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The Effect of Annealing on The Structural and Optical Properties of The Bismuth (III) Iodide (Bii_3) Thin Film Prepared by Vacuum Thermal Evaporation in Order to Lead Free-Perovskite Solar Cells Fabrication

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ABSTRACT

In this study, effect of annealing temperatures in room, 100 and 200 C^0 on the structural and optical properties of Bismuth (III) iodide (BiI_3) thin films is investigated. The deposition process of the specimens was done by physical vapor deposition method on FTO substrate. The samples were prepared at 200 nm thickness. The structural properties, and optical absorption spectra of samples were measured by XRD and UV–Vis spectrophotometer. The Urbach energy and band gap of the samples were obtained by absorption spectrum fitting Tuac methods. The results showed that by increasing the annealing temperature up to 100 C^0, the crystallinity of samples increased, the band gap and Urbach energy decreased about 1.60 and 0.17 eV, respectively. The results show that by increasing the annealing temperature up to to 200 C^0, the band gap and Urbach energy increase. Studies on the structural and optical properties of thin films, show that BiI_3 can be used as an active layer in lead-free perovskite solar cells.

Keywords- Annealing, Bismuth triiodide, band-gap energy, Perovskite solar cell, Urbach Energy.

I. INTRODUCTION

In today's era, the development of low-cost and environmentally friendly solar cells is considered an important necessity in order to meet the demands for energy. Perovskite materials based on lead (Pb) are suitable materials for solar cells with high efficiency and low price. On the other hand, the inherent low stability and toxicity of lead is a weakness of this type of solar cells. Hence, replacing lead in perovskite composition and synthesizing perovskite layers with high efficiency will be very challenging. This will be a big obstacle to the development of perovskite-based solar cells. A simple method to develop lead-free perovskites is to replace lead with bismuth (Bi) (Zhang et al., 2018). The crystal structure of bismuth triiodide perovskite makes it an active layer material in solar cells. This material is widely used in solar cells due to its suitable bandgap, mobility and potential "defect tolerance" for thin films. Bismuth triiodide has two types of crystal structure, according to researchers, the success of this material as a semiconductor in solar cells is due to its hexagonal or trigonal crystal structure (Ikram et al., 2022). Bismuth (III) iodide (BiI_3) is a potential candidate for use in solar cells due to its good optical properties and non-toxic elements. The type of substrate and its temperature also have an effect on some properties of the BiI_3 thin film, especially its optical and structural properties (Ikram et al., 2022).

The increasing demand for efficient and environmentally friendly energy sources has driven significant research into the development of lead-free

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perovskite solar cells. Bismuth (III) iodide (BiI_3) has emerged as a promising alternative to lead-based perovskites due to its non-toxic nature and suitable optoelectronic properties. The preparation and post-treatment of BiI_3 thin films are critical in determining their structural and optical characteristics, which directly influence the performance of perovskite solar cells. One of the key post-treatment processes is annealing, which can significantly modify the crystallinity, morphology, and bandgap of the BiI_3 thin films, thereby impacting the overall efficiency of the solar cells.

Annealing is a thermal process that involves heating the thin films at specific temperatures to enhance their crystallinity and remove any residual stresses. Studies have shown that annealing can lead to improved grain size and reduced defects within the BiI_3 films, which are essential for efficient charge transport in solar cell applications (Savenije et al., 2014). Moreover, the optical properties, such as absorption coefficient and bandgap, can be tuned through controlled annealing, enabling the optimization of the material for solar energy conversion (Kim et al., 2019).

In recent years, vacuum thermal evaporation has been extensively used to deposit BiI_3 thin films due to its ability to produce high-purity and uniform layers. The combination of vacuum thermal evaporation with post-deposition annealing provides a robust approach to fabricating high-quality BiI_3 thin films tailored for lead-free perovskite solar cells (Bisquert et al., 2018). The effects of annealing on these films are thus crucial to understanding and enhancing their structural and optical properties, ultimately contributing to the advancement of sustainable solar cell technologies.

