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Defects study in CdSe using positron annihilation lifetime spectroscopy

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Abstract

Positron life time measurement have been done for CdSe. Samples were prepared in pellet form. Two identical scintillation detectors with the time resolution 300 ps have been used to measure start and stop signal. PAL spectra have been recorded by connecting electronics and MCA data acquisition system. PAL spectra have been analyzed by PATFITT88 software to fit the life times. Samples were annealed and measured life times. The variation in positron lifetime as well as intensity for CdSe due to heat treatment is observed. The value of life time (τ_1) is attributed to diffused vacancies at grain boundaries and second life time(τ_2) is attributed to annihilation of positron directly trapped in vacancy like defect in the samples. It is clear from the tables that there is small change in life-time (τ_2) of annealed samples in comparison to pristine life-time (τ_1) in CdSe. Secondary lifetime (τ_2) increases but corresponding intensity decreases respectively, which indicate that concentration of defects is decreased due to annealing

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 is 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. CdSe 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, CdSe 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 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 as a function of temperature. Study of annealing induced defects in semiconductors has been a subject of both basic and technological interest for CdSe .

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

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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 .

2 Experiment

2.1 Sample preparation

Polycrystalline powder of CdSe 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 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

The PAL spectra of pristine, 100^0 C and 300^0 C annealed CdSe samples . There is small change in annealed samples to pristine samples.

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. It is clear that intensity of corresponding peak has been increased and peaks become sharp after the annealing.

Lifetime parameters for pristine, 100^0 C and 300^0 C annealed CdSe 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 is attributed to diffused vacancies at grain boundaries and second life time τ_2 lies (378-388 ps) for CdSe is 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. For this 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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