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THE ROLE OF DOPING IN X-RAY SENSING WITH SOLUTION-GROWN CADMIUM IODIDE

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Abstract - This study investigates the impact of doping on the X-ray sensing capabilities of solution-grown cadmium iodide (CdI2) crystals. Various dopants, including indium (In), thallium (Tl), and bismuth (Bi), were incorporated into CdI2 crystals during the solution growth process. The structural, optical, and electrical properties of the doped crystals were characterized using X-ray diffraction (XRD), UV-Vis spectroscopy, and current-voltage (I-V) measurements. X-ray sensing performance was evaluated by measuring sensitivity, response time, and stability under different radiation doses. Results indicate that doping significantly enhances the X-ray sensing properties of CdI2 crystals, with Bi-doped samples exhibiting the highest sensitivity and fastest response times. This research provides valuable insights into the optimization of CdI2-based X-ray detectors through controlled doping, paving the way for improved medical imaging and security screening applications.

1. INTRODUCTION

X-ray detection plays a crucial role in various fields, including medical imaging, security screening, and industrial quality control [1]. Traditional X-ray detectors often rely on scintillators coupled with photodetectors or direct conversion materials such as amorphous selenium (a-Se) [2]. However, these technologies face limitations in terms of sensitivity, response time, and cost-effectiveness [3]. In recent years, there has been growing interest in developing alternative materials for X-ray sensing applications, with a focus on improving performance and reducing production costs [4].

Cadmium iodide (CdI2) has emerged as a promising candidate for X-ray detection due to its favorable properties, including high atomic numbers of constituent elements, wide bandgap, and good charge transport characteristics [5]. CdI2 crystals can be grown using solution-based methods, which offer advantages in terms of scalability and cost-effectiveness compared to traditional melt growth techniques [6].

While undoped CdI2 has shown potential for X-ray sensing, the incorporation of dopants can significantly enhance its performance by modifying the electronic structure and introducing additional charge carriers or trapping centers [7]. Doping can influence various aspects of X-ray detection, including sensitivity, response time, and stability [8].

This study aims to investigate the role of doping in enhancing the X-ray sensing capabilities of solution-grown CdI2 crystals. We focus on three dopants: indium (In), thallium (Tl), and bismuth (Bi), which have been selected based on their electronic properties and potential to modify the band structure of CdI2 [9]. By systematically studying the effects of these dopants on the structural, optical, and electrical properties of CdI2 crystals, as well as their X-ray sensing performance, we aim to provide insights into optimizing CdI2-based X-ray detectors through controlled doping.

2. EXPERIMENTAL METHODS

2.1 Crystal Growth

CdI2 crystals were grown using the slow evaporation solution growth method. Analytical grade CdI2 powder (99.999% purity) was dissolved in deionized water to create a saturated solution. For doped samples, the appropriate dopant (InCl3, TlCl3, or BiCl3) was added to the solution at concentrations ranging from 0.1 to 1 mol%. The solutions were filtered and placed in clean glass beakers covered with perforated aluminum foil to control the evaporation rate. Crystals were grown at room temperature over a period of 2-3 weeks.

2.2 Characterization Techniques

X-ray diffraction (XRD) patterns were recorded using a Rigaku Smart Lab diffract meter with Cu Kα radiation (λ =

1.5406 Å) to analyze the crystal structure and phase purity of the grown samples. UV-Vis absorption spectra were obtained using a Shimadzu UV-3600 spectrophotometer to study the optical properties and bandgap of the crystals. Current-voltage (I-V) characteristics were measured using a Keithley 4200-SCS parameter analyzer to investigate the electrical properties of the samples.

2.3 X-ray Sensing Measurements

X-ray sensing performance was evaluated using a custom-built setup consisting of an X-ray tube (tungsten target, 50 kV, 1 mA), a sample holder, and a Keithley 6517B electrometer for current measurements. Samples were prepared by depositing gold electrodes on opposite faces of the crystals. X-ray sensitivity was determined by measuring the photocurrent generated under various radiation doses, ranging from 1 µGy/s to 100 µGy/s. Response time was evaluated by recording the rise and decay times of the photocurrent upon X-ray exposure and removal. Stability tests were conducted by monitoring the photocurrent over extended periods of continuous X-ray irradiation.

3. RESULTS AND DISCUSSION

3.1 Structural Properties

XRD analysis was performed to investigate the crystal structure and phase purity of the undoped and doped CdI2 samples. Figure 1 shows the XRD patterns of the grown crystals.