II. EXPERIMENTAL SECTION

In this research, the effect of annealing temperature on the structural and optical properties of bismuth iodide thin films, which was done by physical evaporation deposition method in vacuum and on FTO substrate, was investigated. First, the glass substrates were washed using distilled water and soap for 15 minutes, then by acetone for 15 minutes in an ultrasonic bath, and then dried by pure nitrogen gas. Bismuth (III) iodide (BiI_3) was used in powder form with a purity of 99.9% from Aldridge Company. Layering was done at an initial pressure of $5\times10^{-5} mbar$. Layering was done by VAS BUC layering device (model 78535). The distance between the source and the crystal of the thickness gauge was considered to be 15 cm in this process. The deposition rate of the layers was about 1 nm/s and was controlled, and the thickness of the prepared layers was chosen to be 200 nm. The thickness of the layers was controlled by a quartz thickness gauge crystal, and after the layering process, the samples were annealed at 100 and 200 degrees Celsius. In order to determine the structural properties of the prepared thin films, XRD (ADVANCE-D8) test was used. The optical properties of these layers were measured based on the absorption and transmission spectra of the layers by Ocean Optics (HR400) UV/Vis Spectrophotometers in the wavelength range of 300 to 900 nm.

III. RESULTS AND DISCUSSION

Figure 1 shows the X-ray diffraction pattern for the samples**.** As can be seen from the figure, the diffraction pattern of BiI_3 layers matches well with the standard pattern of rhombohedral BiI3 (PDF#48-1795) and no additional peaks are observed (Wang et al., 2020). In the XRD diffraction pattern, the peaks at 2θ positions of 7/12, 1/27, 3/35, and 7/41 corresponded to the crystallographic directions of (003), (113), (116), and (300) respectively. In the direction of (003), the peak intensity is greater than in other directions. Moreover, with the increase in the annealing temperature up to 100°C, the intensity of peaks rises which indicates higher crystallinity in this sample. The weaker intensity of scattering peaks in samples without recrystallization can be due to incomplete crystallization with small, boundary-less grains and the rice grain morphology. However, reheating at a temperature of 200°C does not significantly change the crystalline structure and morphology of the layers. The grain size for page (003) was obtained using the Scherrer equation.

$$D = \frac{0.9\lambda}{\beta \cos\theta} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

In the equation, θ is the scattering angle, λ is the wavelength of the X-ray beam, and β is the peak width at half-maximum intensity. The grain size for the samples without annealing, annealed at temperatures of 100°C and 200°C, were found to be 24, 79, and 105 nanometers, respectively.

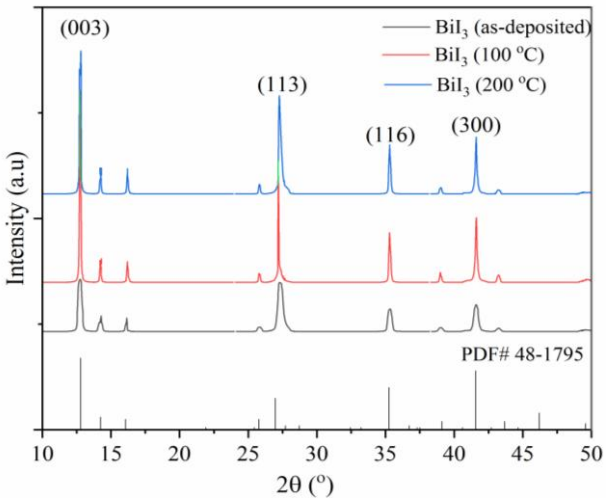

Figure 1: X-ray diffraction pattern of thin layer of annealed BiI_3 at different temperatures.

Calculating the band gap of samples using the Tao-Equation method is dependent on the absorption

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coefficient (α) of incident photons, which is calculated from equation (2**).**

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

A fixed amount, Plank constant, is equal to 2 for indirect energy gap and is equal to 5/0 for direct energy gap (Jean et al., 2017). The chart in Figure 2 shows a direct band gap of bismuth. The band gap chart based on photon energy shows that the band gap increases with increasing annealing temperature of the crystal, so the band gap decreases.

