Band Gap Tuning of Copper Based Inorganic Perovskite Scintillator

Yatharth Thakar[1],* Divya Pandya[1], Yashvanti Sondarva.[1], and Sheetal Rawat[1]

[1]*Department of Physics, Pandit Deendayal Energy University, Gujarat - 382007, INDIA*

Introduction

Perovskite scintillators are revolutionizing the field of X-ray imaging due with their tunable bandgaps, good light yield & ease of synthesis through solution processing [1]. Unlike conventional scintillators, which are typically fragile and limited to rigid substrates, perovskite scintillating thin films offer a versatile and cost-effective alternative, paving the way for advancements in flexible and high-performance X-ray detectors. Traditional scintillators, such as those made from bulk crystals, often face challenges related to fragility and inflexibility, limiting their application in scenarios that require flexible detection surfaces. Additionally, many high-performance perovskite scintillators contain lead, raising toxicity concerns that hinder their widespread adoption in medical environments. To overcome these issues, this study explores the use of $Cs_3Cu_2I_5$ doped with thallium (Tl) as a promising lead-free alternative. $Cs_3Cu_2I_5$:Tl has demonstrated remarkable stability and an exceptionally good light yield which is 98,200 photons/MeV, making it an ideal candidate for X-ray imaging [2]. The primary objective of this research is to develop and characterize high-quality $Cs_3Cu_2I_5$Tl thin films using cost-effective and scalable synthesis methods. Techniques such as spin-coating, the anti-solvent approach, and drop casting are employed to fabricate the scintillating films on ITO-coated PET substrates. These methods are chosen for their simplicity and potential for large-scale production, which are crucial for practical medical imaging applications. Initial synthesis involves preparing $Cs_3Cu_2I_5$:Tl powder using the anti-solvent approach, a technique known for producing high-purity perovskite materials. The synthesized powder is then used to create thin films through spin-coating and drop casting.

*Electronic address : yatharth.tmscp22@sot.pdpu.ac.in

These films will undergo comprehensive characterization Which assess their optical & scintillating properties. UV-Vis spectroscopy and photoluminescence measurements reveal a bandgap of 3.72 eV and a strong emission peak at approximately 450 nm, consistent with previously reported data [15]. These findings confirm the high emission stability and quantum light yield of the $Cs_3Cu_2I_5$:Tl films. Further radiation characterization and imaging studies are underway to evaluate the performance of these films in real-world X-ray detection scenarios. The anticipated results are expected to demonstrate the practicality and effectiveness of $Cs_3Cu_2I_5$:Tl thin films in medical imaging.

Experimental synthesis

Anti-solvent method has two step approach first is dissolution of salt in suitable polar solvent. [3] Then add the dissolved mixture in non-polar anti-solvent to form crystallize formation of salt. In this work, CsI and CuI salts are dissolved in DMSO (Di-methyl Sulfoxide) with 1.088 gm of CsI & 0.532 gm of CuI and for different thallium (Tl) doping of 1%, 3%, 5% were added. now further this mixture is constantly stirred on the magnetic stir for 8-12 hrs. Second step involves anti-solvent preparation. Here, IPA (Iso-Propyl Alcohol) is used as an anti-solvent. Dissolved salt solution is added drop wise in an IPA and microcrystalline $Cs_3Cu_2I_5$ formed immediately. Powder is extracted by centrifuge process.

Spin coated thin film - Dissolve $Cs_3Cu_2I_5$ in the chosen solvent to create a uniform solution. The concentration of the solution will depend on the desired thickness of the final film. Filter the solution using a micro filter to remove any particulates that could cause defects in the thin film. Then at slow rpm drop wise solution is dropped and after rpm is increased IPA is dropped on the films now film is fabricated with small layer of micro powder of $Cs_3Cu_2I_5$ is deposited on the glass substrate.

Results & Discussion

The UV-Vis spectra of the spin-coated $Cs_3Cu_2I_5$ thin films were analyzed to determine the excitation wavelength of the $Cs_3Cu_2I_5$ powder. An absorbance peak was observed at approximately 315-316 nm. indicating that this wavelength is absorbed maximally. This information facilitates the calculation of the band gap using the Tauc plot method, which is a well-established technique for estimating the optical band gap of materials.

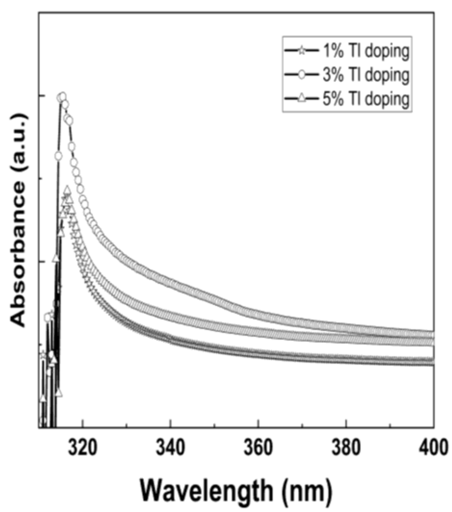

Fig. 1 UV-Vis Graph of the Film

$(\alpha h\nu)^2 = A(h\nu - E_g)$

where α is the absorption coefficient, hν is the photon energy, A is a constant, and E_g is the band gap energy. As the doping concentration decreases from 5% to 1%, a corresponding decrease in the band gap of the material is observed. Additionally, photoluminescence characterization corroborates the excitation wavelength of 315 nm, which aligns with the maximum absorbance observed in the UV-Vis spectra. The Tauc plot method reveals the band gap energy of the $Cs_3Cu_2I_5$ thin films. The plot demonstrates that as the doping concentration decreases, the band gap narrows. Which can be studied by below table.

Doping Concentration	**Band gap**
$Cs_3Cu_2I_5$ 1%	3.68 eV
$Cs_3Cu_2I_5$ 3%	3.71 eV
$Cs_3Cu_2I_5$ 5%	3.73 eV

Table 1. band gap & concentration

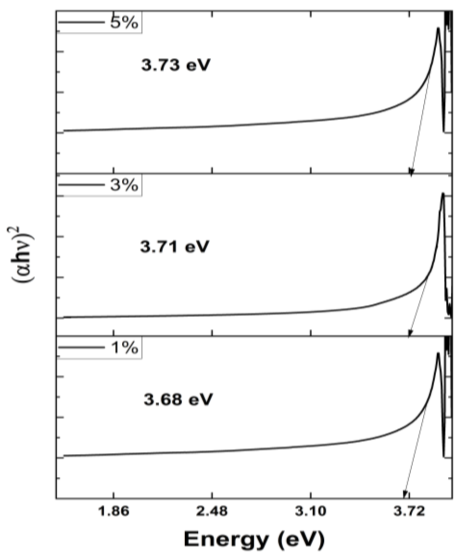

Fig. 2 Tauc Plot of the Thin Film

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