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Characteristic Analysis on the Physical Properties of Nanostructured MgSe Thin Films – Substrate Temperature Effect

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Abstract: Magnesium selenide (MgSe) thin films were synthesized on glass substrates by spray pyrolysis technique at different substrate temperatures. Effect of substrate temperature on the physical properties of the films was investigated. XRD studies revealed that all the films exhibit cubic structure with a preferential orientation along the (2 0 0) plane irrespective of the substrate temperature. The band gap value decreases from 2.87 eV to 2.72 eV with increase in substrate temperature. The type of functional groups present in the samples is verified using FTIR spectrum.

Keywords: Crystal structure; semiconductors; structural; particles, nano-size; FTIR; thin films.

1 Introduction

Selenium based metal chalcogenide nanostructures have potential applications in optoelectronics, thermoelectric, photoelectric devices and solar selective coatings due to their improved structural, electrical, optical and magnetic properties. Among the various metal selenide thin films, MgSe is a wide band gap semiconductor which may exist in various crystal structures such as zinc blende, wurtzite and rocksalt. Due to its hygroscopic nature and unstable zinc blende structure, a detailed investigation on the physical properties of MgSe is not clear till now and only few reports are available in the literature. MgSe thin films have been deposited by various methods such as MOCVD [1], MBE [2], chemical bath deposition [3], spray pyrolysis [4], etc. However, reports on the properties of spray deposited MgSe thin films based on substrate temperature is very scarce in the literature. So in the present investigation, MgSe thin films were fabricated by the spray pyrolysis technique at three different substrate temperatures. The effect of growth temperature on the physical properties of the films has been studied and the results are presented here.

2 Experimental

MgSe thin films were deposited on glass substrates from aqueous solution (30 ml in volume) containing $MgCl_2$, 0.025M and SeO_2, 0.025M at different substrate temperatures (280, 340 and 400°C). The films were characterized by X-ray diffractometer (PANalytical PW 340/60 X'pert PRO), scanning electron microscope (HITACHI-S-300H) and Perkin Elmer LAMBDA-35 spectrophotometer. The thicknesses of the films estimated using profilometer (SurfTest SJ-301) were found to be equal to 452 nm, 313 nm and 115nm for the films coated at 280, 340 and 400°C respectively. It is observed that film thickness decreases with increase in substrate temperature which might be due to the reduction of precursor mass transfer to the substrate. The reduced mass transport is due to gas convection from the chamber, pushing the droplets away, which induces formation of crystallites in the vapor itself. This is in accordance with Suganya et al.[5] for spray deposited lead oxide thin films.

3 Result and Discussion

3.1 Structural studies

Fig. 1 shows the XRD patterns of MgSe thin films coated at different substrate temperatures.

All the films have polycrystalline structure of cubic phase

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with a preferential orientation along the (2 0 0) plane irrespective of substrate temperature. Other weak peaks present in the patterns are associated with the (1 1 1) and (2 2 0) planes of MgSe (JCPDS: 65-2922). The film coated at 280°C is slightly amorphous in nature. As the deposition temperature is increased, the peaks became sharper suggesting improved crystallinity.

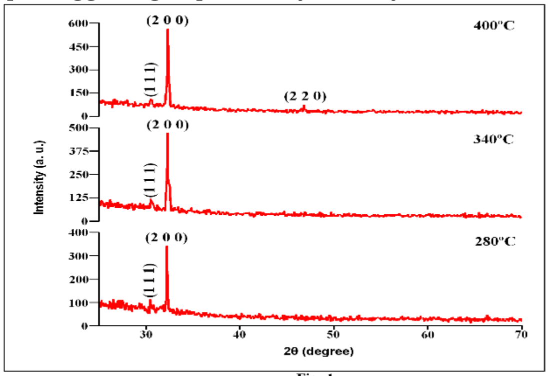

Fig. 1

Fig. 1: XRD patterns of MgSe thin films prepared at different substrate temperatures.

The crystallite size (D) values of the films for the (2 0 0) plane calculated using the Scherrer formula, $D = {0.9\lambda}/{\beta \cos\theta}$ were found to be equal to 17.76, 19.61 and 21.34 nm for the films coated at 280, 340 and 400ºC respectively. Increased crystallite size with increase in substrate temperature confirms that crystallization improves with increase in the growth temperature.

3.2 SEM analysis

Fig. 2 shows the SEM images of the MgSe thin films.

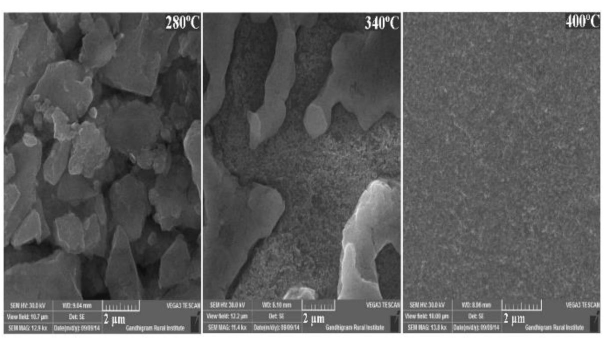

Fig. 2

Fig. 2: SEM images of MgSe thin films.

In the case of the film coated at 280°C, the agglomeration of crystallites appears to be substantial, thereby showing a remarkable increase in the size. As the substrate temperature is increased to 340ºC, the film surface is partially filled with nanosized grains and with patches of interconnected crystallites which showed that at this temperature, the film morphology undergoes a transition from crystallites to nanosized grains. At 400°C, the film morphology undergoes a complete transition to nanoregime with its surface fully covered with nanosized grains which becomes a supporting evidence for its improved crystallinity.

3.3 Elemental analysis

EDS spectra (Fig. 3) confer the presence of expected elements Mg and Se in the films.

