band gap of synthesized materials have been estimated with the help of absorbance spectra using Tauc relation [15].

$$Z(h\nu - E_g) = (\alpha h\nu)^n \text{ --------------(1)}$$

Where,Z is constant,h is the plank constant, E_g is the band gap, and 2 for indirect band gap semiconductor material and n = 1/2 for direct band gap semiconductor material. In our case, the synthesized CdS nanoparticle and Ag-PANI@CdS nanocomposite, the direct transition rule is followed and is expressed as

$$Z(h\nu - E_g) = (\alpha h\nu)^2 \text{----------------(2)}$$

Fig. 3 (a-c) are presented the band gap of prepared materials.The evaluated band gap value for CdS nanoparticle and Ag-PANI (0.5%, 10%)@CdS are 2.47 eV, 2.69 eV, and 2.93 eV respectively. It is clear from the Fig -3, that the optical band gap values are found to be increase with the increase in the content of Ag and PANI in CdS nanoparticles.This increase in the optical band gap may be due to various reasons such as stoichiometries defects, quantum confinement effect and high density of localized states etc. [16,17].

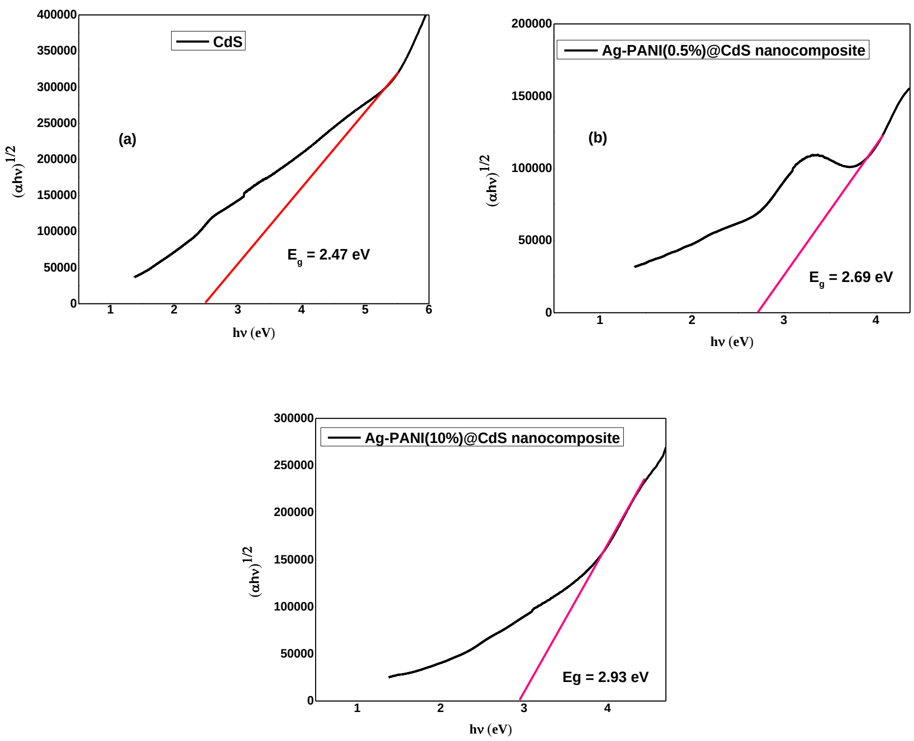

Fig. 3. Band gap of CdS nanoparticle and Ag-PANI@CdS nanocomposite. (**a**) CdS nanoparticle, (**b**) Ag-PANI(0.5%)@CdS nanocomposite, (**c**)Ag-PANI(0.5%)@CdS nanocomposite.

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