

# Influence Of Deposition Temperature On The Structural Properties Of ZnTe Thin Films Prepared By Pulsed Laser Deposition

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## Abstract:

In the pulsed laser deposition (PLD) technique, the substrate deposition temperature is the main parameter controlling the thin film crystallisation and growth characteristics. While previous research has provided valuable insights, the present study aims to extend the understanding by controlling the deposition temperature to obtain an ideal crystal structure. Raising the substrate temperature to extremely high values does not guarantee better film properties. Increasing the temperature above 500 °C permanently damages the film, degrading the physical and chemical properties. The research used a comparative practical strategy to identify the best crystal structure and the lowest defect formation while minimising structural distortion. The XRD results demonstrated that three zinc telluride (ZnTe) thin films with increasing growth temperatures from 100 °C to 300 °C preferred the crystallographic plane orientation (111). The temperature control showed apparent differences in peak intensity and sharpness because the structural quality varied. The film processed at 300 °C demonstrated the most prominent peak, indicating superior crystal order with better atomic motion and reduced overall structural defects. The structural defects that prevail in thin films lead to disturbed growth that might sometimes result in enduring material deformation. Our research provides crucial insights into the effects of thermal energy on PLD-manufactured thin film quality, which future scientists can use to specify process parameters for practical use. The SEM image of the film produced at 300 °C showed a uniform surface that contained aligned grain structures evenly distributed across the surface of the thin film.

**Keywords:** ZnTe thin films; Pulsed laser deposition (PLD); Deposition temperature; Crystal structure; X-ray diffraction (XRD); grain size; crystallinity.

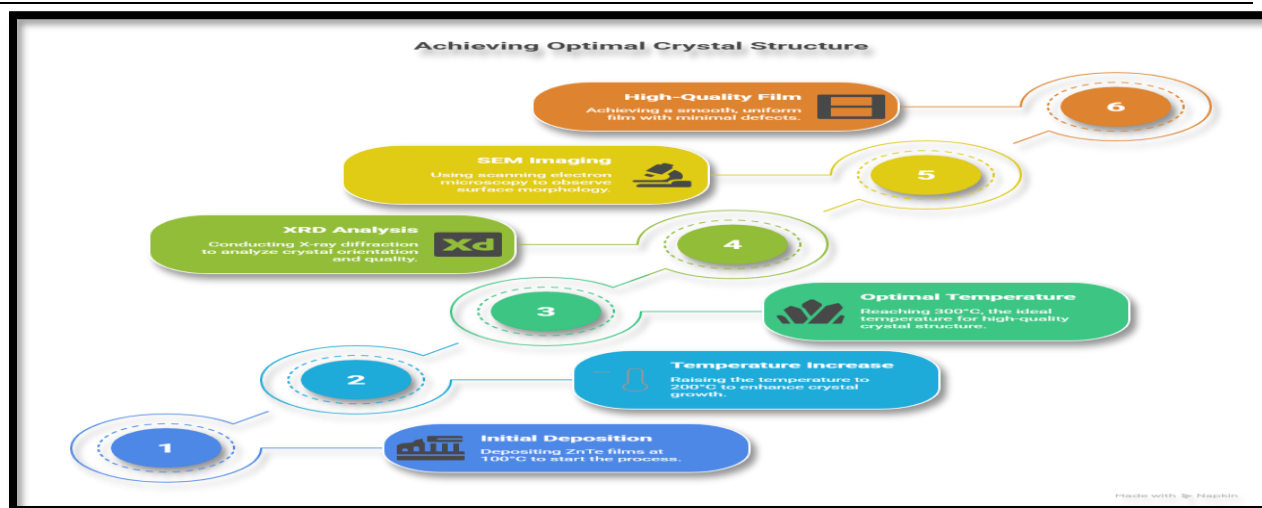


Figure 1: Detailed flow chart of thin-film preparation and structural investigations.

