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Research Article

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Structural and optical characterization of molybdenum oxide thin film synthesized by thermal evaporation method

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ABSTRACT

In this research work, a Molybdenum trioxide (MoO_3) thin film of thickness 0.5μm was synthesized on a glass substrate by thermal vacuum evaporation technique. The deposition was performed at the rate of 1.2Å/s. The structure and optical characterization of the film was carried out by XRD and UV visible spectroscopy respectively. The band gap of the film was 2.82eV. The results of XRD depicts sharp peaks at 2θ angles of 12.74° ,23.32°,25.54°,27.4°,53.76° and 38.91° with respect to the planes (020),(110),(040),(021),(060) and (001).

Keywords: MoO_3, Thermal evaporation, Undoped films, Characterization

INTRODUCTION

Molybdenum trioxide is an orthorhombic solid powder which is considered harmful for human health [1]. Distorted layers of MoO_6 which are in octahedral form make up the structure of MoO_3 [2]. Molybdenum trioxide is an odorless substance with colour varying in accordance to temperature from white, pale or little bluish. Its melting point is 1068K and its boiling point is 1428K [3]. As far as solubility is concerned it is very less soluble in water, highly soluble in alkaline solutions, in concentrated nitric and sulphuric acids. It produces polymeric compounds with the acids [4].

Molybdenum trioxide occurs in oxidation state of +6. It shows aggressive reactivity towards chlorine trifloride (ClF_3), lithium, potassium and sodium metals. Molybdenum is a transition metal and MoO_3 is its oxide. Molybdenum oxide shows electrochromic properties because of its cross linked structure [5]. Apart from this it is used for manufacturing molybdenum (Mo). Molybdenum (Mo) can be used as co- catalyst and its potential use lies as an antibacterial material [6].

EXPERIMENTAL SECTION

The MoO_3 films were prepared by thermal vapor deposition by using HINDHVAC 525 which was evacuated by a rotary pump (V1-2015) followed by a diffusion pump. Thickness was measured simultaneously with deposition by real time monitoring by quartz crystal model (CTM-200). Chamber for deposition was cleaned thoroughly with acetone. A piece of Molybdenum trioxide was kept in the boat shaped sample holder in a chamber. Initially, the rotary pump was used to evacuate the chamber followed by roughing to create a base pressure of 10^{-2} Torr. After half an hour, the diffusion pump was used to further evacuate the chamber and reach a base pressure of 4×10^{-6} Torr. Throughout the runtime of the pumps, continuous water supply was maintained for cooling of outer surface of pumps, so that pressure difference should be retained otherwise action of pumps can be reversed. Penning and pirani gauges are used for monitoring diffusion and rotary pump respectively. A current in the range of 34-38 amp was supplied to the boat which heated the MoO_3 piece in the chamber until it starts evaporating and subsequently depositing on the glass substrate placed near the roof of chamber. Along with it a quartz crystal monitor is placed to monitor the rate of deposition of film and its thickness. The film was deposited in 8 minutes.

RESULTS AND DISCUSSION

An optical characterization was done of the films by UV-Vis spectroscopy. The wavelength range of UV-VIS analysis was kept 200-1100 Ǻ. **Fig. 1** shows a plot between energy in eV and $(\alpha h\nu)^2$. The energy band gap was noted where the tangent to the line intersects the x-axis. It came out to be around 2.8eV which is approximately equal to reported values of 3.04eV at room temperature.

$$\text{Absorption coefficient, } \alpha = 2.303 \times (A/d)$$

Where "A" is called the absorption and "d" is called the film thickness.

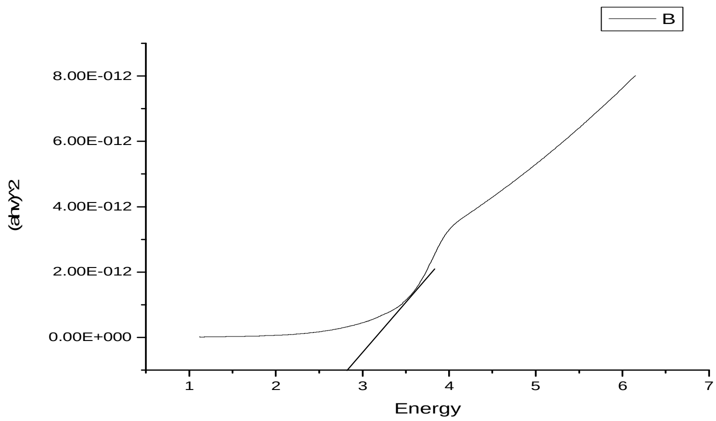

Fig.1 The above figure is the UV-VIS data plotted for hν in eV against $(\alpha h\nu)^2$ to find the band gap

Structural Characterization: The structural characterization of thin films was done with x-ray diffraction. **Fig. 2** shows the diffractograph of this study. The planes of crystal from which strong diffraction peaks were observed are (020),(110),(040),(021),(060) and (002). So the film produced is primarily crystalline in nature.

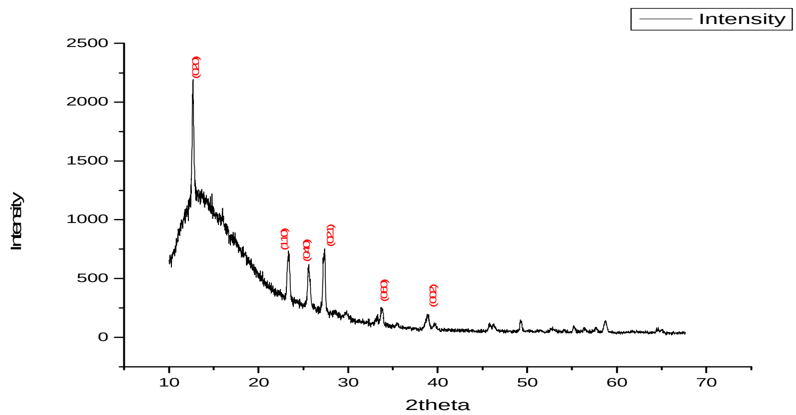

Fig.2 shows graph between grazing angle 2θ and intensity of x-rays

The grain size of the film was calculated using Debye-Scherer equation:

$$D = 0.9/\lambda\ (\beta \times \cos\theta)$$

Where "λ" is the fixed wavelength of x-rays used (1.54Ǻ), β is known as Full width at half maximum(FWHM). The average grain size was found to be 70 nm.

CONCLUSION

The Molybdenum trioxide thin film was successfully deposited by thermal vapor deposition method. The deposited film had good adherence properties with the glass substrate. The x-ray diffraction (XRD) of film annealed at 300^oC confirms that the deposited film has an orthorhombic structure. The preferred growth of crystals along the planes (020),(110),(040),(021),(060) and (001) is observed. The UV-Vis spectroscopic analysis of film was used to find the band gap of film which came out to be 2.82eV which is near the with reported value. This film appears to have the potential application as an additive to corrosion resistant alloys and an anti microbial agent.

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