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Microstructural Features of Ni²⁺ Doped PVA Capped CdTe Nanoparticles

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ABSTRACT

II-VI group semiconductor nanocrystalline materials show enhanced luminescent properties. Surface capping agents are used to control the size of nanoparticles. Surface passivation, prevention of particles from agglomeration can be done by polymers which are in favour of controlling the particles size effectively. Cadmium telluride is a semiconductor material. It has been widely used for different applications. The direct bandgap and high optical absorption coefficient in the visible spectrum makes CdTe an ideal material for photovoltaics and other applications. CdTe nanoparticles doped with Ni²⁺ ions were prepared by Co-precipitation method using PVA as capping agent. The structural studies revealed that the crystal system is indexed to be cubic (zinc blende) phase. The average crystallite size is calculated and it is found to be 9 nm. The characteristic vibrational modes of constituent elements are evidenced by FTIR. SEM showed irregular shaped particle size clusters and EDS analysis confirms the presence of constituent elements of prepared material.

Keywords: CdTe, PVA, Co-precipitation, Ni²⁺ions, XRD, SEM and FTIR.

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INTRODUCTION

The size-quantization effect in semiconductor nanoparticles and nanostructures has become a flourishing field in chemistry, physics and material science [1, 2]. Inorganic materials synthesis is vast developing field, not only due to new materials but because tuning of the reaction schemes. These schemes enable the creation of nanocrystals with a precise control of their size, shape and composition [3, 4]. In semiconductors, shape is an important parameter which affects strongly the electronic spectrum of charge carriers as well as optical properties of nanocrystals. Thin films which are based on nanoparticle synthesis have great potential for next generation of semiconductor devices including solar cells and transistors. The high surface to volume ratio of nanoparticles in thin film form can trap electrons and forms a limit device performance.

Shape is very important parameter in semiconductor materials because it results strongly on the electronic charge carriers as well as optical properties of nanomaterials. Semiconductor nanocrystals for harvesting light energy has drawn great attention towards metal chalcogenide based systems of CdTe, CdS has great interest nowadays [5]. Cadmium telluride (CdTe) is a semiconductor material which is used for variety of applications. The direct bandgap is 1.5 eV at room temperature. Because of its high optical absorption coefficient in the visible spectrum makes CdTe an ideal material for photovoltaics [6]. The growth of CdTe is very important because of its applications in solar energy, X-ray detection, gamma ray detection and infrared detectors [7, 8]. CdTe usually crystallizes with the cubic zinc blend structure [9]. The techniques like electrochemical synthesis, close space sublimation, vapour transport deposition, electron beam evaporation, metal organic chemical vapour deposition, sputtering etc were used to deposit CdTe materials.

CdTe photovoltaic cells have low cost because of its direct bandgap and high absorption coefficient. Large number of preparation methods/techniques was identified for doping CdTe with both n- and p- type materials. Many fabrication techniques have been attempted for depositing CdTe nanoparticles [10-12]. Among these, Co-precipitation is the simple one, low cost one, easy to add doping materials and the possibility of varying the film properties by changing composition of starting solution. Rao et al. have presented the results on different oxide materials in their earlier studies [13-22]. In the present investigation, Ni²⁺ doped CdTe nanoparticles were prepared by co-precipitation and characterized by techniques like XRD and SEM to collect the microstructural information of the synthesized sample.

EXPERIMENTAL

Materials and Synthesis

Analytical Reagent (AR) grade of cadmium chloride (CdCl₂), Sodium hydrogen telluride (NaHTe), polyvinyl alcohol (PVA), Nickel Oxide (NiO) were used as starting materials. These materials were used directly without further purification. In the present experiment double distilled water was used as a solvent. 0.045g of cadmium chloride was added to 2.3g PVA and volume of the solution was completed to 50 mL by double distilled water. The complete solution was left for 24 hours at room temperature to swell. After that the solution was warmed up to 80°C and stirred for 6 hours until viscous transparent solution was obtained. One milliliter (mL) of sodium hydrogen telluride (NaHTe) was dropped into the solution with gentle stirring and then 0.01 mol % nickel oxide was added to it to get the transparent solution. The prepared solution was casted on flat glass plate dishes. After the solvent evaporation, a thin film containing iron doped PVA capped CdTe nanoparticles was obtained. The excess of insoluble salts were removed from the surface of the films by washing the films using de-ionized water before characterization.