## 1. INTRODUCTION:

The zinc telluride (ZnTe) semiconductor compound has gained considerable attention because it shows promising potential for use in photovoltaic cells and optoelectronic devices that benefit from the properties of the photodetector, infrared sensor, and light-emitting diode (LED) [1]. ZnTe demonstrates properties from its II-VI group semiconductor status and its zinc blende crystal structure to generate efficient photovoltaic operation as a buffer or window layer in heterojunction thin film solar cells because it enables direct band gap energies of 2.26 eV at room temperature [2,4]. The semiconductor technology ZnTe finds everyday use within tandem solar cell technologies with CdTe or CIGS to extract maximum light absorption benefits and improved energy conversion outcomes. Buffer layer materials that contain ZnTe have been proven to be environmentally friendly because they do not contain toxicants or cadmium. The growth of high-quality ZnTe thin films benefits most from pulsed laser deposition (PLD), which represents one of the multiple suitable deposition techniques. PLD surpasses sputtering, thermal evaporation, and chemical vapour deposition because it provides targeted substance transfer and fast deposition speeds and allows film delivery at lower temperatures [3]. Thin-film formation begins when a ZnTe target receives pulses from a laser beam directed at it to initiate a plasma plume, which releases material toward the substrate [4]. The multiple variables determining the outcome of deposited films include substrate temperature, ambient gas pressure, target-substrate distance, and laser energy. The temperature of the substrate base determines the fundamental characteristics of ZnTe films with respect to crystal structure and optical and surface features [5]. Numerous research studies show that correctly controlled deposition parameters generate high-quality structural, optical, and morphological features in ZnTe thin films that improve their use in solar cells and optoelectronic applications [5,6]. Currently available information regarding PLD-produced films and substrate temperature effects fails to explain their complete properties when using established procedures. This research analyses how substrate deposition temperature affects the microstructure and optical properties of zinc telluride thin films made by PLD to find parameters which generate photovoltaic-quality materials.

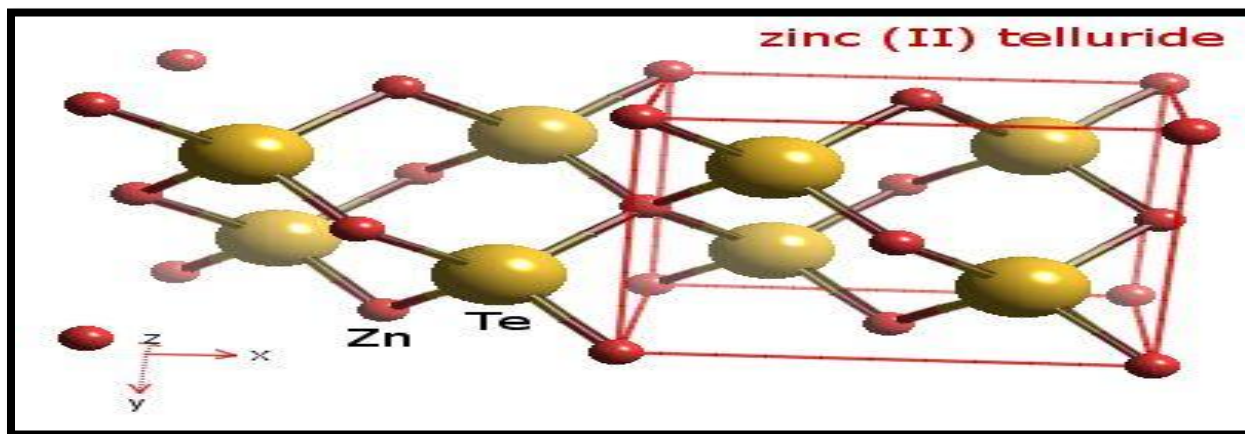


Figure 2: Crystal structure of zinc telluride.

## 2. Experimental details:

Within a vacuum chamber, a high-energy laser focuses on a target material, so a plasma plume develops to deposit material onto the substrate (Figure 3). Oxygen or other background gases within a chamber play an essential or a non-essential role when deposition occurs or may occur under vacuum conditions below  $10^{-10}$  torr. Various approaches within pulse laser deposition (PLD) have been established to improve thin film quality, allow thin polymer and biomaterial layers to be deposited, and create multiple layered two- and three-dimensional systems. Various elements that shape the quality of deposited films stem from their composition, thickness level, laser parameters, deposition circumstances, target treatment approaches, and processing steps after film formation. The wavelength of the laser, the pulse energy, the repetition rate, and the pulse duration

