Studies on structural characteristics of Ag:CdTe nanoparticles by precipitation method

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Abstract:
This work deals with the synthesis and structural characterization of silver (Ag) doped cadmium telluride **(**CdTe) nanoparticles which were prepared by using conventional co-precipitation method and the samples were characterized by X-ray powder diffraction. The doping concentration varies from 0.1 **-** 0.3% of Ag atoms. X-ray diffraction (XRD) studies reveal that silver (Ag) doped cadmium telluride **(**CdTe) nanoparticles have ahexagonal crystal structure highly orientated with the hkl values of (401) plane along with Ag_7Te_4, Ag:CdTe ($Ag_2Cd_{1+x}Te$) and Ag:CdTe ($Ag_2Cd_{5+x}Te$) phases. The crystalline size of the particle varies from 62.51 nm to 72.01nm and is found to be increased with increase in concentration of Ag.

Keywords: II-VI semiconductors, cadmium compounds, Ag, X-ray diffraction (XRD), Crystal structure.

1. Introduction

The intense interest in the science of materials confined within the atomic scales stems the fact that these semiconducting nanomaterial's exhibit fundamental unique size dependent optical and electrical properties with potential of next generation technologies

in electronics, optics, biotechnology, computing, medical imaging, drug delivery, aerospace and energy etc. [1]. As size of the particle reduces to nano and increased surface states, which influence the chemical reactions by altering transitions of electrons and holes. Metal oxides and telluride's play a very important role in many areas of chemistry, physics and materials science. The structural geometries with an electronic structure can exhibit metallic, semiconductor or insulator character. Since the discovery that nanocrystalline materials have interesting chemical and physical properties, these materials have found many applications. Incorporation of semiconductor nanocrystals (NCs) into functional polymers is a highly desirable approach to generate novel materials for use in optoelectronic devices, such as light emitting diodes (LEDs), photovoltaic cells, chemical/biological sensors and photo catalysis [2]. There has been growing interest in the synthesis of nanometer-sized II-VI binary semiconductor materials.

Nanoparticles based on II-VI and III-V semiconductors have been the most widely studied systems in the recent years. Among different semiconductor materials, II-VI semiconductor nanoparticles are considered to be an important group with considerable progress in the synthesis and utilization of their unique properties [3, 4]. CdTe is an important II-VI semiconductor material, which is very useful for a variety of electro-optical devices and solar energy conversion [5]. CdTe nanoparticles have been the subject of numerous investigations, because of high quantum efficiency and multicolour availability.CdTe nanoparticles can find applications in solid-state lighting, displays, optical communications, sensors, as well as in biological imaging and detection. In the recent years, the use of nano particle coatings such as CdTe semiconductor has experienced a significant boom because of its ideal band gap, high absorption coefficient; low-cost, diversified manufacturing methods and their applications compared to other thin film coatings [6]. The most important applications of cadmium telluride thin films are using of these in the solar cells [7-9], detectors [10] and photovoltaic [11]. Doping is widely used method to improve electrical, optical and luminescent properties of semiconductor compounds, facilitating the construction of many electronic and optoelectronic devices.

In the present work, Ag doped CdTe nanoparticles with various concentration of Ag ion were prepared by precipitation method. These nanoparticleswere characterized for structural properties.

2. Experimental details

2.1 Preparation of Precursor Solution

In the present work, raw materials used for synthesis of Ag doped CdTe nanocrystalline materials were cadmium acetate dehydrate 99% AR grade $Cd(CH_3COO)_2.2H_2O$, Tellurium dioxide (TeO_2) and Silver nitrate ($AgNO_3$) (Loba) as a source materials.All chemicals are used in this work without further purification. All the solutions were prepared in fresh double distilled water (Merck) and acetone is used for glassware cleaning purpose. For preparation of precursor solutions of desired concentrations, we have used the formula**Eq. (1)**,

$$\mathbf{W=\frac{M \times C \times Q}{1000}} \quad \mathbf{(1)}$$

where, W is the weight of solute in gm, M is the molecular weight of the solute/salt, C is the concentration (molarity) and Q is quantity of solvent in ml. Different powders can be prepared for each composition by precipitation method.

