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Positron Life time Study of CdSe and CdT

Mahesh Chander Mishra, Ph.D
R R Govt. Autonomous College,Alwar Alwar, Rajasthan INDIA

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Corresponding Author:	mahesh chander mishra, Ph.D R R Govt. Autonomous College,Alwar Alwar, Rajasthan INDIA
Corresponding Author Secondary Information:	
Corresponding Author's Institution:	R R Govt. Autonomous College,Alwar
Corresponding Author's Secondary Institution:	
First Author:	mahesh chander mishra, Ph.D
First Author Secondary Information:	
Order of Authors:	mahesh chander mishra, Ph.D
Order of Authors Secondary Information:	
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Abstract:	The positron annihilation studies have been presented on II-VI group polycrystalline CdSeand CdTe compound semiconductor. Samples were prepared in form of 1 mm thick pellets having 12 mm diameter using hydraulic pressure at 3 ton. These pellets annealed at different temperature under vacuum (10-5 torr) then characterized using positron annihilation spectroscopy and X-ray diffraction (XRD) techniques after and before annealing. Structural properties have been observed for both the pristine as well as annealed samples. It has been found that concentration of defects is decreased and crystallinity of samples is increased after annealing.
Suggested Reviewers:	yogesh kumar vijay, Ph.D professor, VIT,Jaipur vijayyk@gmail.com
	mangej singh, Ph.D Assot.professor, University of Rajasthan singh-mangej@uniraj.ernet.in
	Dolia s.n., Ph.D Assot.professor, University of Rajasthan sndolia@uniraj.ernet.in
	mukesh kumar mishra, Ph.D Assot.professor, University of Rajasthan mishra-mk@uniraj.ernet.in
	kunj bihari joshi, Ph.D professor, Mohanlal Sukhadia University k_joshi@yahoo.com
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1.Introduction

The II-VI group compound semiconductors are technologically important materials. Their widespread applications in optoelectronic devices, detectors and photoelectro-chemical reactions have increased interest in the study of the properties of these materials. CdSe and CdTe are the most established II-VI group compound semiconductors. These have great importance in the fields of fundamental research and technical applications because of its structural, optical and electronic properties. Due to large atomic number of Cd, Se and Te, high density, sufficiently wide optical band gap and good carrier mobility. CdTE is used both as X- ray as well as γ- ray detector at room temperature [1, 2]. It is also used as photon absorber in solar cells because of strong absorption and high detection efficiency of high energy photons [3, 4]. CdSe is used as photovoltaic, acousto-optic applications and photoconductive material [5]. Among the various applications, CdSe has been studied intensively in recent years as a photo anode in photo electrochemical cells [6]. The transport and optical properties of n-type CdSe crystals together with microanalysis of residual impurities was carried out by Tenne et al. [7]. At atmospheric conditions, both CdSe and CdTe occur in two modifications, one having the hexagonal wurtzite structure and the other having the cubic zincblende structure. Usually the cubic modification exists in thin layers, while bulk CdSe has the hexagonal structure. Under pressure CdSe undergoes a structural transformation into the rocksalt structure [8]. Presence of defects in the form of vacancies, vacancy–impurity complexes and dislocations play a major role on the performance of compound semiconductors. Defects trap charge carriers and modify the optical properties in terms of optical absorption or emission of photons in radiative recombination mechanisms. So for understanding the material properties, it is necessary to understand the defects. Many researchers have studied defects dynamics of II-VI group compound semiconductors [9-16]. During growth, the material is often subjected to annealing under controlled temperature and partial pressures to getter impurities and to reduce native defects introduced during the growth at high temperatures [17]. Although, high-pressure growth produces the material with the highest resistivity, large single crystals are difficult to produce, and material inhomogeneities remain. While more conventional growth results in lower

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resistivity material, if postgrowth annealing can be employed to reduce the native defect concentrations, resistivities comparable to or in excess of those obtained in the high pressure growth method. The question remains as to how to select these annealing conditions so as to optimize the desired materials properties. In this chapter, I studied that the equilibrium native defect concentrations in CdSe and CdTe as a function of temperature. Study of annealing induced defects in semiconductors has been a subject of both basic and technological interest for CdSe and CdTe.

