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# Synthesis and Characterization of Single Crystals of Cadmium Iodide as Gamma-ray Radiation Sensor

Alka Garg[a*] & Ritu Dhingra[b]

[a]Department of Physics, Gargi College, University of Delhi, Delhi 110 049, India
[b]Department of Physics, Maitreyi College, University of Delhi, Delhi 110 021, India

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Single crystals of Cadmium iodide have been grown by solution method and characterized by X-ray Diffraction (XRD) to determine the structural parameters and miller planes which are responsible for X-ray diffraction. The Crystals were subjected to UV spectroscopy to determine the optical band gap. The value of optical band gap was found to be 3.22 eV, well matched with the value reported in the literature. The presence of well-defined reflections with low FWHM confirms the good crystalline quality of single crystals. Single crystals of cadmium iodide have been chosen to design a radiation sensor as it has high absorption coefficient, wide band gap, and high resistivity. These are the required parameters for a compound semiconductor to act as a radiation sensor at room temperature. Single crystals were exposed to low dose of gamma radiation emitted by the source Cobalt-60 to explore their usage in detecting high energy gamma radiations at room temperature. It was observed that on irradiation the optical band gap decreased but there was no variation in the peak positions of XRD, although the intensity of XRD peaks decreased. The results have been explained in terms of structural defects produced due to gamma irradiation.

**Keywords:** Single crystals; Cadmium iodide; Solution method; XRD; UV-Spectroscopy

## 1 Introduction

Radiation exposure can pose serious health risks to humans and the environment. Radiation detectors are essential for monitoring and controlling exposure to ionizing radiation, which can come from sources such as nuclear reactors, medical equipment, and industrial processes. Detecting and quantifying radiation levels help ensure the safety of workers, the public, and the environment. Designing radiation detectors is important and crucial for their application in radiation monitoring of environment, safety of workers in and around nuclear reactors , and for scientific research.

Metal iodides are considered as suitable material for sensing high energy radiation due to their remarkable sensitivity to ionizing radiations, driven by their distinctive structural and optical properties[1].Among these, Cadmium iodide stands out as a notable candidate. It possesses several desirable characteristics including a high atomic number, a wide energy band gap and a high absorption coefficient[2]. Cadmium iodide unit cell is hexagonal which is typical of the compounds of the form $MX_2$. Cadmium ions are sandwiched between two identical layers of iodine atoms. The aim of the present work is to grow single crystals of cadmium iodide. These single crystals were subjected to a comprehensive characterization process employing X-ray diffraction and UV spectroscopy. Subsequently underwent irradiation with gamma rays, allowing for the investigation of alterations in their structural and optical properties resulting from exposure to gamma irradiation.

## 2 Materials and Methods

The solution of cadmium iodide in water was made by dissolving 15.1 g of cadmium iodide in 20 ml of water. This solution was kept undisturbed for almost two days for the preparation of the crystals under ambient conditions of temperature, moisture and pressure. Single crystals were dried and characterized by XRD (Model Bruker D8 Discover) and UV-spectroscopy (Perkin Elmer, lambda 35). Crystals were then irradiated with gamma rays from a cobalt-60 source with a dose of 20 Gy at a rate of 1 Gy per minute performed at INMAS Delhi. The irradiated crystals were characterized by XRD and UV to determine any changes in the structural and optical properties.

## 3 Results and Discussion

Single Crystals of $CdI_2$ were characterized by XRD for structural measurements. The XRD results are

*Corresponding author: (E-mail: alka.garg@gargi.du.ac.in)

depicted in Fig. 1. Sharp and well- defined diffraction peaks are observed at angles 2θ equal to 12.93°, 25.91°, 39.11° and 53.27° corresponding to the miller planes (002), (004), (006) and (008) respectively, which are in good agreement with the corresponding reflections reported in the card no. JCPDS data file 00-012-0574-hexagonal[3].XRD analysis reveals the hexagonal structure of crystals. All the diffraction peaks are obtained from the planes of symmetry (00l), which are perpendicular to the c-axis. Sharp and well-defined diffraction peaks confirm the formation of single crystals. As all planes are oriented in the same direction, it can be inferred that most of the crystallites are oriented with their c-axis normal to the basal plane[4].