2.2 Synthesis of Ag doped CdTe nano powder

In the present work, simple chemical precipitation method were employed to synthesize $Cd_{1-x}Ag_xTe$ (x = 0.1, 0.2 and 0.3) nano powder where x is the doping concentration of Ag. Chemical reaction was carried out at room temperature. Depending on the value of 'x', initially the 50 ml solutions of cadmium acetate, silver nitrate and telluride dioxide were prepared separately using deionized water. For the preparation of $Cd_{1-x}Ag_xTe$ powder samples, 50 ml solution of silver nitrate was added drop wise into 50 ml solution of cadmium acetate in beaker and stirrer vigorously by using magnetic stirrer at room temperature. Then 50 ml solution of tellurium dioxide was slowly mixed drop wise in a beaker containing the mixed solution of cadmium acetate, silver nitrate and then the mixture continuously and vigorously stirred for 3 hours at constant stirring 800 rpm and consequently a dark gray $Cd_{1-x}Ag_xTe$ precipitate formed which was filtered out and washed several times with double distilled water and methanol to remove all impurities. Finally, the product was dried for 24 hours in dry air. After drying, the precipitate was crushed to fine powder by grinding process using a mortar and pastel.

2.3 Characterization of Ag doped cadmium telluride ($Cd_{1-x}Ag_xTe$) powders

The synthesize $Cd_{1-x}Ag_xTe$ (x = 0.1, 0.2 and 0.3) nanopowder where x is the doping concentration of Ag were characterized for structural properties by X-ray Diffractometer of Bruker (D8 ADVANCE) in scanning angle of 20°-80° (2θ) using CuKα1 radiation with wavelength 1.5406 Å.

3. Results and Discussion

3.1 Structural properties of $Cd_{1-x}Ag_xTe$ powders

The X-ray diffraction pattern of the synthesized Ag doped CdTe nano powders at different Ag concentrations are shown in **Fig. 1**. The structure is composed of hexagonal phase with (310), (401) and (422) as preferred orientation and can be indexed based on a hexagonal Ag_7Te_4 lattice with constant a = 13.48 Å as a dominated one as polycrystalline in nature. As seen a main peak is observed at position 2θ ≈ 32.258° which is corresponding to strong (401) preferential orientation for hexagonal crystal system of Ag_7Te_4 and (213) for hexagonal phase system of CdTe. However, it reveals that the high concentration of Ag helps to growAg_7Te_4 crystals with (401) orientation.

The peaks intensity at position 2θ ≈ 27.84°, 32.25°, 46.26°, 54.81° and 57.49° for (310), (401), (422), (105) and (603) oriented Ag_7Te_4 phase gets increases continuously with increase Ag concentration which may be attributed to the growth of the materials that revealed to an improvement in the crystallinity [12]. The controversial result was observed by the different authors [13]. It is also revealed that the presence of peak related to Ag:CdTe at 46.24° indicate the presence of Ag doped CdTe alloy in all concentrations depicted the behaviour of alloy formation even the concentration varied. The next major peak is at 2θ ≈ 27.84° for Ag_7Te_4 (310), Ag (220) and hexagonal CdTe (210) again next major peak is at 2θ = 46.26° for Ag_7Te_4 (422), cubic CdTe (311), Ag (420) and Ag:CdTe. These results are matched with the reference JCPDS card numbers 75-1022, 01-1167, 19-0193, 75-1022, 10-0207, 01-1164, 42-1221 and 42-1222 for Ag_7Te_4, Ag, H-CdTe, Ag_7Te_4, C-CdTe, Ag, Ag:CdTe ($Ag_2Cd_{1+x}Te$) and Ag:CdTe ($Ag_2Cd_{5+x}Te$) respectively. The results of XRD pattern show the formation of Ag doped CdTe nano powder.

In this XRD pattern, it can be seen that the change in intensities of all the peaks for all concentrations of Ag was observed as shown in **Fig 1**. The two peaks at 2θ ≈ 23.34°, 26.17° have appeared showing hexagonal crystal system with (300) and (220) orientation respectively. The intensity of both peaks decreases for higher concentration. The peak at 2θ ≈ 23.34° is the mixture of cubic CdTe (111) and hexagonal CdTe (100)[14].

