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Characterisation of Spray Deposited Nanostructured MoS_2 Thin Film

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ABSTRACT

The molybdenum disulphide thin film was deposited using ammonium molybdate tetrahydrate and thiourea on glass substrate by spray pyrolysis technique. The X-ray diffraction spectrum of the MoS_2 thin film shows polycrystalline nature with hexagonal structure. The field-emission scanning electron micrograph reveals the formation of nanorods over the film surface. The optical parameters such as optical band gap, refractive index and Urbach energy of the MoS_2 thin film were studied and reported.
Keywords: Molybdenum disulphide; Spray pyrolysis; nanorods; Urbach energy;

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INTRODUCTION

The confinement of layered structure materials, particularly transition metal dichalcogenides (TMD) has attracted great interest due to their distinct properties. Hence, TMDs are utilized in diverse fields for several applications such as hydrodesulphurization [1], lubricants [2], energy storage devices [3], photo active materials [4], field effect transistors [5] and lithium batteries [6] etc.

Among many TMDs ($MoTe_2$, WTe_2, $MoSe_2$, WSe_2 and MoS_2), molybdenum disulphide (MoS_2) is considered as an important semiconducting materials due to its physical properties similar to that of graphene and electronic properties similar to boron nitride [7]. The crystal structure of MoS_2 is hexagonal in which each layer of Mo atoms is bonded between two layers of sulphur atoms. Also, each Mo atoms are surrounded by six sulphur atoms to form a trigonal prism arrangement and each sulphur atoms are surrounded by three Mo atoms to form a stratified arrangement.

MoS_2 in bulk form exhibits an indirect band gap of 1.2 eV [8] and are used in the application of photo-catalytic [9] and solar cells [10]. Due to quantum confinement, the band gap of monolayer MoS_2 has direct band gap of 1.8 eV [8]. This band gap conversion from indirect to direct is due to the hybridization beneath the Fermi level of d-state of Molybdenum and p-state of Sulphur [11]. Hence, used in photovoltaic devices due to its effective absorption in solar spectrum [8].

Molybdenum disulphide thin films were deposited using various techniques such as chemical vapour deposition [12], RF sputtering [13], chemical bath deposition [14], electro deposition [15], spin coating [16] etc. In the present work MoS_2 thin film was prepared by simple home-build spray pyrolysis system [17] and its structural, morphological and optical properties were analysed and reported.

Experimental

To prepare molybdenum disulphide thin film, precursor solution containing 0.61 g of ammonium molybdate tetrahydrate ($(NH_4)_6Mo_7O_{24}.4H_2O$) and 0.19 g of thiourea ($(SC(NH_2)_2$) in 50 mL of deionized water was prepared. The precursor solution was sprayed as fine mist over a glass substrate kept at 230 ºC to obtain MoS_2 thin film. The prepared thin film was then characterized and for structural, morphological and optical properties. The structural studies were analysed using X-ray diffractometer (XPERT-PRO Model) with $CuK\alpha_1$ source and its wavelength is 1.5406 Å. The morphological studies were investigated using field-emission scanning electron microscopy (FE-SEM, JSM 6701F, JEOL). The optical studies of the thin film were obtained using UV-Visible spectrophotometer (Perkin Elmer, Lambda 25).

RESULTS AND DISCUSSION

Structural studies

The X-ray diffraction pattern of the prepared thin film is shown in Fig. 1. The different peaks indicate polycrystalline nature of the film and planes were indexed to (0 0 2), (0 0 4) and (1 0 3) with respect to the standard JCPDS card no 73-1508 of hexagonal structure. The crystallite size and microstrain were calculated from the well known Scherrer relation:

$$D = \left(\frac{K\lambda}{\beta \cos\theta} \right) \text{-----------------------------------} (1)$$

$$\varepsilon = \frac{\beta \cot\theta}{4} \text{-------------------------------------} (2)$$

where, K is the shape factor, λ is the wavelength of X-ray and β is the Full Width at Half Maximum (FWHM, in radians), θ is the diffracting angle (in radians). The crystallite size and microstrain was found to be 20 nm and 0.0065 respectively.

Morphological studies

Fig. 2(a) shows the field emission scanning electron micrograph of the MoS_2 thin film deposited at 50 mL of precursor solution volume, shows the presence of nanorods. From Fig. (2b) shows the cross-sectional scanning electron micrograph in which the thickness of the deposited thin film was found to be 540 nm.