are key parameters that significantly influence the absorption efficiency and the ablation process. Other substrate temperatures, background gas pressures, distances between the target and substrate, and deposition rates affect the crystallinity of the thin film of the material, grain size, and surface roughness to which the film is coated. At the same time, the ablation efficiency of cinema is determined by characteristics of the target material such as purity, density, composition, and surface condition[8,9,10]. Additionally, the substrate material on which the film is coated is crucial because it determines the film compatibility, the quality of the crystal structure, the surface preparation method, and the treatment applied after deposition. Figure 3 illustrates the design of our “PLD system with an Nd: YAG laser source. In contrast to the Krf excimer laser, which features a substantial and heavy cabinet (e.g., 1182 × 375 × 793 mm and weighing 275 kg), the laser head of the Nd: YAG laser can be positioned directly in front of the entry window. This potential is enabled by the significantly reduced dimensions and weight of a standard Nd: YAG laser head. The laser head of the Innolas SpitLight Compact 400 used in our experiment measures 390 × 135 × 91 mm (L × W × H) and weighs about 10 kg”[4,7].

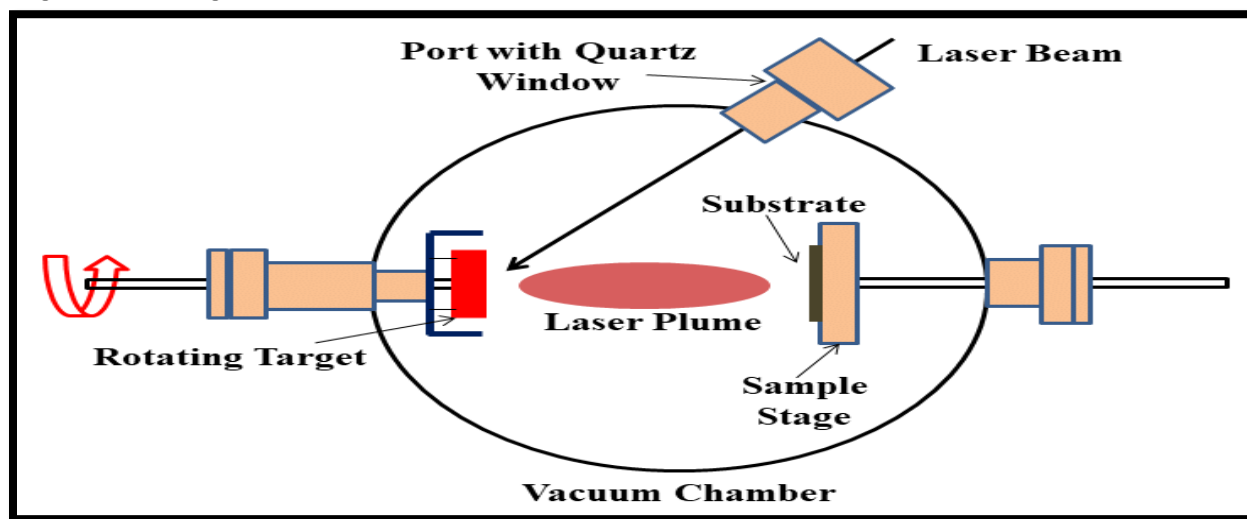


Figure 3: Schematic of the pulsed laser deposition technique.

The location does not need reflecting mirrors to direct the laser pulses within the deposition chamber, accommodating various geometries, including those from above or the planar configurations depicted in Fig. 3, respectively. Furthermore, “the laser's complete output energy is allowed for usage. The laser emits a constant energy of approximately 700 mj, with a beam diameter of around 6 mm and a maximum repetition rate of 10 Hz. Reduced repetition rates can be readily achieved by adjusting the aperture of the optical cavity and controlling the precise number of laser pulses within a specific timeframe. It is essential to emphasise the remarkable stability in the energy of the laser pulse (ie, <0.7%), which ensures a consistently stable ablation rate over time. Unlike Krf excimer lasers, which allow for controllable laser output energy, the inability of Nd: YAG lasers to adjust to energy levels has been addressed by implementing a specific process protocol for the growth and optimisation of epitaxial thin films. An alumina ceramic component featuring a variable diameter aperture (eg, 1-2mm or larger/smaller) is used as a laser mask to diminish the overall fluence of the laser pulse. Subsequently, a focusing lens was positioned in the laser path to concentrate the laser pulses onto the targets at a 45 ° angle of incidence”[11].

