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Substrate Temperature Effect on the Optical and Structural Properties of ZnS Thin Films Prepared by Nd:YAG Pulsed Laser Deposition

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ABSTRACT

Zinc sulfide (ZnS) thin films were deposited on glass substrates using pulsed laser deposition technique. The laser used is the Q-switched Nd:YAG laser with 1064nm wavelength and 1Hz pulse repetition rate and a varying substrate temperature (50^0C -200^0C) . The laser energy was kept constant at 1000mJ with 21 pulses for each sample. The structural, morphological and optical properties of ZnS thin films were characterized with X-ray diffraction (XRD), scanning electron microscopy (SEM), atomic force microscope (AFM) and UV-VIS spectrophotometer.
Keywords:ZnS thin film, PLD, surface roughness.

1.INTRODUCTION

Zinc sulphide belongs to II-VI group compound material with large direct band gap between (3.4-3.7)eV depending upon composition. It is potentially important material to be used as an antireflection coating for heterojunction solar cells [1], for light emitting diode [2, 3], and other optoelectronic devices such as blue light emitting diode [4], electro luminescence devices and photovoltaic cells which enable wide application in the field of displays [5,6], sensor and Laser [7,8]. In recent years ZnS attracted much attention because the properties in nano form differ significantly from those of their bulk counter parts. Therefore much effort has been made to control the size, morphology and crystalline of ZnS thin films. There has been growing interest in developing techniques for preparing semiconductor nano particles and films.

2.EXPERIMENTAL

ZnS thin films were deposited by using the pulsed laser deposition technique. The chamber was evacuated to a base pressure of (10^{-3} mbar) at varying substrate temperature (50^oC- 200^oC). Q-switched Nd: YAG laser with a wavelength of 1064 nm and laser energy of 1000mJ and fixed number of pulses (21 pulses) was used; the focal length for the lens was about 13cm with a repetition rate of 1 Hz. The distance between the target and the substrate was kept at 2.5 cm. Figure (1) shows the setup of PLD. After deposition, the structural, morphological and optical properties of ZnS thin films were characterized with X-ray diffraction (XRD), atomic force microscope (AFM) and UV-VIS spectrophotometer.

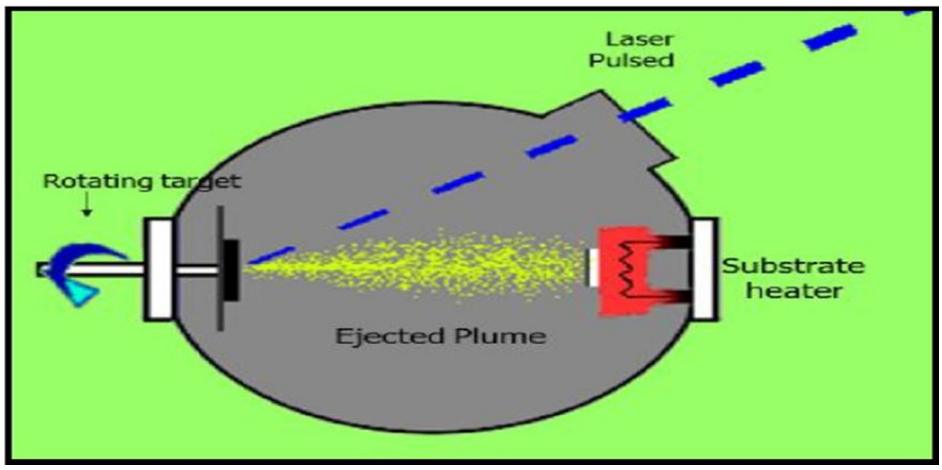


Figure (1): Schematic diagram of PLD setup [13].