Figure 2 shows the XRD of single crystals irradiated with gamma rays with a dose of 20 Gy. It is observed that on irradiation, the intensity of the planes represented by miller indices (002) and (004) is comparatively reduced. The positions of the peaks are identical for both un-irradiated and irradiated crystals, which suggests that no change in lattice parameters occurred within the resolution of XRD. This indicates that gamma irradiation can result in the weaker interface bonding between the single crystalline grains which reduces the volume fraction of single crystalline phase[5]. The crystallite size of the unirradiated and radiated crystals was estimated by fitting the prominent peak corresponding to dominant (004) plane using Scherrer's formula:

$$D= K \lambda / \beta \cos \theta \quad \text{... (1)}$$

where K is Shape factor constant, λ is X-ray wavelength, β is full width at half maxima (FWHM) in radians, and θ is Bragg's diffraction angle. The estimated value of crystallite was found to be 55nm for unirradiated crystals and for radiated crystals it was calculated to be 53nm within experimental errors. Thus it can be concluded that irradiation with low doses of gamma rays has not changed the structural properties much.

The value of optical band-gap was determined by plotting the graph between $(\alpha h\upsilon)^2$ and photon energy with the linear portion extrapolated to the X-axis which is referred to as the Tauc's plot[6]. Figs. 3 & 4 show the Tauc's plot of a single crystal of cadmium iodide before and after gamma irradiation.

It is observed that on irradiation the optical band gap decreased from 3.22 eV to 3.14 eV. It is thus evident that irradiation creates a band tail which shifts towards the higher energy range leading to a decrease in the optical band gap. The decrease in optical band

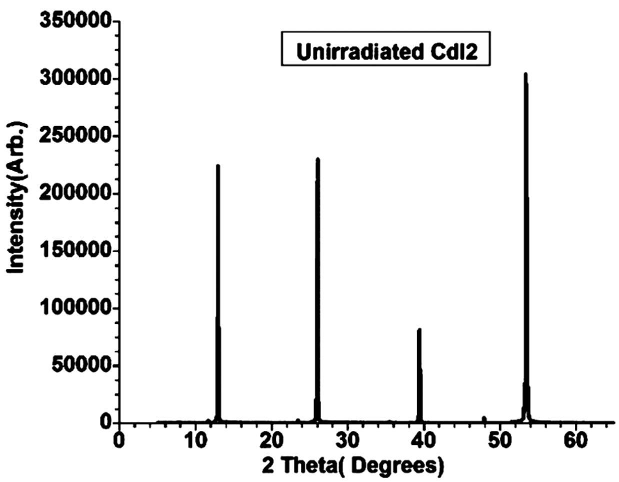


Fig. 1 — XRD pattern of as-grown single crystals of Cadmium Iodide.

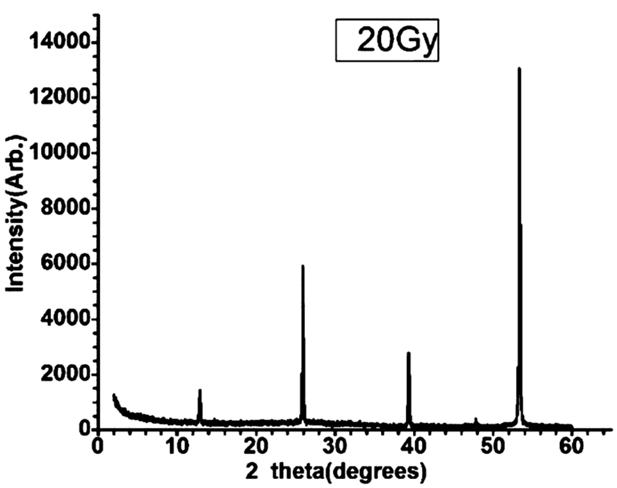


Fig. 2 — XRD pattern of radiated single crystal.