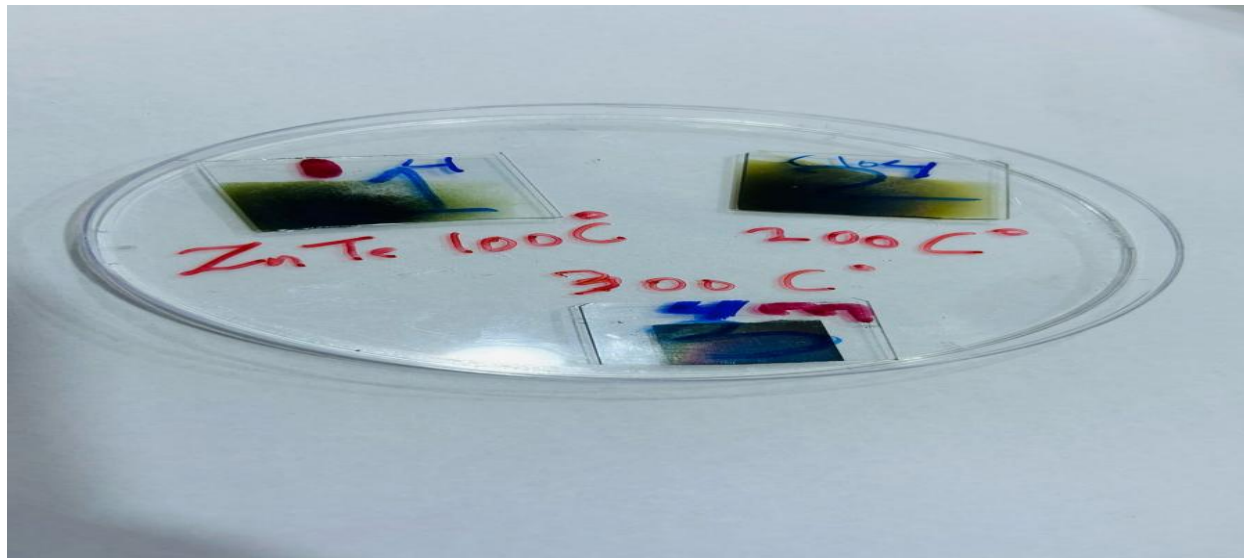


Figure 4: Three thin zinc telluride films via (PLD) at substrate temperatures of 100 ° C, 200 ° C and 300 ° C .

### 3. RESULTS AND DISCUSSION

#### 3.1: XRD results:

XRD analysis is one of the most widely used and reliable techniques in characterising solid materials, particularly in materials science, physics, chemistry, and nanotechnology. The significance of this technique lies in its ability to provide both qualitative and quantitative information about the crystal structure of materials, which is fundamental to understanding their physical and chemical properties. Primarily, XRD is employed for phase identification because the technique is based on the diffraction of X-rays when they interact with a crystalline material. The resulting diffraction pattern is unique to each crystalline phase and can be considered a “fingerprint” of the material. By comparing this pattern with standard reference data, such as PDF files from the International Centre for Diffraction Data (ICDD), the precise identification of crystal phases is achieved, even in complex multiphase systems. In addition to phase identification, X-ray diffraction (XRD) enables crystallite size estimation using formulas such as the Scherrer equation, offering a non-destructive means of evaluating the influence of synthesis or treatment conditions on crystal growth at the nanoscale. Moreover, the analysis of peak broadening and peak shifting allows for detecting lattice strain and crystallographic distortions, significantly affecting material properties such as conductivity or reactivity. X-ray diffraction (XRD) is also a powerful tool for tracking the evolution of materials over time or under varying treatment conditions, which makes it valuable for studying the structural stability of materials under environmental, thermal, or radiation stress. Furthermore, preferred orientation (texture) analysis provides insight into the growth direction of crystallites, which is closely related to material performance in electronic and optoelectronic applications. In summary, X-ray diffraction (XRD) in materials characterisation extends beyond simple phase detection; it constitutes a comprehensive framework for analysing subtle structural changes, thereby enabling a deeper understanding of material behaviour and guiding its optimisation for various industrial and technological applications. Figure [5] represents an XRD plot that represents the structural properties of ZnTe thin films deposited at different substrate temperatures: 100 ° C (blue, A), 200 ° C (orange, B) and 300 ° C (green, C) via pulsed laser deposition (PLD). The x axis represents  $2\theta$  (degrees), corresponding to the diffraction angles, while the y axis indicates the intensity (arbitrary units), representing the peak strength and crystallinity.