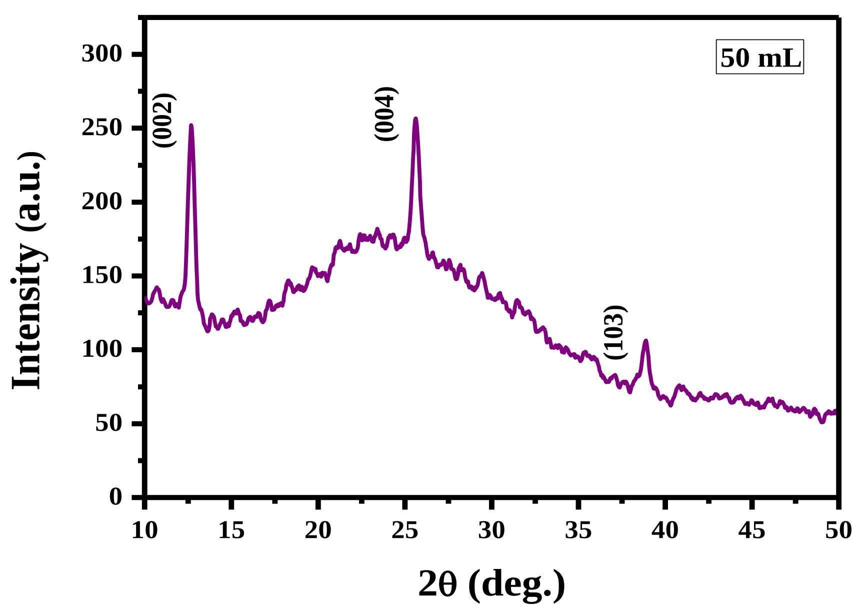

Figure 1: Structural morphology of 50 mL deposited MoS_2 thin film

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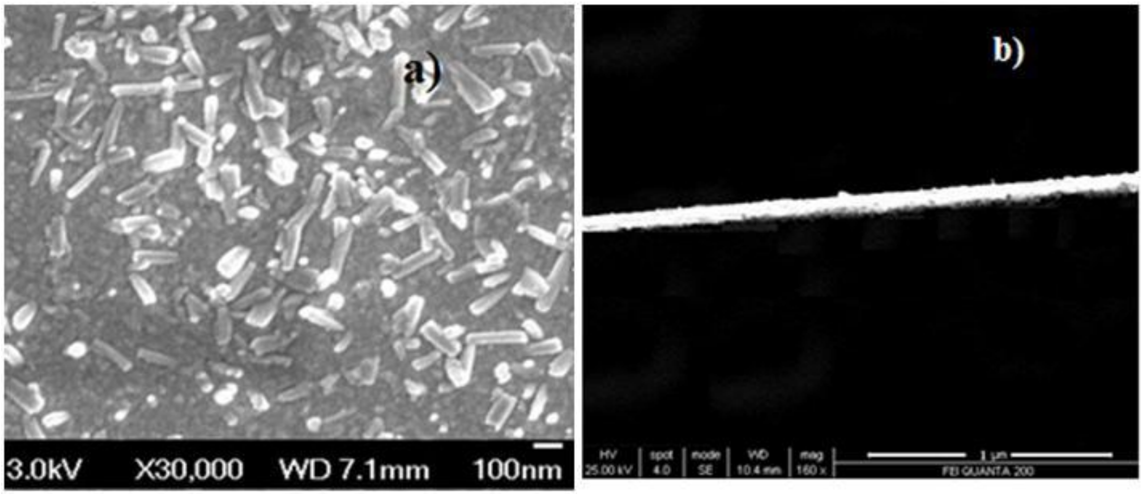
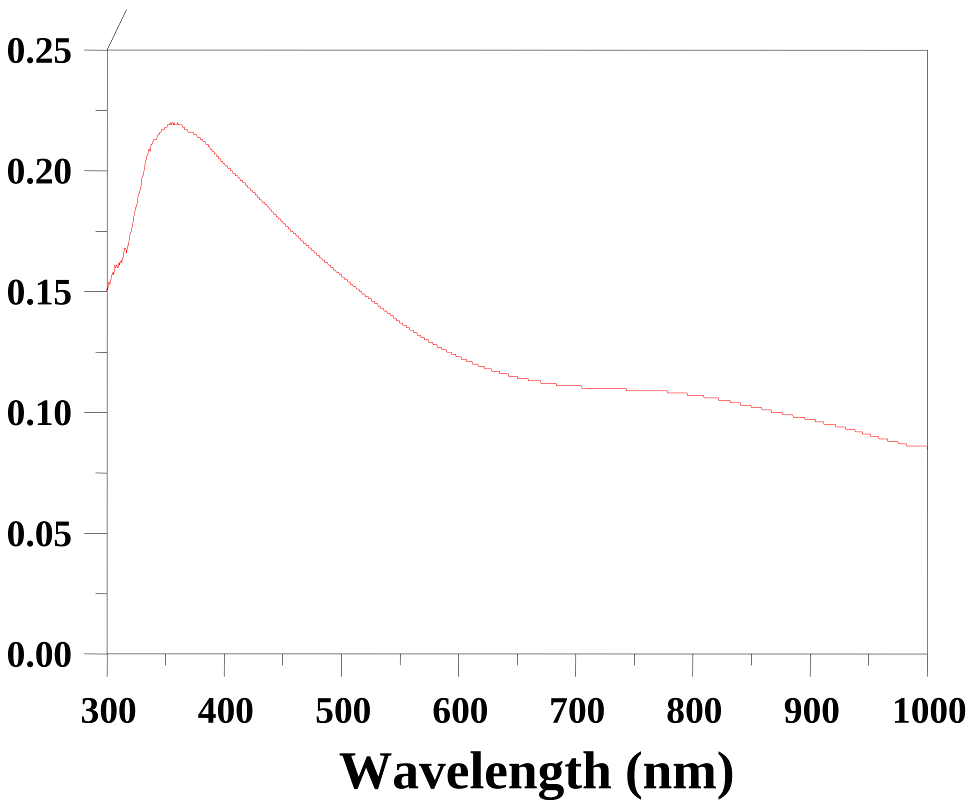