3.RESULTS AND DISCUSSION

3.1 OPTICAL PROPERTIES

Optical properties of ZnS thin films were determined from the transmission and absorption measurements in the range of 300-800 nm. Figures (2) and (3) show the variation of optical transmittance and absorbance as a function of wavelength for the films prepared at different substrate temperatures (50^0C, 100^0C, 150^0C and 200^0C). Figure (2) shows the film formed at 200 ^{0}C was relatively higher than the spectral transmittance for the other films prepared at other growth temperatures moreover the average transmission was reached in the near IR region approximately 98%. Absorption coefficient (α) associated with the strong absorption region of the films was calculated from absorbance (A) and the film thickness (t) using the relation [9, 10]:

$$\alpha = 2.3026\, A / t \qquad (1)$$

The absorption coefficient (α) was analyzed using the following expressionfor near-edge optical absorption of semiconductors:

$$(\alpha\, h\square) = K\,(h\square - E_g)^{n/2} \quad (2)$$

Where: K is constant, Eg is the separation between the valence and conduction bands and n is a constant that is equal to 1 for direct band gap semiconductors. The band gap values were determined from the intercept of the straight-line portion of the $(\alpha\, h\square)^2$ against the h□ axis figure (4). The linear part shows that the mode of transition in these films is of direct nature. The calculated band-gap value of the films was between (3.7-3.95) eV. The band-gap values are higher than bulk value of ZnS (3.68 eV) because of quantum confinement of ZnSnanocrystals.

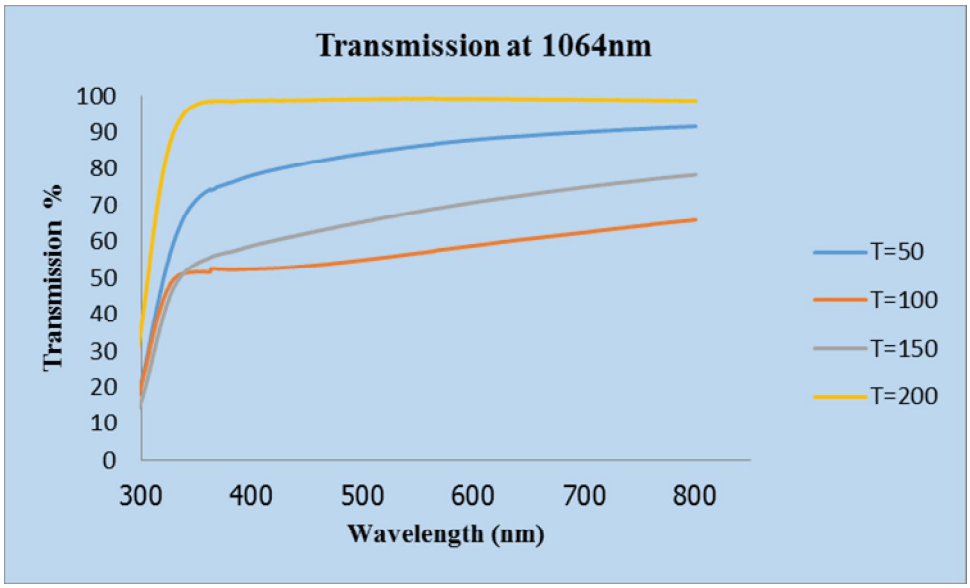


Figure (2): Optical transmissions as a function of wavelength for ZnS/glass at different substrate temperatures.