Characterization

PANalytical Xpert Pro diffractometer with CuK α radiation was used to study the Powder X-ray diffraction pattern. Scanning electron microscope (SEM) and energy dispersive spectrum (EDS) are taken on ZEISS EVO 18. Transmission electron microscope (TEM) images are recorded on HITACHI H-7600 and CCD CAMERA system AMTV-600 by dispersing samples in ethanol. Bruker FT-IR spectrophotometer is used for recording FT-IR spectrum in the wavelength region 400-4000 cm⁻¹.

RESULTS AND DISCUSSION

Here in the present investigation PVA capped CdTe nanoparticles doped with Ni²⁺ were prepared by Co-precipitation method. These samples are characterized by powder X-ray diffraction, SEM with EDS, TEM and FT-IR. The XRD revealed the prepared samples are pure crystalline in nature.

Powder X-ray Diffraction Studies

XRD pattern of Ni²⁺ doped PVA capped CdTe nanoparticles were shown in Figure-1. A high intensity peak is observed at $2\theta = 23.46^\circ$ along with less intensity sharp peak at 40.09° (JCPDS file No. 15-0770), which indicates the crystal system as cubic phase and the corresponding lattice cell parameter $a = 0.637$ nm is calculated. The volume is found to be $V = 26.682$ nm. The crystallite size of the XRD peaks is calculated by Debye - Scherrer's formula,

$$D = (K \lambda / \beta \cos\theta)$$

where

D is the mean crystallite size,

K = 0.9 is Scherrer's constant,

λ is the wavelength of the incident beam,

θ is the diffraction angle,

and β is the full width half maximum intensity of the diffraction peak.

The average crystallite size is calculated as 9 nm from the XRD data and the broadening of diffraction peaks indicate the formation of nano-sized particles.

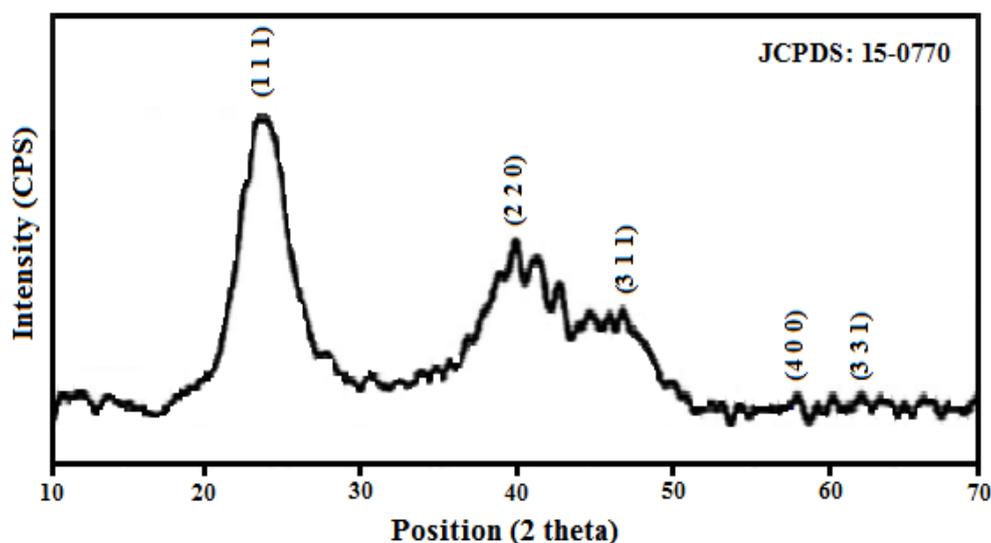


Figure-1: Powder XRD pattern of Ni²⁺ doped PVA capped CdTe nanoparticles

Morphological Studies

Figure-2 shows the SEM images of Ni²⁺ doped PVA capped CdTe nanoparticles at different magnifications. The SEM micrographs showed a little agglomeration of uniformly distributed spherical structures. The agglomeration could be induced by densification resulting from the narrow space between particles. EDS measurements confirm the incorporation of nickel into the host material. The observed EDS pattern was shown in Figure-3. EDS pattern showed the elemental compositions of Cd, Te and nickel. From the data of EDS, it was confirmed that the prepared samples contain doped nickel species. Further, to obtain the microscopic morphology and structural information the TEM analysis was performed. TEM images of Ni²⁺ doped PVA capped CdTe nanoparticles were shown in Figure-4. TEM images represent spherical and sphere like structures. The diameter was found to be around 18 nm.