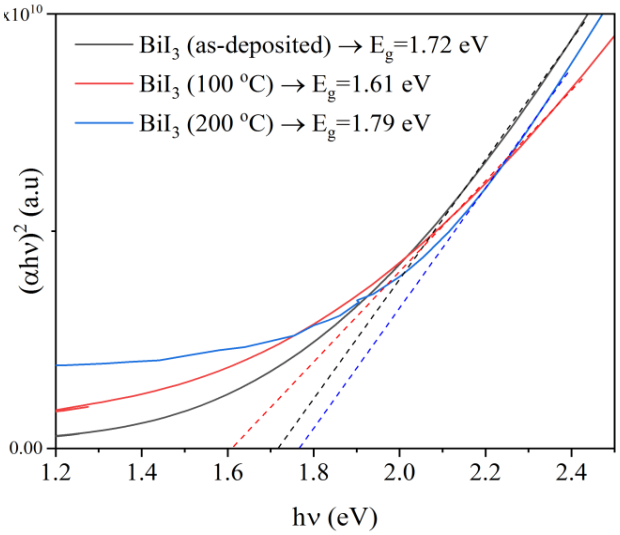

Figure 2: Diagram showing the variation for re-crystallized thin layer of BiI_3 at different temperatures.

Orbital energies of examples are calculated using the TaoK method from equation (3).

$$\alpha = \alpha_0 \exp(\frac{h\nu}{E_u}) \quad \ldots\ldots\ldots\ldots\ldots\ldots (3)$$

E_u is the energy of the orbitals and α_0 is a constant value (Jean et al., 2017).

The graph of ln α as a function of photon energy is presented in Figure 3. The energy of the orbital is obtained from the slope of the ln α graph with respect to photon energy. The obtained gap values and orbital energies for the reheated samples at different temperatures are presented in Figures 2 and 3. The results indicate that as the annealing temperature increases up to 100°C, the energy gap and orbital energy decrease to 61.1 eV and 170 meV, respectively, and at a temperature of 200°C, this value increases. The reason for the decrease in the Orbach energy is due to the improvement in the crystallinity properties of the material with increasing particle size in samples annealed at higher temperatures. One of the reasons for the increase in the Orbach energy is attributed to crystalline defects within the material, and its decrease is evidence of a reduction in crystalline defects and an improvement in the crystallinity properties of the material (Jean et al., 2017).

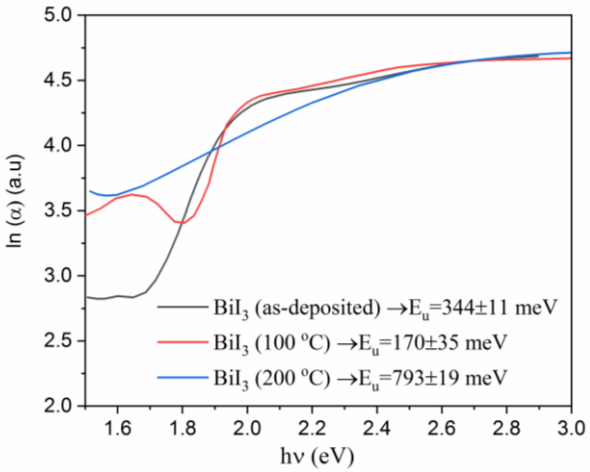

Figure 3: The plot of ln(α) as a function of (hν) for the annealed thin film of BiI3 at different temperatures.

IV. CONCLUSION

In this study, the band gap and orbital energy of newly fabricated bismuth thin films on an FTO substrate were investigated using the Tao method. The orbital sequence is observed due to the disorder near the absorption edge in disordered semiconducting materials and crystalline materials at high temperatures. The obtained results demonstrate that the band gap and Orbach energy of the samples vary with increasing annealing temperature. As the annealing temperature increases from room temperature to 200°C, the band gap and Orbach energy decrease due to the improved crystallinity of the layers. However, with further increase in annealing temperature up to 200°C, these values increase. The X-ray diffraction spectrum also confirms the improvement in crystallinity. The results of this study indicate that the newly fabricated bismuth can be used as an active material in lead-free perovskite solar cells.

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