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Structural, Morphological, Optical & Infrared properties of nanocrystalline MoO_3 thin films

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Abstract: Nanocrystalline MoO_3 thin films were deposited by RF-Magnetron Sputtering on to glass and p-Si (100) substrates at partial pressures of 0.05, 0.1, and 0.5 mbar and annealed at various temperatures (300 K - 673 K). The deposited films were characterized by XRD, AFM, optical, IR spectrophotometer and ellipsometry. The XRD confirms the existence of monoclinic and orthorhombic phase of MoO_3. The AFM measurements confirm the formation of nano particles. The optical energy gap of the films was found to be 3.4eV. The formation of Mo = O and O – Mo– O modes of vibrations of MoO_3 molecule was observed from IR spectra. The thickness of the films was found to be 200 nm.
Keywords: Oxides, Thin films, R.F sputtering, characterization.

Introduction & Experimental:

Nanocrystalline molybdenum trioxide has attracted the attention of many researchers because of the various technological applications. Molybdenum trioxide films can be prepared by various physical and chemical vapour deposition techniques. In the present investigation, nanocrystallineMoO_3 films were prepared by R.F. magnetron sputtering technique and the influence of deposition parameters on the physical properties of the films were studied. The films were deposited on quartz and Si substrates at a sputtering power of 25 W. The films were further annealed at temperatures varied from 300– 673 K and partial pressures from 0.05 – 0.5 mbar. The characterizations of these films were carried out by studying their structure by XRD, morphology by AFM, optical by UV-VIS Spectrophotometer and infrared properties by FT-IR Spectrophotometer.

Results & Discussions:

The XRD (Fig.1) studies reveal that the films deposited at 0.05 mbar and annealed at 373 K, were amorphous in nature as they show no characteristic peaks. This may be due to the low mobility of the atoms reaching the substrate surface and the interaction between molybdenum and oxygen is low. When annealed at 473 K, the films showed a (0 1 1) reflections indicating the presence of monoclinic phase. Films annealed at 573 K showed an intense (0 4 0), (1 0 2) orientations. The intense (0 4 0) reflections indicating the presence of orthorhombic phase of MoO_3 which were in good agreement with the values obtained earlier [1-3]. Thus, the

MoO_3 films annealed at lower annealing temperatures are amorphous and the crystallinity of the films was increased when annealed at higher temperatures and the predominant phase is orthorhombic phase of MoO_3.

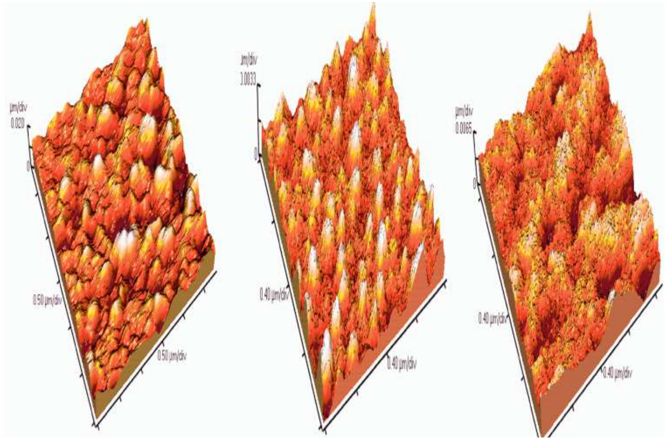

Fig. 1 The XRD spectra of the MoO3 films deposited at a sputtering pressure of 0.05 mbar and annealed at various temperatures.

AFM images (Fig.2) reveal that the films deposited at 0.05 and 0.1 mbar and annealed at 373, 573 K shows a needle like growth of the particles and were wrinkled. Particle size and average roughness of the films were found to be increasing with increasing annealing temperatures [4, 5]. The surface of the film appears to be uniform, grainy and composed of spherical nanoparticles of various sizes for the films deposited at 0.5 mbar and annealed at 373 K. AFM studies reveal that, all the particles are uniformly distributed with small variation in grain sizeand surface roughness of the films was increasing with increasing annealing temperature.