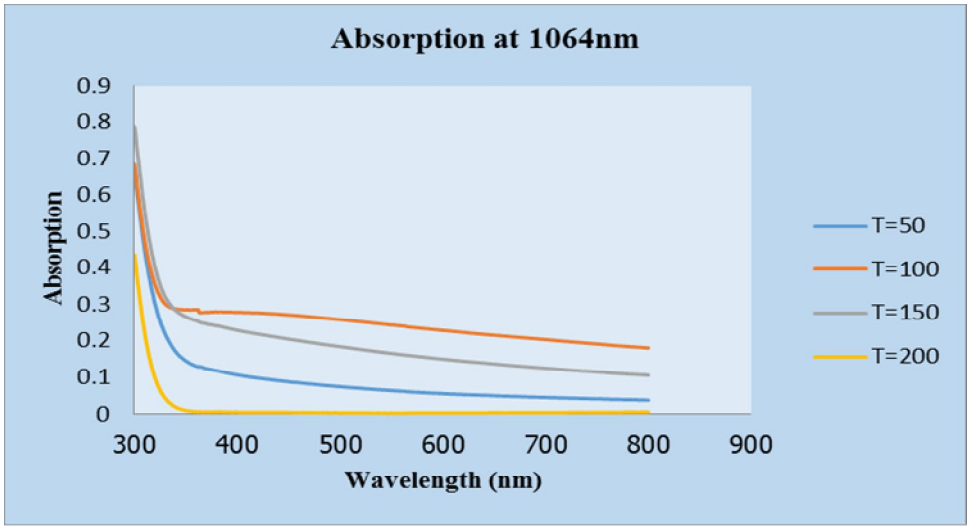


Figure (3): Optical Absorption as a function of wavelength for ZnS/glass at different substrate temperatures.

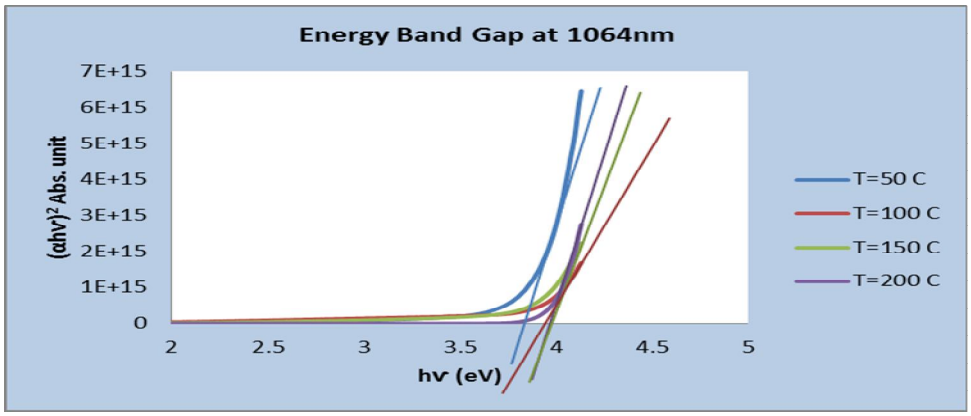


Figure (4): Optical energy band gap for ZnS/glass at different substrate temperatures.