Figure 2: (a) FE-SEM and (b) Cross-sectional SEM of MoS_2 thin film



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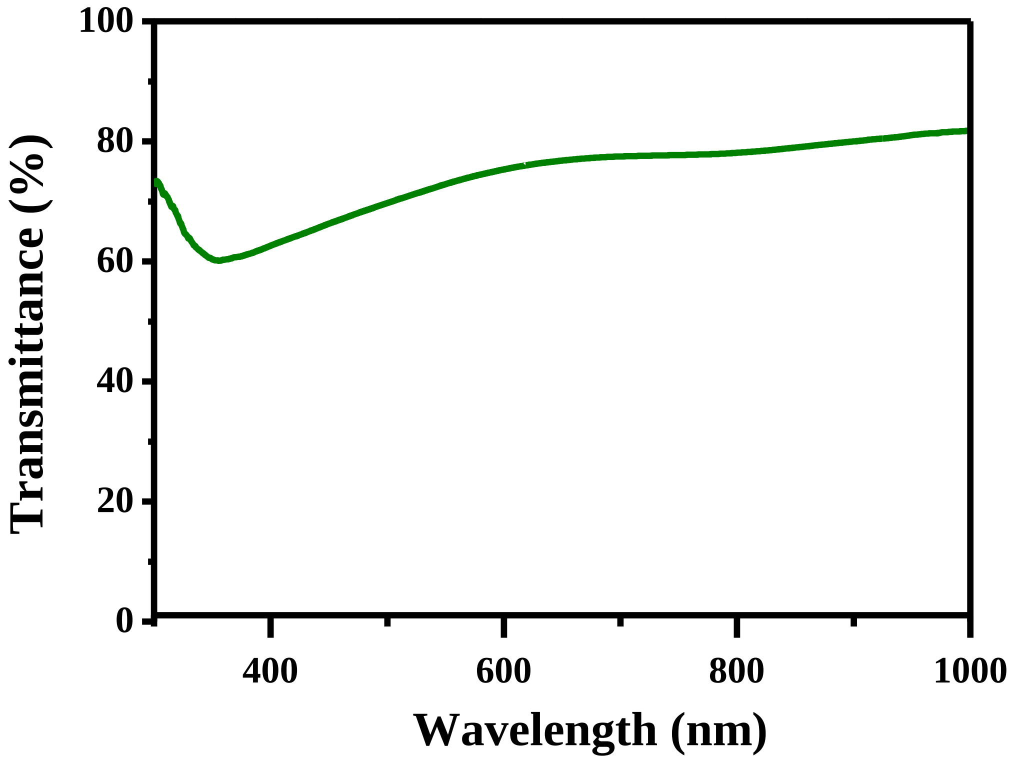
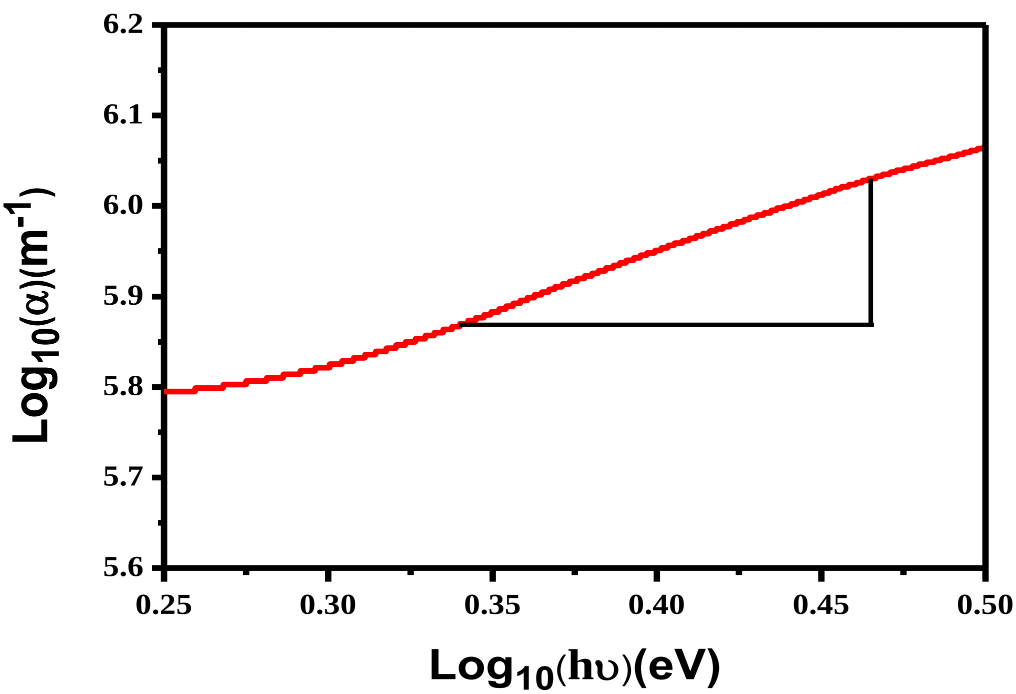


Figure 3: Optical absorbance and transmittance