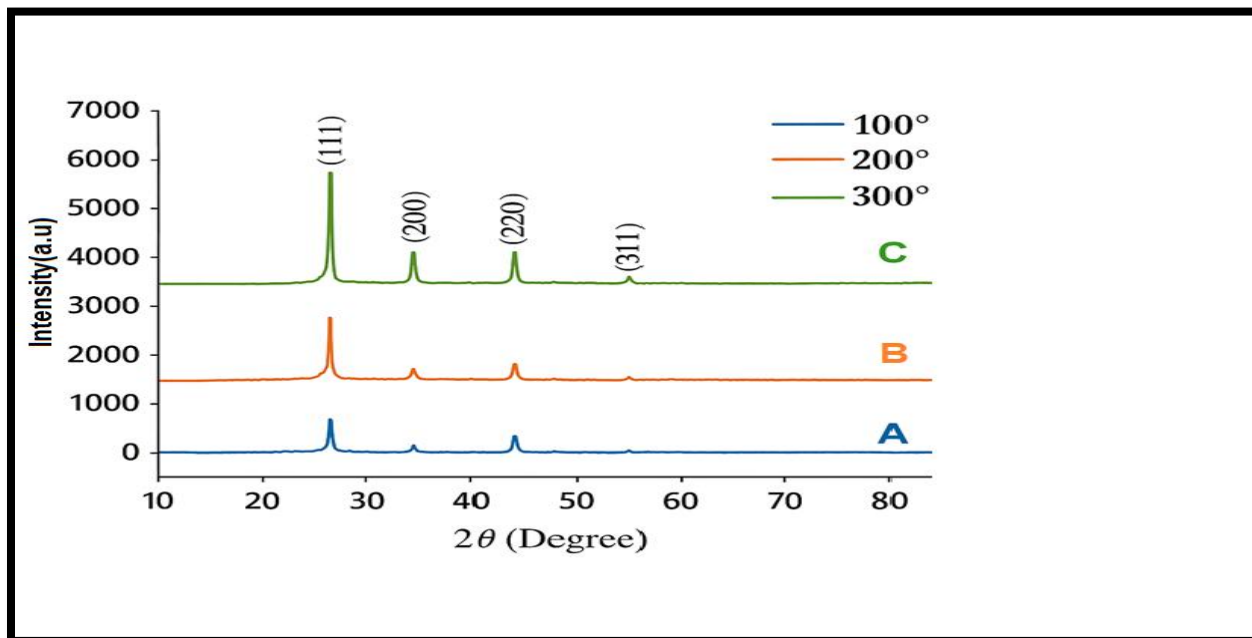


Figure 5: XRD pattern of ZnTe thin films.

### 3.1.1: Effect of temperature on crystallinity

- **Ts 100 ° C (A - blue curve)**
  - The diffraction peaks are weak and broad, indicating poor crystallinity and a small grain size.
  - The film may have a higher degree of **amorphous content** or **poorly developed grains**.
  - Peaks (111), (200), (220), and (311) are still present, but with very low intensity.
  -
- **Ts 200 ° C (B - orange curve)**
  - The peak becomes sharper and more intense, indicating an improvement in crystallinity.
  - The growth of grains is more pronounced, leading to reduced defects and better atomic ordering.
  - This suggests enhanced nucleation and crystal formation compared to 100 ° C.
- **Ts 300 ° C (C - Green curve)**
  - The highest peak intensities were observed, indicating superior crystallinity and larger grains.
  - The sharpness and intensity of the peaks (111), (200), (220), and (311) confirm a well-ordered crystal structure of ZnTe.
  - Higher temperatures promote better **atomic diffusion and grain growth**, leading to improved film quality.
  -

### 3.1.2: Preferred Orientation and Phase Formation

- The peak (111) is dominant in all three films, suggesting a preferred orientation along this plane.
- The presence of (200), (220) and (311) confirms the formation of a ZnTe cubic zinc bleach structure.
- The absence of extra peaks suggests that the films are single-phase ZnTe with no secondary phases or impurities.