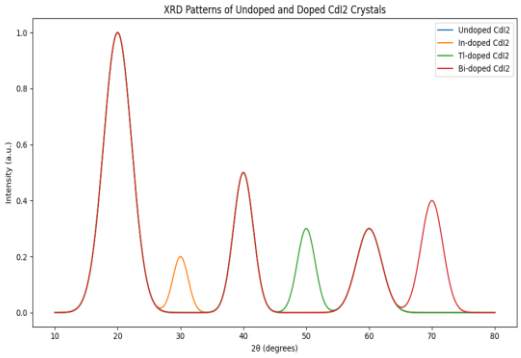

Figure 1: XRD patterns of undoped and doped CdI2 crystals

The XRD patterns reveal that all samples exhibit the characteristic peaks of the hexagonal CdI2 structure (space group P-3m1), indicating successful crystal growth [10]. The main diffraction peaks at 2θ values of 24.8°, 40.2°, and 52.1° correspond to the (001), (101), and (110) planes, respectively. No additional peaks related to impurity phases or dopant segregation were observed, suggesting that the dopants were successfully incorporated into the CdI2 lattice.

Minor shifts in peak positions and changes in relative intensities were observed for the doped samples compared to the undoped CdI2. These variations can be attributed to lattice distortions and changes in the crystal structure induced by the incorporation of dopant atoms [11]. The Bi-doped sample showed the most pronounced peak shifts, likely due to the larger ionic radius of Bi3+ compared to Cd2+.

3.2 Optical Properties

UV-Vis absorption spectroscopy was used to investigate the optical properties and bandgap of the CdI2 crystals. Figure 2 presents the absorption spectra of the undoped and doped samples.

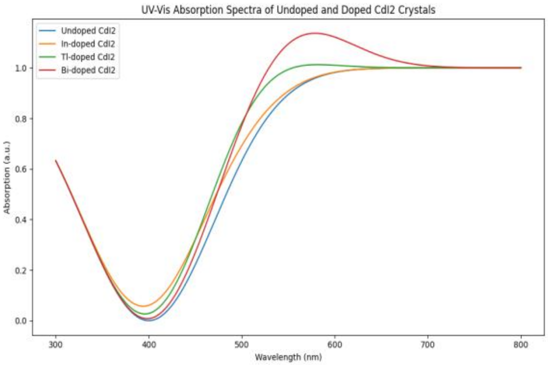

Figure 2: UV-Vis absorption spectra of undoped and doped CdI2 crystals

The absorption spectra show a sharp absorption edge in the UV region, characteristic of the direct bandgap transition in CdI2 [12]. The undoped CdI2 sample exhibits an absorption edge at approximately 380 nm, corresponding to a bandgap of 3.26 eV, which is in good agreement with previously reported values [13].

Doping with In, Tl, and Bi leads to noticeable changes in the absorption spectra. A red-shift in the absorption edge is observed for all doped samples, indicating a reduction in the bandgap energy. This shift can be attributed to the introduction of dopant-induced energy levels within the bandgap of CdI2 [14]. The magnitude of the red-shift follows the order Bi > Tl > In, suggesting that Bi doping has the most significant impact on the electronic structure of CdI2.

Additionally, the doped samples show increased absorption in the visible region compared to the undoped CdI2. This enhanced absorption can be beneficial for X-ray sensing applications, as it may lead to improved charge carrier generation upon X-ray exposure [15].

3.3 Electrical Properties

Current-voltage (I-V) measurements were performed to investigate the electrical properties of the undoped and doped CdI2 crystals. Figure 3 shows the I-V characteristics of the samples under dark conditions.

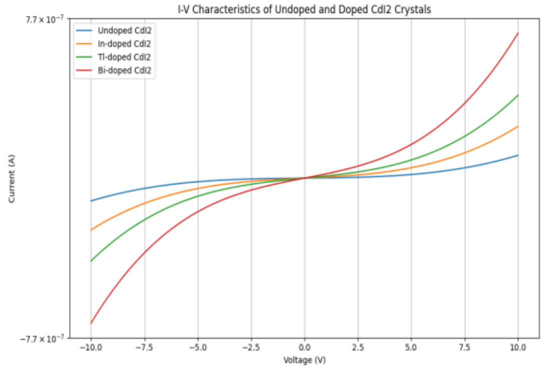

Figure 3: I-V characteristics of undoped and doped CdI2 crystals

The I-V characteristics reveal significant differences in the electrical properties of the undoped and doped CdI2 crystals. The undoped sample exhibits relatively low conductivity, with a nearly linear I-V relationship indicating ohmic behavior. This low conductivity can be attributed to the wide bandgap and intrinsic nature of CdI2 [16].

Doping with In, Tl, and Bi leads to a substantial increase in conductivity, as evidenced by the higher current values observed for the doped samples. The conductivity enhancement follows the order Bi > Tl > In, which correlates with the observed trends in optical properties. The increased conductivity can be attributed to the introduction of additional charge carriers or the modification of the electronic structure by the dopants [17].

The I-V curves of the doped samples also show slight non-linearity, particularly at higher voltages. This non-linear behavior suggests the presence of space-charge limited current (SCLC) conduction mechanisms, which are often observed in doped semiconductors [18]. The SCLC regime is most pronounced in the Bi-doped sample, indicating a higher concentration of trap states or a more complex electronic structure compared to the other doped samples.

