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Influence of Thermal Oxidation Temperatures on the Structural and Morphological Properties of MoO_3 Thin Films

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In this study, molybdenum (Mo) thin films have been deposited on Si substrate by dc magnetron sputtering. Then for preparation of MoO_3 thin films the thermal oxidation of Mo thin films under the oxygen flow was employed in the electrical furnace. The influence of the different thermal oxidation temperatures at 400, 600, 800 and 1000 °C on the structural and morphological properties of MoO_3 thin films were characterized by X-ray diffraction and atomic force microscopy, respectively. The results show that the crystallinity and surface morphology of the films are strongly dependent on the thermal oxidation temperatures.

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1. Introduction

Molybdenum oxide (MoO_3) is a metal oxide with intermediate band gap n-type semiconductors that have attracted much interest for technological applications in recent years, because of its attractive structural, electrical and optical properties [1].

Also, MoO_3 thin films have potential application in important devices, including optical memories [2], gas sensors [3], catalysis [4], electrochromic devices (ECDs) [5] and lithium batteries [6]. However, the device efficiency is essentially related to the structure and surface morphology of the films which in turn invariably depends on the deposition technique and deposition parameters used for the growth of thin films.

In the present investigation the thermal oxidation of Mo thin films was employed for preparation of MoO_3 thin films. The effect of thermal oxidation temperatures on structural and surface morphology of the films are elaborately studied and presented here.

2. Experimental details

In this experiment, in the first step the Mo thin films were deposited by dc magnetron sputtering onto silicon (1 cm × 1 cm) substrates at room temperature with using a molybdenum target (purity 99/995%). The distance between substrate and target is 7 cm. Before the operation, the chamber is evacuated to less than 4×10^{-5} Torr, by means of a rotary and diffusion pumps. The pure argon gas is injected to the system as working gas to deposit the films with discharge current of 180 mA. The films depositions are carried out for 24 min at constant gas pressure of 2×10^{-2} Torr. The thickness of the films and the rate of deposition were controlled using the quartz crystal monitor. The rate of sputtering (1 Å/s) was used to deposit all Mo films to a thickness of 140 nm. Then, for preparation of MoO_3 thin films the thermal oxidation of Mo films under the oxygen flow at different temperatures, namely 400, 600, 800 and 1000 °C were done in electrical furnace. Finally, the effect of the thermal oxidation temperatures on the structures and surface morphology of the prepared films were investigated.

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3. Results and discussion

X-ray diffraction (XRD) patterns of the thin films at different thermal oxidation temperatures were shown in Fig. 1.

The X-ray diffraction patterns showed that for sample without thermal oxidation, only one intensive peak due to the Mo (110) was observed. Thermal oxidation of Mo films at 400 °C showed three peaks due to the Mo (110), (211) and (220) orientations. By increasing the temperature to 600 °C the polycrystal MoO_3 phase appeared. Furthermore, by enhancing the thermal oxidation temperatures up to 1000 °C the crystallinity of MoO_3 films was decreased, maybe for disassembled lattice arrangement. The results show that the optimum temperature of thermal oxidation of Mo films in our experiment was 600 °C, because in this temperature the best crystallinity was observed. The average crystallite sizes were estimated by the Scherrer formula [7]. The measured values were varied between 12–42 nm for the samples (1–5) as are mentioned in Table I.

Figure 2 shows the AFM images of the thin films at different thermal oxidation temperatures. Investigation of the AFM images demonstrates that before the thermal oxidation, the crystal sizes are small. By thermal oxidation at 400 °C, these small crystals gradually combine and make bigger grains. With increasing the thermal oxidation temperature to 600 °C, the grains become bigger and at last it can cause to create clusters. The films roughness also increases during the annealing pro-

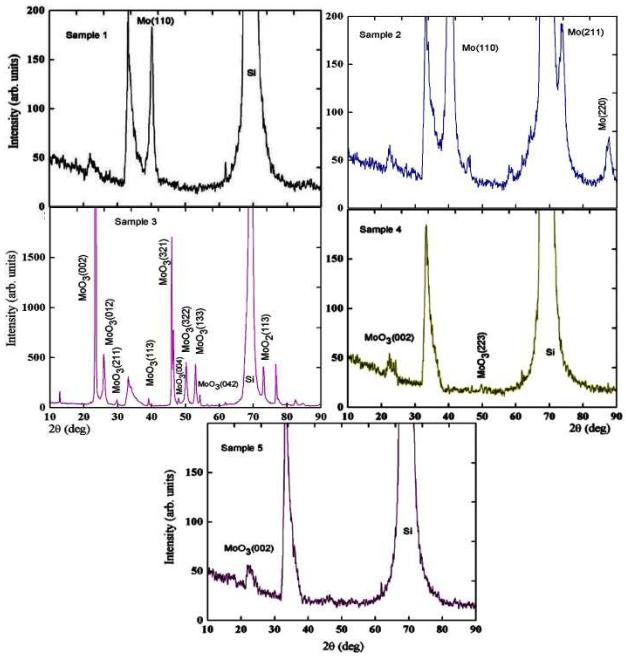

Fig. 1. XRD patterns of the thin films at different thermal oxidation temperatures: sample (1): without oxidation, sample (2): 400 °C, sample (3): 600 °C, sample (4): 800 °C, sample (5): 1000 °C.

TABLE I

Crystal size and crystal phase of films.

Sample number	Crystal phase (hkl)	Average crystal size [nm]
1	Mo(110)	21.53
2	Mo(110)	30.79
3	MoO_3(002)	41.35
4	MoO_3(002)	34.45
5	MoO_3(002)	12.87

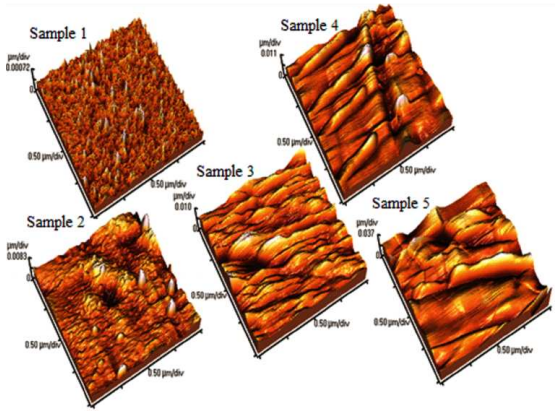

Fig. 2. AFM images of samples: sample (1): without oxidation, sample (2): 400 °C, sample (3): 600 °C, sample (4): 800 °C, sample (5): 1000 °C.

TABLE II

RMS roughness and Ave roughness of films.

Sample number	RMS roughness [nm]	Ave roughness [nm]
1	0.14	0.11
2	2.44	1.91
3	5.11	3.93
4	1.68	1.18
5	2.21	1.59

cess. Table II shows root mean square (RMS) roughness and average (Ave) roughness of films.

4. Conclusion

MoO_3 films have been formed by thermal oxidation of Mo film which has been sputtered on silicon substrate. The results have shown that the effect of thermal oxidation temperatures on MoO_3 films leads to thermal oxidation of Mo films at 400 °C which promotes the crystallinity of Mo film and by increasing the oxidation temperature up to 600 °C the polycrystalline MoO_3 film appeared. Furthermore, by enhancing the thermal oxidation temperatures up to 1000 °C the MoO_3 films crystallinity was decreased, maybe for the disassembled lattice arrangement. The results show that the optimum temperature of thermal oxidation of Mo films in our experiment was 600 °C. AFM results showed the lowest RMS roughness, for Mo films without oxidation, and the highest RMS roughness for the polycrystalline MoO_3 film.

Acknowledgments

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