During the last few decades, there have been many techniques for defects studies but amongst them positron annihilation spectroscopy (PAS) has proved to a valuable tool. It is non destructive, depth resolved and highly defect sensitive technique. The particular importance of positron annihilation spectroscopy for identification of vacancy-type defects in a solid is well known [18-23]. The detection of defects by means of positron annihilation spectroscopy is based on the trapping model [24, 25]. The aim of this model is the quantative analysis of life time spectra in order to calculate the trapping rates and the corresponding defects concentration. The main reason for the binding of positron to an open volume defect is the lacks of repulsive force of nucleus.

Positron annihilation lifetime (PAL) spectroscopy deals with the measurement of the lifetime of positrons in a solid [26]. Positrons injected from a radioactive source (^{22}Na) get thermalized within 1–10 ps inside a sample and annihilate with an electron of that material. The lifetime of positrons trapped in defects is comparatively longer with respect to those that annihilate at defect-free regions. An analysis of the PAL spectrum, thus, throws light on the nature and abundance of defects in the material. Crystallinity of material can be identified by X-ray diffraction (XRD) technique which shows specific peaks at certain diffraction angle [27].

The evolution of defects with increasing annealing temperature is being presented here. This chapter employs the analysis to understand the defect dynamics near annealing temperature in CdSe and CdTe.

2 Experiment

2.1 Sample preparation

Polycrystalline powder of CdSe and CdTe compound semiconductors having purity 99.999 has been prepared in pellets form of thickness 1 mm & 12 mm diameter by applying 3 ton hydraulic pressure. These pellets were annealed in vacuum environment (10^{-5} torr) at different temperature 100^0 C and 300^0 C for constant duration (3h). Slow cooling and heating rate (3^0 C / minute) have been maintained to avoid any strain.

2.2 Characterization:

These samples have been characterized by XRD and PAL techniques.

2.2 (1) XRD

For structural measurement, these samples were analyzed using Philips X'pert Pro X-Ray diffractometer having Cu Kα (λ=1.5460Å) source of X-rays. Bragg diffraction condition has been verified and powder X software has been used for analyzing the results. These results are verified with PCPDF win cards. h, k, l planes have been best fitted for CdSe and CdTe compound semiconductor. For each sample, a scan has been performed from 20^0 to 70^0 angles with step size of 0.05^0.

2.2 (2) Positron annihilation lifetime spectrometer

For the positron life time measurement, two identical scintillation detectors with the time resolution 300 ps have been used to measure start and stop signal. A sodium (^{22}Na) positron source(20 μ Ci activity) has been sandwiched between two identical pallets. Energy pulses have been selected by CFDD unit, these selected pulses converted into shape pulses by time to amplitude converter (TAC). PAL spectra have been recorded by connecting electronics and MCA data acquisition system. After this, PAL spectra have been analyzed by PATFITT88 [28] software to fit the life times.

3. Results and Discussion

Fig. 1.1 shows the XRD pattern of CdSe samples.The diffraction data is in agreement with the JCPDS card no. 08-0459 for CdSe, which depicts the wurtzite structure of the samples. The corresponding peaks at special angle are shown in figure. For the

CdTe samples, the characteristic diffraction peaks 111, 220, 311, 400 and 331, are observed in the patterns in Fig. 1.2. The calculated lattice parameter of CdTe is 6.471Å corresponding to zinc blende structure which is in good agreement with the value in the JCPDS card, no. 15-770. It is clear from Fig. 6.1 and 6.2 that intensity of corresponding peak has been increased and peaks become sharp after the annealing.
Table 6.1 shows lifetime parameters for pristine, 100^0 C and 300^0 C annealed CdSe samples and Table 6.2 shows positron lifetime parameters for pristine, 300^0 C and 500^0 C annealed CdTe samples. The variation in positron lifetime as well as intensity for CdTe and CdSe due to heat treatment is observed. The value of τ_1 lies (187-172 ps) in CdSe and (154-147 ps) in CdTe is attributed to diffused vacancies at grain boundaries and second life time τ_2 lies (378-388 ps) for CdSe and (375-385 ps) for CdTe, attributed to annihilation of positron directly trapped in vacancy like defect in the samples. Here we are interested only in second life time (τ_2) due to defects. It is clear from the tables that there is small change in lifetime (τ_2) of annealed samples in comparison to pristine life-time (τ_1) in CdSe and CdTe respectively. For both sample the secondary lifetime (τ_2) increases but corresponding intensity decreases respectively, which indicate that concentration of defects is decreased due to annealing.