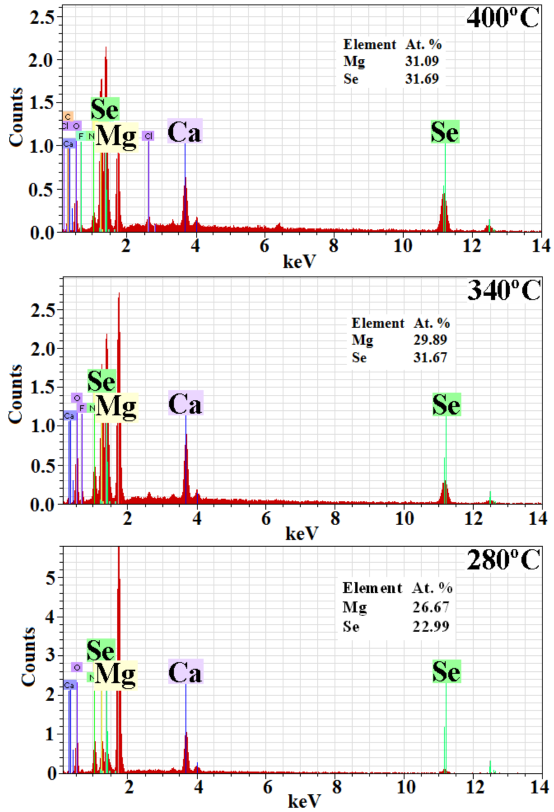

Fig. 3

Fig. 3: EDAX spectra of MgSe thin films.

The compositions of the elements were shown in the insets. It can be seen that the Se/Mg ratio increases as the substrate temperature increases and for the film coated at 400°C, the ratio became equal to 1, confirming its perfect stoichiometric nature. The other impurities Ca and Na observed in the spectra are attributed to the chemical component of glass substrate [6] whereas C, N and O might be due to exposure to the atmosphere.

3.4 Optical characterization

The transmittance spectra of the MgSe films are shown in Fig. 4. Film transparency increases with increase in substrate temperature.

The increase in film transparency with substrate temperature may be attributed to the reduction of defect centers due to lesser thickness obtained. As the density of defect centers decreases, light loss by scattering decreases and hence film transparency increases. The optical band gap (E_g) values are evaluated from the Tauc's plots (inset of Fig. 4) [7]. The band gap value decreases from 2.87 eV to 2.72 eV with increase in substrate temperature. Similar results were observed by Lo at al. [8] for chemically deposited CdS thin films.

The decrease in band gap causes a strong red shift in the optical spectra and this is attributed to the increase of density of localized states in the energy gap. The decrease in the optical band gap may be due to the quantum size effect and variation in the stoichiometry of the films with substrate temperature.

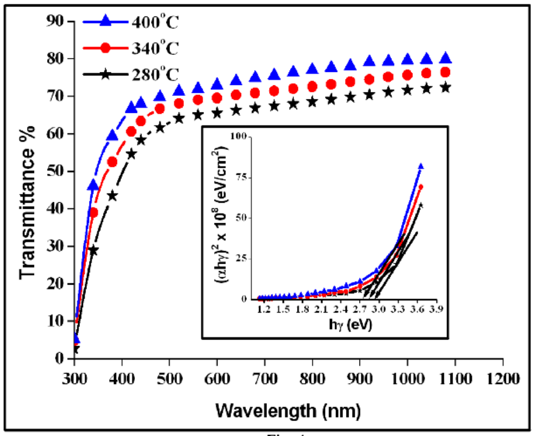

Fig. 4: Transmittance spectra and Tauc's plots (inset) of MgSe thin films.

3.5 FTIR analysis

The FTIR transmittance spectrum of MgSe thin film coated at 400°C which have better structural, morphological and optical properties is shown in Fig. 5.

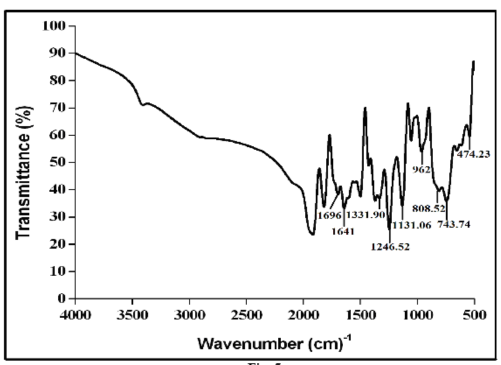

Fig. 5: FTIR spectrum of MgSe thin film coated at 400ºC.

The bands observed at 1696 and 1641 cm^{-1} correspond to asymmetric and symmetric stretching vibrations of carboxyl group (C=O). The bands observed at 1131, 1246.52 and 1331.90 cm^{-1} correspond to C-F stretching which may obscure any C-H bands present in the films. The presence of C and F are very much acknowledged from the EDS spectra. The bands observed in the 800-400 cm^{-1} regions correspond to C-X stretching (X = F, Cl, Br or I). The peaks observed at 1300 – 1420 cm^{-1} correspond to combination C-H stretching mode. The band observed at 962 cm^{-1} is the finger print evidence for the presence of Mg in the octahedral sites of the sample. Fingerprint peaks related to monophase MgSe are seen in the spectral region of 808 to 474 cm^{-1}.

4 Conclusion

The effect of substrate temperature on the properties of spray deposited MgSe thin films were investigated. XRD studies revealed that the films have a preferential orientation along the (2 0 0) plane. The size of the crystallites was approximately 17 – 22 nm for all the films. It was observed that film crystallinity increases with increase in substrate temperature. From the SEM images, it was observed that growth temperature largely governed the surface morphology of the MgSe films. Optical band gap was red shifted with increase in substrate temperature.

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