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OPTICAL STUDIES AND SEM ANALYSIS OF DOPED AND UNDOPED SILVER TELLURIDE THIN FILMS

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Abstract

Thin films of silver telluride of thickness between 25 nm to 150 nm were deposited on highly cleaned glass substrates at a high pressure better than 10⁻⁵ mbar. These films are doped with selenium by stack layer deposition method and annealed at 110°C for three hours. X-ray Diffraction Analysis (XRD) is used to confirm the structure of the thin films. Optical studies reveals that the optical band gap of silver telluride thin films was decreased with selenium doping, as the absorption decreases. High absorption coefficient in recorded spectra indicates the presence of direct band gap transition. The optical band gap is depending on the thickness of the films. The average crystal size decreased from 23nm to 17 nm with the doping. SEM images are reported in this report for the surface morphology and EDAX analysis for the elemental composition.

Keywords – Silver telluride, Stack layer, XRD, Optical band gap, Morphology.

1. Introduction –

The chalcogenides semiconductor compounds having excellent properties, they receive attention from both experimental and theoretical point of view. They have potential application in visible and infra-red

light emitting diodes, optical sensors and solar cells [1]. Optical studies on AgXTe₂ (X= Al, Ga, In) compounds developed on 77 K reported, they confirm the practical applications of AgXTe₂ in optical fibre communication and non-linear optics [2]. Ag₂Se_{0.5}Te_{0.5} having orthorhombic structure and it undergoes phase change to body centred cubic (BCC) around 400 K with increasing temperature [3]. They also reported that the thermoelectric properties of ternary chalcogenides Ag₂Se compound are superior to that of binary chalcogenides in the hole doped region. They have many current applications in optoelectronics, chemistry, optics and magnetic field etc. [4-5]. The structural transformation takes place in Ag₂Se with increase in temperature. Ag₂Se exists in two phases, β -Ag₂Se (at low temperature) and α -Ag₂Se (at high temperature) β -Ag₂Se and α -Ag₂Seused as a solid [6]. photosensitizes in photographic film and solid electrolyte in photochargable secondary batteries [7]. At room temperature $Ag_{2+\delta}Se$ and $Ag_{2+\delta}Te$ shows that the resistance of up to 200% in the magnetic field of 55 kOe, which are comparable with the colossal- magnetoresistance materials [8]. Ag2Se nanowires and ternary Ag₂Se_{1-x}Te_x nanowires were fabricated by electrochemical deposition method [9]. Crystalline β -Ag₂Sewas prepared in different shapes

by solvothermal reaction of silver carbonate and selenium at low temperature [10]. β -Ag2Se thin films prepared by pulsed-laser deposition have orthorhombic structure reported [11]. Optical study is an important tool to analyse the properties of semiconductor materials. In this report thin films of Ag₂Te and Ag₂Se_{0.3}Te_{0.7} of various thicknesses between 25 nm to 150 nm developed by thermal evaporation method and their optical properties discussed in detail. The optical band gap decreased with the doping of Se; this effect is explained by the possible reason.

2. Experimental Details

2.1. Thin film preparation

The Silver (I) telluride (Ag₂Te) in the form of powder and chunks are purchased from M/s Sigma Aldrich and used for the formation of thin films using technique Thermal vapour evaporation. The Ag₂Te thin films of thickness between 25 nm to 150 nm were thermally evaporated on highly cleaned glass substrates by evaporating the Ag₂Te pellets, placed in the molybdenum boat. The starting material is powder and chunks which is pelletized for evaporation. The deposition rate of 0.2nm/s is maintained in the chamber under a high pressure better than 10⁻⁵ mbar. High value current is passed in the molybdenum boat so that the material vaporises and sticks on the glass substrate [12]. Glass substrates are well cleaned by acetone and distilled water. These films are doped by selenium, the selenium powder convert in to the form of pellets, and process is repeated as mentioned above. The thickness and deposition rate are monitored by the digital quartz crystal thickness monitor. High vacuum thermal unit (Model BC-300 HHV) is used for depositing thin films.

2.2. Measurement procedure

The X-Ray plots of Ag₂Te and Ag₂Se_{0.3}Te_{0.7} thin films of different thickness is recorded and is used to confirm the structure of the thin films. The UV-Spectra is used to find the optical band gap of Ag₂Te and Ag₂Se_{0.3}Te_{0.7}thin films. Scanning Electron Microscopy (SEM) images are recorded to confirm the smoothness of the Ag₂Te and Ag₂Se_{0.3}Te_{0.7} film with the thickness of 100 nm. Energy Dispersive X-Ray Analysis (EDAX) for 100 nm thin film of Ag₂Te and Ag₂Se_{0.3}Te_{0.7} is also done for the elemental composition of silver telluride thin films.

The UV- Spectra study is carried out by UV-VIS NIR spectrophotometer (LAMBDA 750 Perkin Elmer) at room temperature. The XRD is carried out by X-Ray Diffractometer (Panalytical X Pert Pro). The SEM Images and EDAX are recorded by the Field emission gun SEM (FE-SEM 450).