The optical transmittance spectra of the films showed a high transmittance of an average 65% in the range of 400 – 600 nm. The decrease in optical transmittance with increasing annealing temperature for the all deposited films is due to the formation of more oxygen-ion vacancies in the films at higher temperatures. The energy gap of the films annealed at 0.05, 0.1 and 0.5 mbar pressures are 3.20, 3.22, 3.4 eV. The high value of energy gap at 0.5 mbar is due to the formation of lower crystallite size. This is in good agreement with grain size obtained by AFM at 373 K. The shift in absorption edge towards lower wavelength side [2, 6] with increasing sputtering pressure is due to the formation of crystallites of lower grain size which cause the broadening of the band gap between the filled level and unfilled levels of electrons.

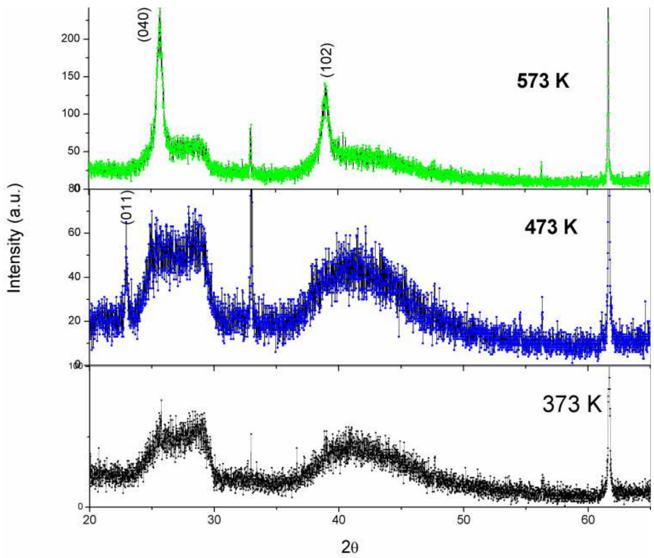

Fig. 2 The 3-dimensional AFM image of MoO_3 deposited at a sputtering pressure of 0.05 mbar, 0.1 mbar and 0.5 mbar and annealed at 373 K

The FT-IR spectra of MoO_3films deposited at a sputtering pressure of 0.05 mbar and annealed at 373 Kare shown in Fig.3 which shows weak absorption bands at 841, 996 cm^{-1}. When annealed at higher temperatures these absorption bands are strong and additional peaks were observed at 942, 1020, 1067, 1160 cm^{-1}due to Mo – O groups in MoO_3 [7, 8]. The absorption band observed at 952 $cm^{-1}$when annealed at 373 K in

0.1 mbar was due to the formation of molybdenum species of lower oxidation state Mo^{5+}. The peak at 934 cm^{-1} represents Mo–O–Mo stretching. The intensity of IR bands was increasing with increasing annealing temperatures which is due to the ad-atom mobility at higher temperatures that improves the crystallinity of the films and sharpness of the peaks.

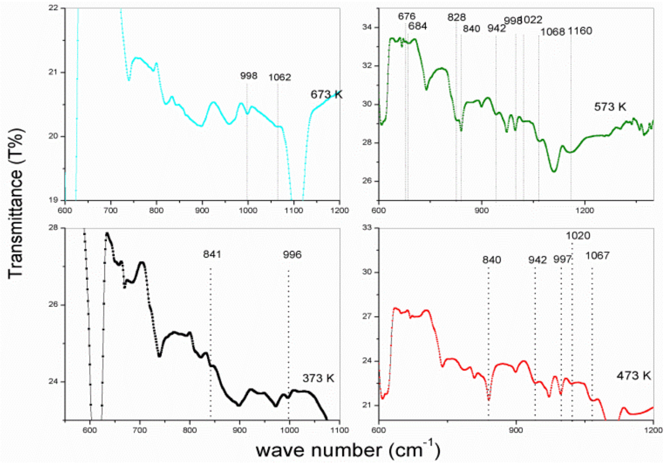

Fig. 3 The FT-IR spectra of MoO_3 films deposited at various annealing temperatures and at a fixed pressure of 0.05 m bar

Conclusions:

The nanocrystalline thin films were deposited by r.f. magnetron sputtering technique and their structural, morphological, infrared and optical properties have been extensively studied. The XRD confirms the existence of monoclinic and orthorhombic phase of MoO_3. The AFM studies confirm the formation of nano particles.The optical energy gap of the films was found to be 3.4eV. The formation of Mo = O and O – Mo– O modes of vibrations of MoO_3 molecule was observed from IR spectra.

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