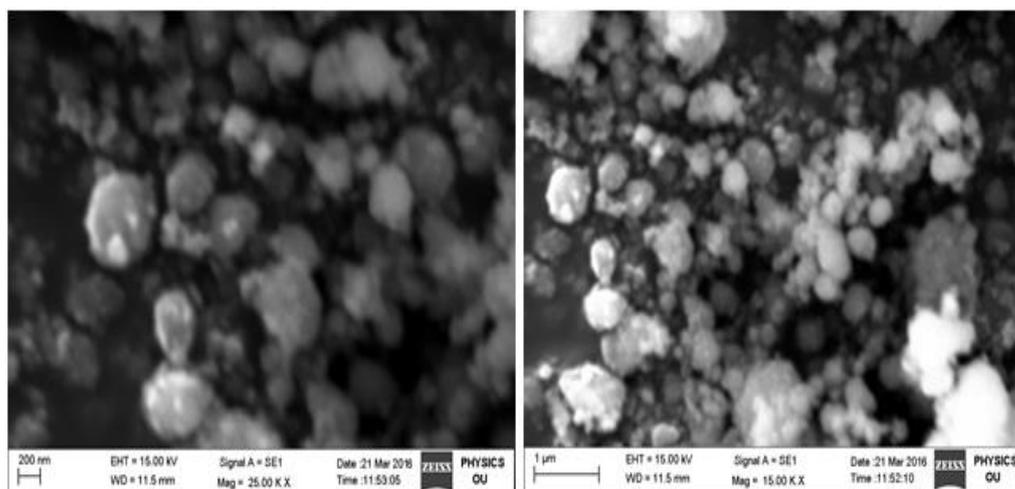


Figure-2: SEM images of Ni²⁺ doped PVA capped CdTe nanoparticles

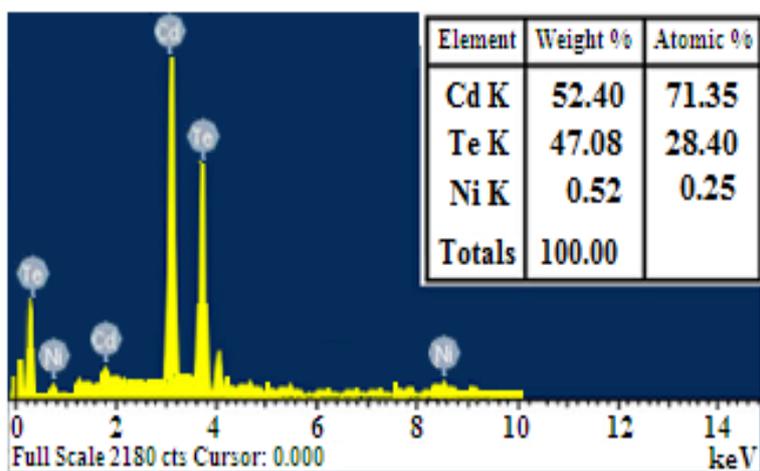


Figure-3: EDS spectrum of Ni²⁺ doped PVA capped CdTe nanoparticles

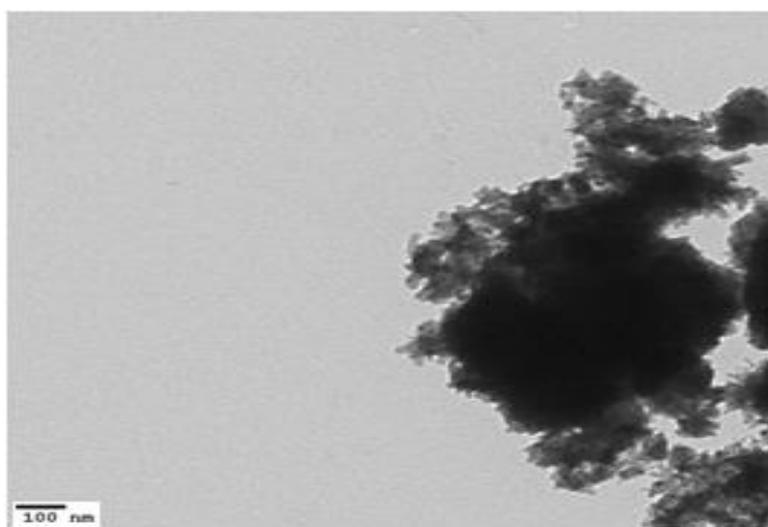


Figure-4: TEM images of Ni²⁺ doped PVA capped CdTe nanoparticles

FT-IR Studies

FT-IR spectrum of Ni²⁺ doped PVA capped CdTe a nanoparticle in the wavenumber range 500- 4000 cm⁻¹ is shown in Figure-5. The absorption peaks at 1381 cm⁻¹ and 1645 cm⁻¹ were due to C=C stretching vibration [23]. The absorption peak at 2956 cm⁻¹ was assigned to C-H stretching vibration [24]. Additionally, the characteristic peak of O-H group was appeared in the spectrum at 3382 cm⁻¹ regarded as the associated hydrogen bonds among the molecules [25].