spectum of spray deposited MoS_2 thin film



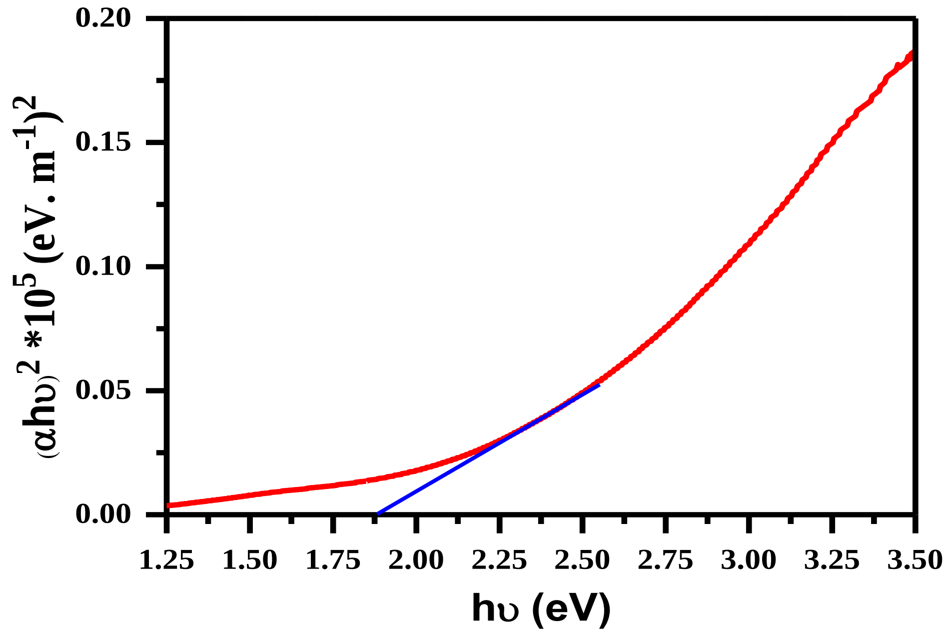


Figure 4: (a). α Vs hν graph in log-log scale to find the transition probability
Figure 4: (b). Optical band gap of MoS_2 thin film obtained from Tauc's plot