3. Result and discussion

3.1 X-Ray Diffractogram studies

The X-Ray diffractogram studies of the silver telluride thin films with the variety of thicknesses are shown in Fig. 1. Fig. 1(a) shows the diffraction pattern for Ag₂TeThin films and Fig. 1(b) shows the diffraction pattern for Ag₂Se_{0.3}Te_{0.7} thin films. For the film with thickness of 25nm and 50nm, we did not observe any strong peaks, reveals its amorphous nature but for the film with thickness 100 nm and 150 nm we found some prominent peaks reveals its polycrystalline nature for the both thin films developed by thermal evaporation method. For the film with thickness 150 nm of Ag₂Te and Ag₂Se_{0.3}Te_{0.7}, the films have prominent peaks at 2Θ values. By comparing the recorded data with Pearson's crystal data, the structure of Ag₂Te thin films is found to exhibit cubic structure without any preferred orientations and the structure of Ag₂Se_{0.3}Te_{0.7}thin films is found to exhibit orthorhombic structure without any preferred orientations [13, 14].



Fig. 1(a): X-ray diffractogram of various thicknesses Ag₂Te



Fig. 1(b): X-ray diffractogram of various thicknesses Ag₂Se_{0.3}Te_{0.7}

The grain size of the thin films are calculated by the Debey - Scherrer relation

$$D = \frac{k\lambda}{\beta Cos\theta}$$

Where **D** is the grain size in nm, **k** is the Scherrer constant (0.94), λ is the wavelength, β is the half-maximum of the peak and θ is the diffraction angle. We have calculated grain size for most intense peak. The grain size of 150 nm thin film of Ag₂Te is 27 nm, while 150 nm thin

film of $Ag_2Se_{0.3}Te_{0.7}$ have 18 nm. The average grain size of Ag_2Te thin film is 23 nm and $Ag_2Se_{0.3}Te_{0.7}$ thin film has 17 nm.

3.2 UV Spectroscopy Studies

The Variations of absorption coefficient with the wavelength for Ag_2Te and $Ag_2Se_{0.3}Te_{0.7}$ films of various thicknesses is shown in the Fig. 2 the absorption coefficient is calculated by the relation-

$$\alpha = \frac{2.303 A}{t}$$

Here α is the absorption coefficient **A** is the absorbance and **t** is the thickness of the film. The graph reveals that all the films show more absorbance in the ultraviolet region corresponding to 350-450 nm spectral regions. The value of absorption coefficient is found to be of the order of 10^6 cm⁻¹, which means that direct band transition is there in the thin films. [15].



Fig. 2: Plot of Absorption verses wavelength for thin films of various thicknesses Ag₂Te and Ag₂TeSe.



Figure- 3(a). Plot of (ahv)² verses hv (eV) for thin films of various thicknesses Ag₂Te



Fig. 3(b) Plot of (αhv)² verses hv (eV) for thin films of various thicknesses Ag₂Se_{0.3}Te_{0.7}.

The optical measurements were performed using the UV- visible dual beam spectrophotometer. Fig. 3 shows the graph plotted between $(\alpha hv)^2$ on X-axis and the photon energy (hv) on the Y-axis as shown in the Fig. 3. This technique is sometimes referred as the Tauc plot. Fig. 3(a) shows the Tauc plot for Ag₂Te thin films and Fig. 3(b) shows the Tauc plot for Ag₂Se_{0.3}Te_{0.7} thin films of various thicknesses. For direct transition films such as silver chalcogenides, and assuming the parabolic bands the optical band gap was determined by plotting the graph between $(\alpha hv)^2$ and photon energy (hv). The direct band gap is obtained by the intersection of the slopes of Tauc plots on the X-axis. The relation between absorption coefficient and (α) and photon energy (hv) is given by the relation-

$$\alpha = \frac{k(hv - E_g)^{\frac{n}{2}}}{hv}$$

Where α is the absorption coefficient in cm⁻¹, hv is the energy in eV, E_g is the band gap in eV, n takes the value 2 for the indirect allowed band transition and $\frac{1}{2}$ for the direct allowed band transition. The optical band gap of Ag₂Te thin films is reported and it is to be varied from 1.63 eV to 1.61 eV. for the thickness 50 nm to 150 nm and for Ag₂Se_{0.3}Te_{0.7} thin films it is to be varied from 1.60 eV. to 1.58 eV. In this report the optical band gap of the doped sample is decreased with the doping and it is explained by the possible reason. In the past only few papers are dedicated to the optical studies on silver telluride thin films, and there is an uncertainty in band gap calculations. This report helps us to find the reliable optical studies of silver telluride thin films.

Damodardas and Karunakaran [16] have measured the electrical band gap of silver telluride thin films and it is varied from 0.02 eV to 0.08 eV. Dalven and Gill [17] have measured the band gap of silver telluride thin films by Hall coefficient measurement and it is found to be 0.064 eV. Appel [18] has measured the optical band gap of silver telluride thin films by transmission studies and it is found to be 0.7 eV. Prabhune and Fulari [19] calculated the band gap of silver telluride thin films by optical studies and it is reported 1.7 eV at room temperature

4. Conclusions

The authors conclude that thermal evaporation can produce Ag_2Te and $Ag_2Se_{0.3}Te_{0.7}$ thin films of high quality. Xray diffraction study confirm that crystal structure of Ag_2Te is cubic whereas that of $Ag_2Se_{0.3}Te_{0.7}$ is orthorhombic. The optical band gap of $Ag_2Se_{0.3}Te_{0.7}$ is less than that of Ag_2Te and its value is around 1.58eV.

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