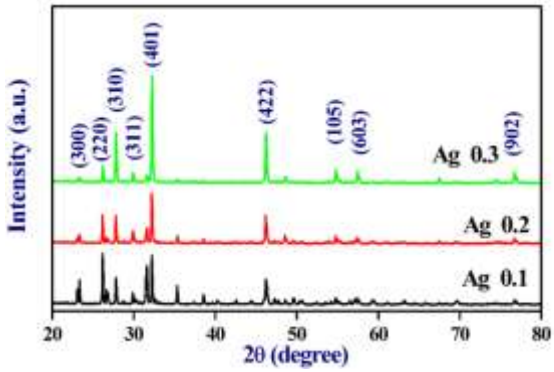

Fig. 1: X-ray diffraction spectra of Ag doped CdTenanopowders with Ag (x = 0.1, 0.2 and 0.3)concentrations

To know more about the effect of Ag concentrations on structural properties, the structural parameters such as lattice constants (a, c), crystalline size (D) and inter planar spacing (d) were calculated using relations concerned [15, 16] and tabulated in **Table 1 & 2**.

The lattice constant is found 9.61 Å which is slightly lower than the powder sample (13.48 Å).

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The inter-planner spacing is varied in the range 2.7745-2.7726 Å and observed to decrease with Ag concentration. The average crystalline size (D) was calculated using the Scherer's relation and found in the range 62.51-72.01 nm. The XRD analysis results of Ag:CdTe powders for different concentrations of Ag are given in **Table 3**

Table 1: The structural parameters of $Cd_{1-x}Ag_xTe$ powder with different values of x = 0.1, 0.2, and 0.3%

Composition	2θ °	(hkl)	d (Å)		a (Å)		D (nm)
			Obs.	Std.	Obs.	Std.	
$Cd_{0.9}Ag_{0.1}Te$	32.236	(401)	2.7745	2.7599	9.611	13.48	62.51
$Cd_{0.8}Ag_{0.2}Te$	32.239	(401)	2.7742	2.7599	9.610	13.48	64.08
$Cd_{0.7}Ag_{0.3}Te$	32.258	(401)	2.7726	2.7599	9.604	13.48	72.01

Table 2: The structural parameters of $Cd_{1-x}Ag_xTe$ powder with different values of x = 0.1, 0.2, and 0.3%

Composition	2θ °	(hkl)	FWHM	a = b (Å)		c (Å)		Volume
				Obs.	Std.	Obs.	Std.	$(Å)^3$
$Cd_{0.9}Ag_{0.1}Te$	32.236	(401)	0.1322	9.611	13.48	8.323	8.49	768.80
$Cd_{0.8}Ag_{0.2}Te$	32.239	(401)	0.1290	9.610	13.48	8.322	8.49	768.55
$Cd_{0.7}Ag_{0.3}Te$	32.258	(401)	0.1148	9.604	13.48	8.317	8.49	767.13

Table 3: The XRD results of $Cd_{1-x}Ag_xTe$ powders at different concentrations of Ag (x= 0.1%)

Concentrati-on of Ag	2θ °	Formation	Crystal system	Millar indices (hkl) of observed peaks
Ag 0.1%	23.34	Ag_7Te_4+CdAgTe+CdTe	Hex+Cubic	Ag_7Te_4(300),H-CdTe(100), C-CdTe(111)
	26.17	Ag_7Te_4+CdTe	Hexagonal	Ag_7Te_4(220),H-CdTe(003)
	27.81	Ag_7Te_4+CdTe+Ag	Hexagonal	Ag_7Te_4(310),H-CdTe(210), Ag(420)
	32.23	Ag_7Te_4+CdTe	Hexagonal	Ag_7Te_4(410),H-CdTe(213)
	46.24	Ag_7Te_4+CdAgTe+CdTe + Ag_5Cd_8+Ag	Hex+Cubic	Ag_7Te_4(422),Ag_5Cd_8(510), C-CdTe(311),Ag(420)
	76.71	Ag_7Te_4+CdTe+Ag_5Cd_8+ Ag	Hex+Cubic	Ag_7Te_4(902),Ag_5Cd_8(800), C-CdTe(511),H-CdTe (300),Ag(105)

4. Conclusion

Precipitation method has been used to synthesize Ag doped CdTe crystals with different concentration of Ag. Structural studies have been demonstrated the influence of Ag concentration on crystal growth of CdTe in their preferred orientation. The Ag^{2+} doped CdTe has three distinct (310), (401) and (422) planes as preferred orientation and can be indexed based on a hexagonal Ag_7Te_4 lattice with constant a = 13.48 Å as a dominated one as polycrystalline in nature. Increase of Ag concentration supports Ag_7Te_4 growth and increase in crystalline size.

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