3.2 STRUCTURAL AND MORPHOLIGICAL PROPERTIES

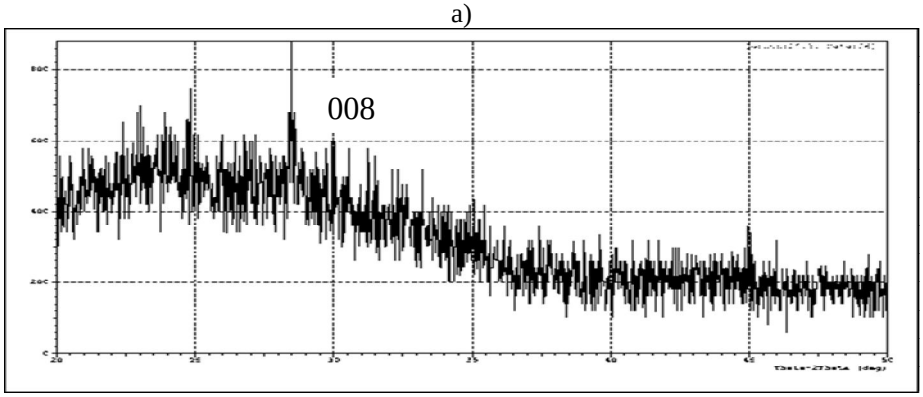
3.2.1XRD STUDIES

All the deposited ZnS films were white, homogeneous with a good adherence to the substrate. Generally ZnS material has the hexagonal, wurtzite type structure or cubic, zinc blend-type structure. X-ray diffraction patterns of ZnS thin films prepared at different substrate temperatures (100^0C and 200^0C) are shown in fig. (5(a & b)) respectively. Fig. (5(a)) shows a crystalline phase with orientation at (008) plane exhibited a hexagonal wurtzite structure. As the temperature increased to 200 ^{0}C (fig. 5(b)),the XRD pattern of ZnS thin films exhibit two distinguished peaks corresponding to diffraction of (008) and (104) planes of hexagonal wurtzite It has been noticed that the diffraction pattern sharpen with increase in substrate temperature and the growth rate was found to be depend on substrate temperature [11, 12]. The highest peak value of the XRD measurement came from ZnS film grown at 200 ^{0}C, indicating that the film had the best preferred orientation structures. . The grain size of the nanocrystalline films is estimated using the Scherrer formula [9].

$$D = K\lambda / \beta \cos\theta \quad (3)$$

Where K is a constant taken to be 0.94, λ the wavelength of X-ray used (λ = 1.54056 A°) and β the full width at ha lf maximum. The peak broadening in the XRD patterns clearly indicates the formation of ZnSnanocrystals of very small size. The grain sizes were found to be within the range of 33.8-71.7 nm.

a)



b)

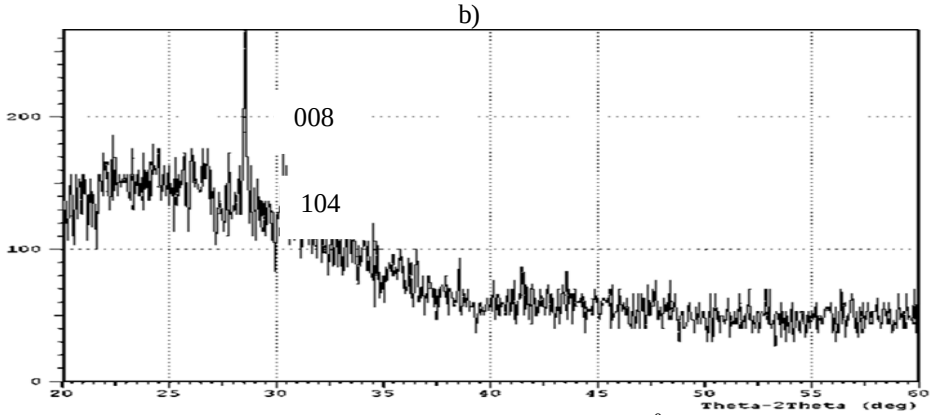


Figure (5): XRD diffraction pattern of ZnS a) at substrate temperature 100^0C and b) at substrate temperature 200^0C

3.2.2 SEM ANALYSIS

Scanning electron microscopy is a convenient technique to study the microstructure of thin films. Figure (6) shows a picture of ZnS powder observed by SEM. The particle size from the SEM is found to be in the range of 210 nm.