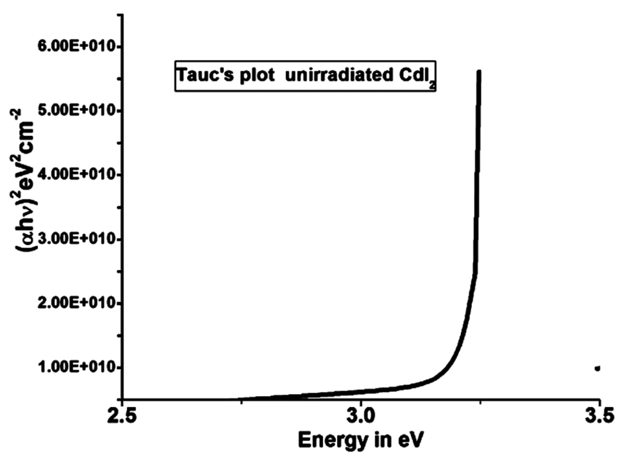


Fig. 3 — Tauc's plot of unirradiated single crystal of Cadmium iodide.

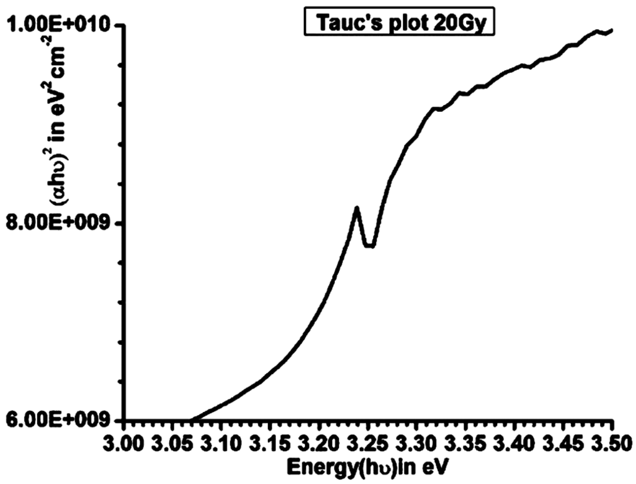


Fig. 4 — Tauc's plot of radiated single crystal of Cadmium Iodide.

gap may be due to the change in average bond energy after irradiation because optical band gap is a bond sensitive property[7]. The irradiation of the crystals may cause the loss of iodine ions and induce the detachment of ions from lattice sites. This contributes to the structural defects and may be responsible for occurrence of localized states between valence and conduction bands and thus in optical band gap[8] reduction.

When gamma radiation interacts with the material it results in either bond-breaking or bond rearrangement. Both processes lead to change in local structure of the material. This could lead to a shift in the absorption edge and a change in the atomic and molecular arrangement of the material.

## 4 Conclusion

In this work, the effect of gamma radiations on the structural and optical properties of single crystals of cadmium iodide were explored because of their importance in designing of cost effective and compact room temperature radiation detector. A Cobalt source was used for exposing the crystals to gamma radiations at a dose rate 1Gy/min. XRD (X-ray diffraction) pattern confirmed the single crystalline nature of cadmium iodide crystals. Gamma irradiation resulted in the weaker interface bonding between the single crystalline phase resulting in reduction in volume fraction of single crystalline phase. Transmission spectra for single crystals were recorded. It was found out that optical band gap showed a decrease in value on gamma irradiation. This decrease in optical band gap can be attributed to the arising structural defects in the crystals.

Research highlights the sensitivity of single crystals of $CdI_2$ to a low dose of gamma radiation and their ability to undergo quantifiable modifications in structural characteristics and optical band gap. These findings suggests the potential use of $CdI_2$ single crystals in designing real-time room temperature gamma-ray radiation sensors, emphasizing their relevance in dosimetry applications.

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