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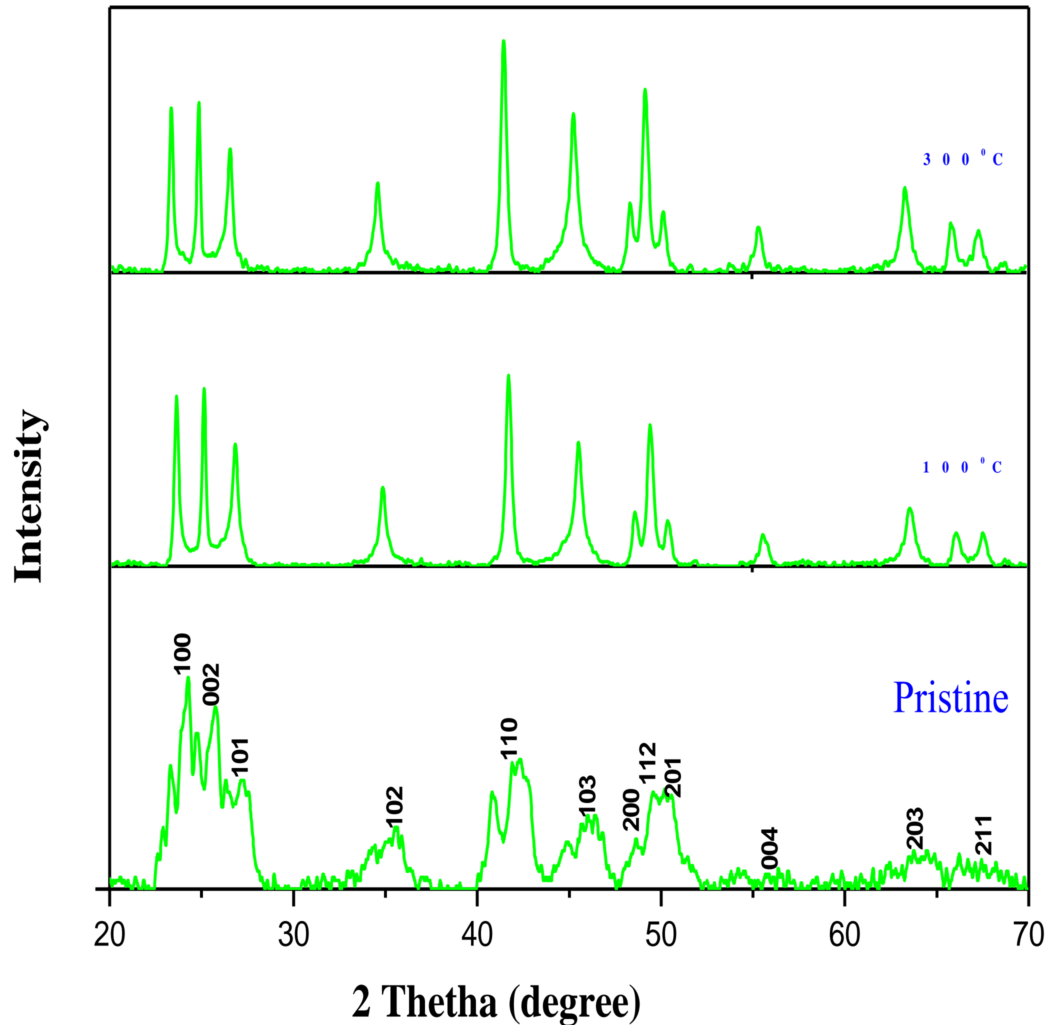

Fig. 1.1 X-ray diffraction pattern of CdSe.