### 3.1.3: Peak Broadening and Grain Size Estimation

- At lower temperatures (100 ° C), the peaks are larger due to a smaller grain size and greater strain.
- At higher temperatures (300 ° C), the peaks become sharper, indicating larger grains and lower strain.
- The grain size can be estimated using the Scherrer equation:

$$D = \frac{K\lambda}{\beta \cos \theta}$$

Where:

- 'D' is the crystallite size,
- K is the shape factor (~ 0.9),
- $\lambda$  is the X-ray wavelength,
- $\beta$  is the full width at half maximum (FWHM) of the peak,
- $\theta$  is the Bragg angle."

Applying this equation would indicate that grain size increases with increasing deposition temperature [6, 7, 14]. Increasing the deposition temperature from 100 ° C to 300 ° C leads to improved crystallinity, higher peak intensity, and larger grain size. The orientation (111) dominates, indicating a firm texture along this plane. The best structural quality is achieved at 300°C, making it the most suitable condition for high-quality ZnTe thin films.

Temperature (°C)	Crystallinity	Peak Intensity	Grain Size	Defect Density
100°C	Low	Weak peaks	Small	High
200°C	Moderate	Stronger peaks	Larger	Lower
300°C	High	Sharp, intense peaks	Largest	Lowest

Tab1. Effect of increased temperatures on the grain size of thin films

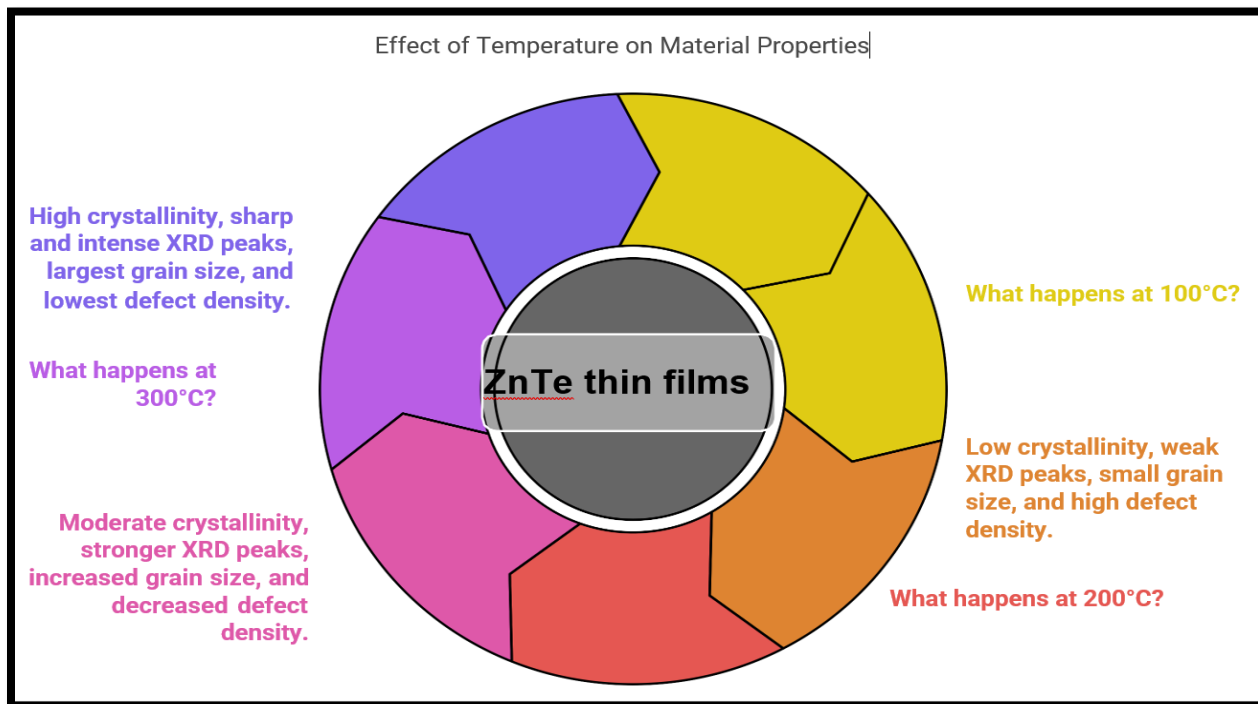


Figure 6:Effect of temperature on ZnTe thin films structure.