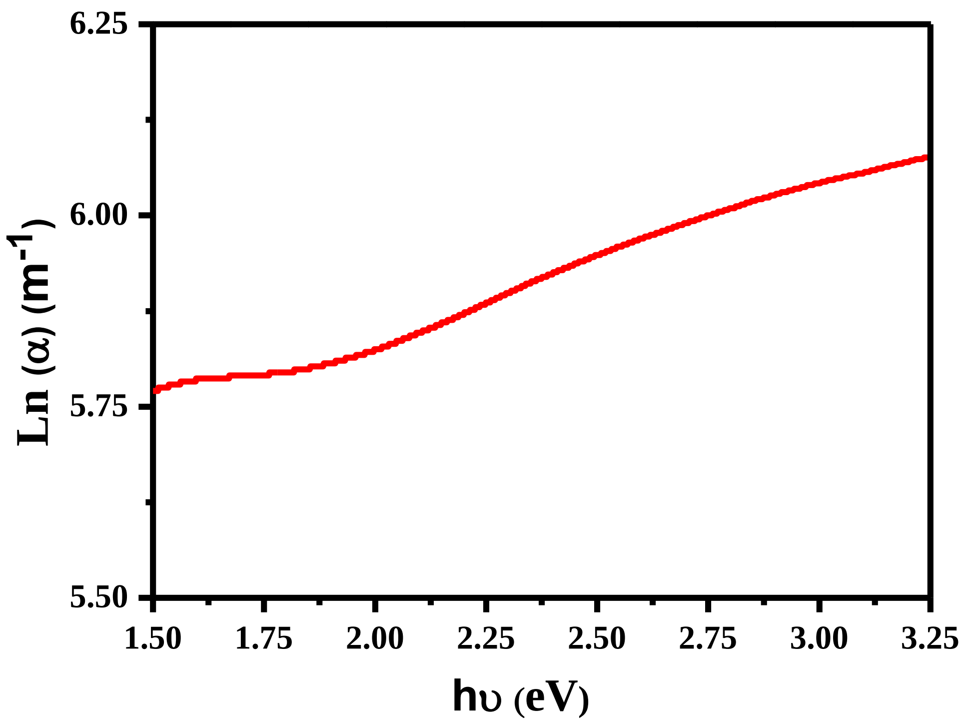


Figure 5: Urbach energy plot for the MoS_2 thin film

Optical properties

The optical absorbance and transmittance spectra of the MoS_2 thin film was shown in Fig. 3. It shows maximum absorbance at 350 nm and good transparency in the entire visible region. The value of absorbance co-efficient (α) was calculated from the following equation [18]:

$$\alpha = \frac{2.303 * absorbance}{t} \text{-----------------------------------} (3)$$

Where α is the absorbance co-efficient, t is the film thickness and was found to be 540 nm, obtained from the cross sectional SEM shown in Fig. 2(b).

The slope from the plot Log (α) and Log (*hv)* shown in Fig. 4 (a) has value of ~1 and indicates the nature of transition is of direct allowed. The band gap was obtained from the Tauc's plot shown in Fig. 4 (b) and found to be 1.8 eV. The refractive index (n) with respect to reflectance (R) of the MoS_2 thin film was calculated using the relation [18]:

$$n = \frac{1+\sqrt{R}}{1-\sqrt{R}} \text{-----------------------------------} (4)$$

The refractive index is 1.2596 at the wavelength of 328 nm. The value of the refractive index decreases with increase in wavelength. Fig. 5 shows the Urbach energy of the MoS_2 thin film which was obtained by plotting a graph between Ln (α) and Energy (eV).

CONCLUSION

The MoS_2 thin film was deposited on glass substrate by home-made chemical spray pyrolysis technique. XRD pattern reveals polycrystalline nature with grain size and microstrain of 20 nm and 0.0065. FE-SEM micrograph determines the formation of nanorods and the thickness of the deposited film was analysed using cross sectional SEM. Optical band gap of the deposited MoS_2 thin film was obtained as 1.8 eV.

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