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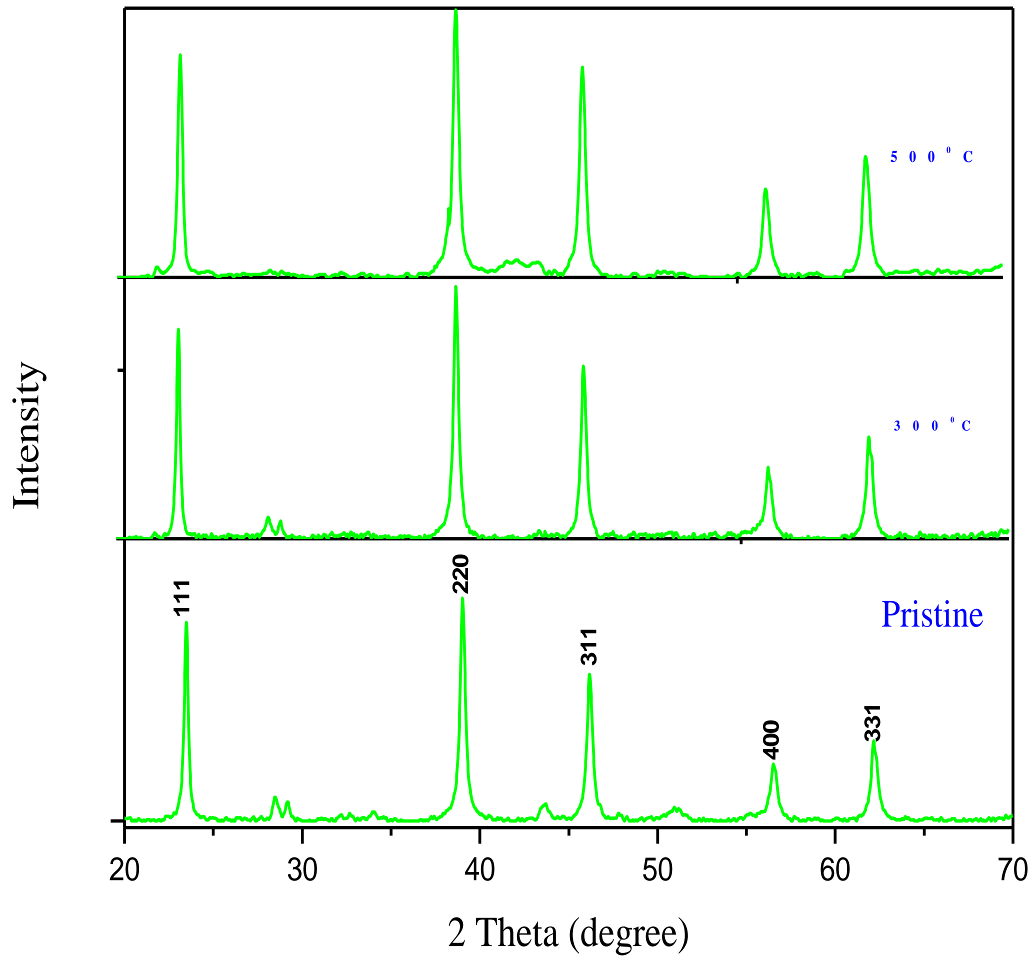

Fig. 1.2 X-ray diffraction pattern of CdTe.

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Table 6.1

Positron lifetime parameter for CdSe samples

S. No.	Sample	τ_1 (ps)	τ_2 (ps)	I_1 %	I_2 %
1.	CdSe (Pristine)	187±004	378±003	39.40±1.92	58.10± 1.77
2.	CdSe (100 ^{0}C)	182±004	386±003	44.40±1.92	56.10± 1.77
3.	CdSe (300 ^{0}C)	172±004	388±004	46.20±1.97	53.10± 1.99

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Table 6.2

Positron lifetime parameter for CdTe samples

S.No.	Sample	τ_1 (ps)	τ_2 (ps)	I_1 %	I_2 %
1.	CdTe (Pristine)	154±006	375±006	38.605±1.924	61.10±1.798
2.	CdTe (300 ^{0}C)	150±006	385±006	42.605±1.924	58.101±1.798
3.	CdTe (500 ^{0}C)	147±006	380±006	44.406±1.925	55.502±1.793

4 Conclusions

The defects and structural properties in CdTe and CdSe samples due to annealing process at different temperature have been characterized by PAL and XRD techniques. It is clear from above discussion that due to annealing concentration of defects is decreased and crystallinity of the samples is increased.

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April 2017

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