The sharp, high-intensity diffraction peaks suggest that the deposited films exhibit excellent crystalline alignment. The FWHM of the peak (111) is 35°, so the ZnTe films made at a substrate temperature of 300 °

C had a good crystalline structure, with all crystallites orientated in the (111) direction. The investigation revealed that direction (111) is the most prominent crystallographic orientation for all ZnTe films deposited on substrates at temperatures ranging from 100 °c to 300 °c. This indicates that the crystallites are well oriented toward the basal plane direction and grow in the C-axis direction. The increase in peak intensity with increased substrate temperature indicates a concomitant increase in the crystallite size. The substrate temperature becomes the predominant parameter that influences the improvement of crystalline perfection in ZnTe films. Crystalline ZnTe thin films can be grown using MBE [4] and MOCVD methods at 300-350 °c growth and 325-400°C [12, 13]. Hence, we conclude that ZnTe films with the best crystalline characterisation can be synthesised at substrate temperatures much lower than those required for MBE and MOVPE. This is attributed to the relatively non-equilibrium nature of the PLD process, which imparts a high energy [15].

### 3.2. Surface Morphology Analysis by SEM:

SEM analyses revealed the surface features of ZnTe thin films deposited with PLD at various substrate temperatures ranging from 100 to 200 °c, then 300 °c. Figure 7: (A-F) supports the findings. Surface structures vary directly with deposition temperature according to micrograph images. When deposition occurs at 100 ° C (Figures A and B), the films develop an uneven surface that contains tightly packed grain clusters. The restricted atomic movement on the substrate at lower temperatures results in poor crystallinity and an unorganised growth pattern. An increase in the deposition temperature to 200 ° C leads to a significant improvement in surface uniformity in the results (Figures C and D). Better surface migration and grain coalescence occur because atomic diffusion produces distinct and enlarged grains inside the structure. The process of improving crystal formation has begun. The films show a uniform, smooth surface pattern at 300 ° C (Figures E and F). The surface exhibits uniformly dispersed grains, demonstrating the perfect level of crystallinity with the highest possible uniformity. Higher temperature levels furnish enough thermal energy to allow atoms to reach energetically favourable positions, resulting in decreased structural defects and increased crystallinity. When the deposition temperature increases, the microstructural properties of the ZnTe thin films undergo improvements, resulting in better grain growth and surface smoothness and enhanced crystalline quality.