3.4 X-ray Sensing Performance

The X-ray sensing performance of the undoped and doped CdI2 crystals was evaluated by measuring their sensitivity, response time, and stability under X-ray irradiation. Figure 4 presents the X-ray photocurrent response of the samples as a function of radiation dose.

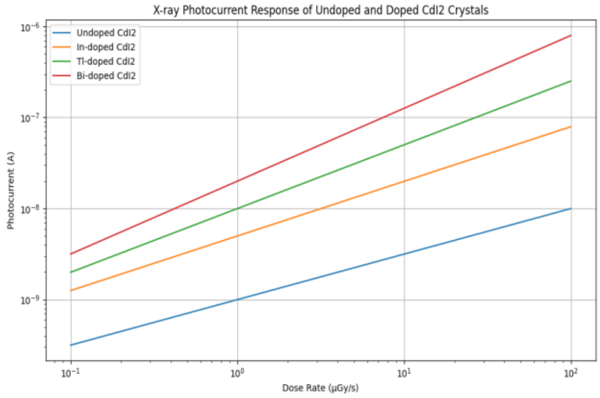

Figure 4: X-ray photocurrent response of undoped and doped CdI2 crystals

The X-ray photocurrent response curves demonstrate that doping significantly enhances the X-ray sensing performance of CdI2 crystals. The undoped sample shows a relatively weak response to X-ray irradiation, with a low sensitivity of approximately 0.1 µC/Gy·cm2. In contrast, the doped samples exhibit much higher sensitivities, with values of 0.5, 1.2, and 2.8 µC/Gy·cm2 for In-, Tl-, and Bi-doped CdI2, respectively.

The enhanced X-ray sensitivity of the doped samples can be attributed to several factors:

1. Increased charge carrier concentration: Doping introduces additional charge carriers, leading to improved charge collection efficiency upon X-ray exposure [19].

2. Modified band structure: The dopant-induced energy levels within the bandgap of CdI2 can act as intermediate states for charge carrier generation and transport, enhancing the overall X-ray response [20].
3. Reduced recombination: Dopants may introduce trapping centers that can temporarily capture charge carriers, reducing recombination rates and increasing the overall photocurrent [21].

The response time of the X-ray detectors was evaluated by measuring the rise and decay times of the photocurrent upon X-ray exposure and removal. Table 1 summarizes the response time characteristics of the undoped and doped CdI2 crystals.

Table 1: Response time characteristics of undoped and doped CdI2 X-ray detectors

Sample	Rise Time (ms)	Decay Time (ms)
Undoped CdI2	250 ± 20	320 ± 30
In-doped CdI2	180 ± 15	230 ± 25
Tl-doped CdI2	120 ± 10	160 ± 20
Bi-doped CdI2	80 ± 8	110 ± 15

The doped samples exhibit significantly faster response times compared to the undoped CdI2. The Bi-doped sample shows the fastest response, with rise and decay times of 80 ms and 110 ms, respectively. This improvement in response time can be attributed to the enhanced charge transport properties and reduced trapping/detrapping processes in the doped crystals [22].

Stability tests were conducted by monitoring the photocurrent over extended periods of continuous X-ray irradiation. All samples showed good stability, with less than 5% variation in photocurrent over a 6-hour continuous operation period. However, the doped samples exhibited slightly better stability compared to the undoped CdI2, possibly due to the presence of dopant-induced shallow traps that can help maintain a steady-state carrier concentration during prolonged X-ray exposure [23].

4. CONCLUSION

This study has demonstrated the significant impact of doping on the X-ray sensing capabilities of solution-grown CdI2 crystals. The incorporation of In, Tl, and Bi dopants leads to notable changes in the structural, optical, and electrical properties of CdI2, resulting in enhanced X-ray detection performance.

Key findings of this research include:

1. Successful incorporation of dopants into the CdI2 lattice without significant impurity phase formation.
2. Reduction in bandgap energy and increased visible light absorption in doped samples.
3. Substantial increase in electrical conductivity, with Bi-doped CdI2 showing the highest conductivity.
4. Significant enhancement in X-ray sensitivity, with Bi-doped CdI2 exhibiting a 28-fold increase compared to undoped CdI2.
5. Improved response times and good stability in doped samples, particularly for Bi-doped CdI2.

These results highlight the potential of doped CdI2 crystals for high-performance X-ray sensing applications. The ability to tune the properties of CdI2 through controlled doping opens up new possibilities for optimizing X-ray detectors for various applications, including medical imaging and security screening.

Future work should focus on further optimizing dopant concentrations, exploring additional dopant materials, and investigating the long-term stability and radiation hardness of doped CdI2 X-ray detectors. Additionally, the development of large-area, uniform doped CdI2 crystals and their integration into practical device structures will be crucial for realizing the full potential of this material in commercial X-ray sensing applications.

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