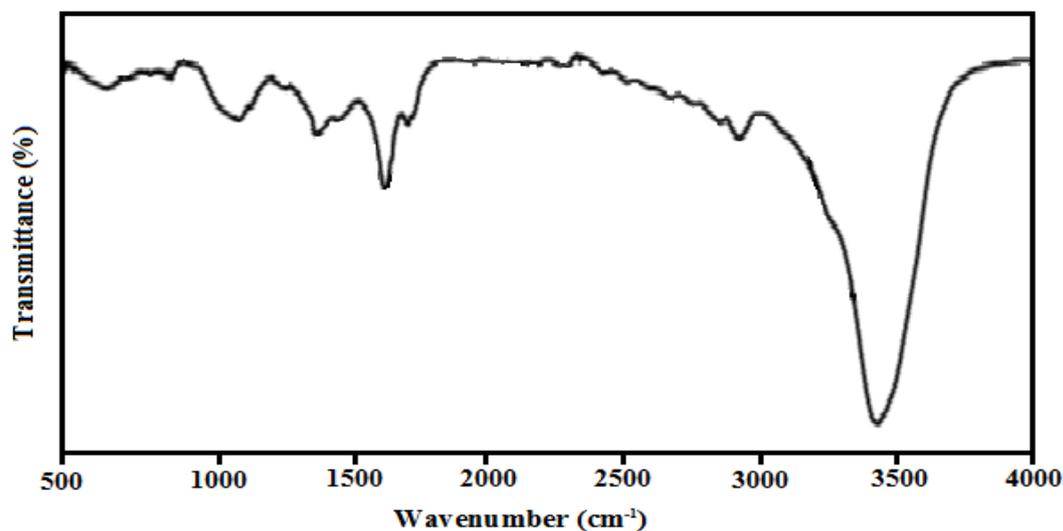


Figure-5 FT-IR spectrum of Ni²⁺ doped PVA capped CdTe nanoparticles

CONCLUSIONS

PVA capped CdTe nanoparticles were prepared by doping Ni²⁺ ions successfully by Co-precipitation method. X-ray diffraction studies revealed the crystal system is indexed to be cubic phase and the lattice cell parameters are evaluated. The calculated average crystallite size of Ni²⁺ doped PVA capped CdTe nanoparticles is around 9 nm. SEM micrographs show irregular shaped sphere like structures. The presence of constituent elements in the prepared material was confirmed by EDS analysis. TEM images clearly show the formation of nanorods. The characteristic vibrational modes in the host lattice were confirmed by FT-IR analysis.

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