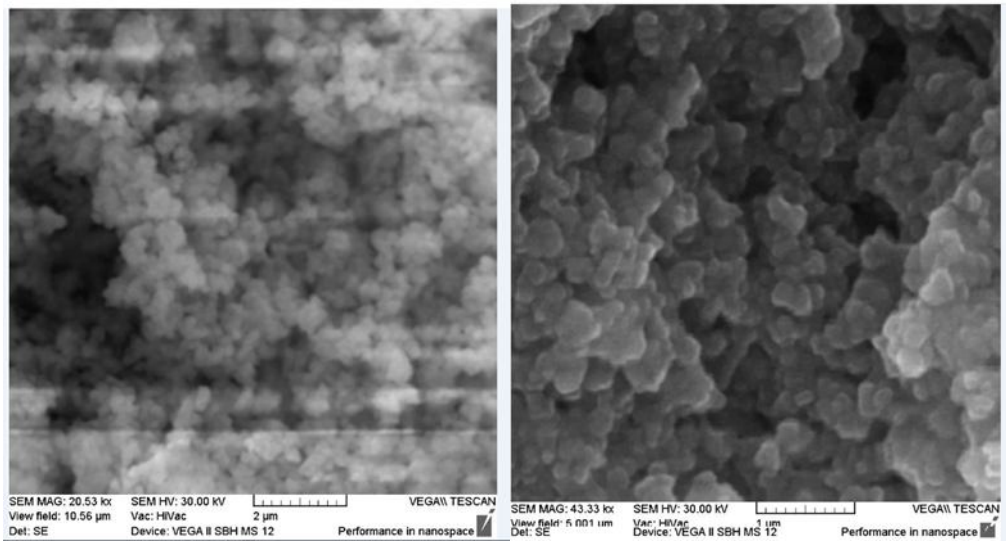
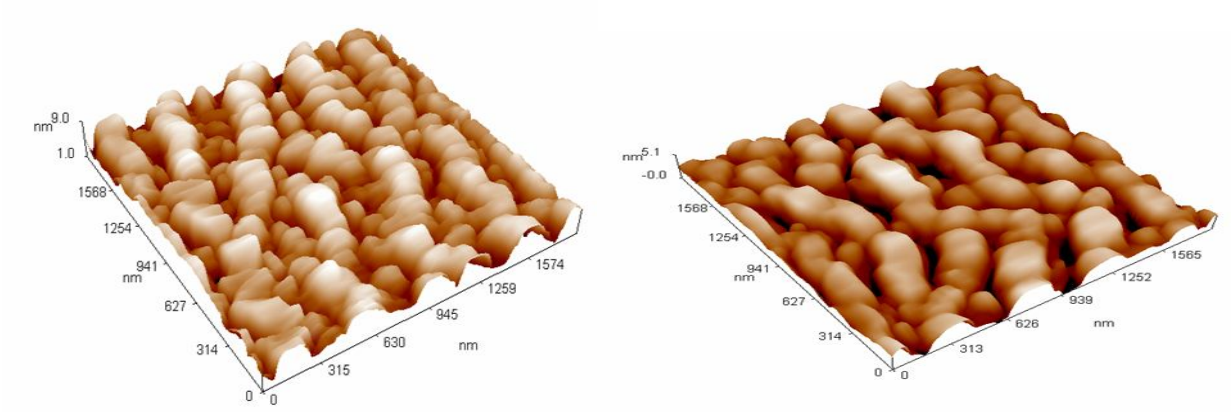


Figure (6): SEM picture of ZnS powder.

3.2.3 AFM ANALYSIS

AFM images which have been taken to the samples are shown in figure (7 (a & b)) which corresponding to the 100^0C and 50^0C samples respectively. The surface roughness and average diameter were tabulated in table 1.



a) b)

Figure (7): AFM images at a) 100^0C and b) 50^0C.

Table (1): The surface roughness and average diameter.

Substrate temperature (^{0}C)	Surface roughness (nm)	Average diameter (nm)
100	1.41	92.77
50	0.966	90.02

4.CONCLUSIONS

Thin films of ZnS prepared by PLD technique are found to be nanocrystalline. The crystallite sizes measured by XRD studies are found to be within 33.8-71.7 nm. XRD shows that samples are of wurtzite hexagonal phase which is important for device performance. Powder SEM studies showed irregular distributions of particles with particle size at

a range of 210nm. The films formed at 200 ^{0}C exhibited good optical properties with a relatively high transmittance reach up to 98% in the UV–VISNIR regions; hence,they could be effective as thermal control window coatings for cold climates and antireflection coatings. The films clearly show an increase in band gap with reduction in particle size as compared to bulk materials, and this fact supports the formation of nanocrystallites in these films.

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