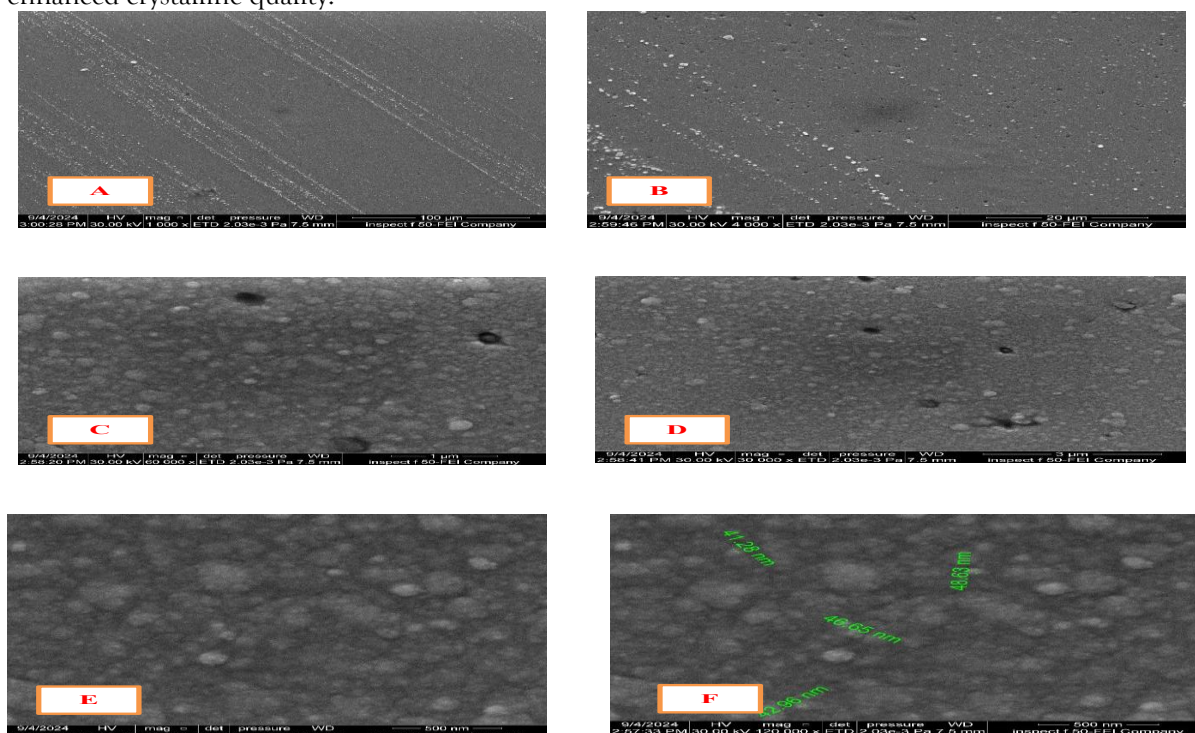


Figure 7: SEM Surface Morphology images of ZnTe thin films

### **Comparison with previous studies:**

Research on II-VI semiconductors combined with ZnTe shows that higher deposition temperatures produce superior surface characteristics and crystal formation based on results from previous investigations. The study shows that the influence of substrate temperature produces better crystal formation and surface characteristics, as previously reported. Dergacheva et al. (2020) researched how ZnTe films developed through PLD produced crystals and smooth surfaces at different temperatures. The films produced larger grains with smoother surfaces at higher substrate temperatures because high temperatures promote better atomic movement and improved nucleation kinetics. Controlled nuclear motion and faster nucleation rates appeared due to higher temperatures. The ZnTe thin films showed better optoelectronic properties, emerging from both a denser film microstructure and a decreased defect density with higher heat temperatures. The research proves that elevated temperature produces denser film microstructures and reduced defect density, according to Lee et al. (2018). Sahoo et al. (2016). The CdTe films underwent structural changes from deteriorated to crystalline versions at elevated deposition temperatures, according to Sahoo et al. (2016). The overall value of thermal energy comes to light as the thin film structures transition to crystalline qualities. The microstructure quality of chalcogenide films is improved by applying PLC deposition techniques. The results obtained. The experimental findings in this work prove that the substrate temperature is a key parameter determining the quality of ZnTe thin films.

### **Challenges and future prospects:**

The technical challenges in this research were caused by producing ZnTe thin films using the pulsed laser deposition (PLD) technique. The main obstacle in this research involved obtaining consistent film coverage under low-temperature deposition conditions because atomic movement was restricted and substandard crystal formation was produced, together with irregular grain patterns. The study discovered that increasing substrate temperatures resulted in structural degradation and mechanical instability. Hence, researchers needed to optimise various deposition factors, such as the target-to-substrate distance and laser pulse repetition rate, to enhance crystal quality. The results of this research project present fundamental knowledge about how temperature affects the structural makeup of the ZnTe thin film and its physical characteristics, leading to its development for photovoltaic and optoelectric applications. Future development includes thermal treatments after deposition to improve crystalline quality and doping methods for modification of optical and electronic properties. The leading research methods, transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS), should be used for detailed structural and interfacial analysis. High-quality ZnTe thin films can be produced effectively through advanced structural engineering and analytical tools.

## **CONCLUSIONS**

The researchers deposited three thin zinc telluride films through pulsed laser deposition (PLD) at substrate temperatures of 100 ° C, 200 ° C and 300 ° C, where X-ray diffraction (XRD) showed that all samples preferred orientation (111). The film created at 300 ° C produced the most intense and sharp diffraction peaks correlated with the highest crystalline quality and the largest grain size properties. The obtained structural stability and minimal disorder within the film point to 300 ° C being the optimal temperature to provide excellent performance in solar cells. The film produced at 300 ° C exhibited the most regular surface pattern that scanning electron microscopy (SEM) analysis showed alongside a well-arranged crystal grain distribution while maintaining a uniform structure.

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