Investigation of Properties of $Se_{(1-x)}Sb_x$ Heterostructure

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Received 27.10.2018 received in revised form 03.01.2019, accepted 05.01.2019

Abstract : $Se_{(1-x)}Sb_x$ Heterostructure of 200nm Nano Crystalline Thin Films with different stoichiometry ratio (x = 0.25 ,0.50 , 0.80) of Se:Sb have been deposited on glass substrate by thermal evaporation method under the vacuum of about 10^{-5} torr using vacuum coating unit under the deposition rate of 10 A^0/sec. Nano Crystalline thin films were kept at without annealed, annealed at 150^0 C and 200^0 C (for 1 hr) to examine the effect of annealing in recrystallization. It was observed that optical band gap decreases exponentially with increases the photon energy. It is observed that absorption coefficient in optical band gap decreases exponentially with increasing Sb content. UV- VIS NIR Spectrometer is used to measure optical properties of thin films. X-ray diffraction and scanning electron microscopy used to obtain comprehensive and consistent micro structural information.

Keywords – Optical band gap, Vacuum coating unit, UV-VIS NIR Spectrometer, comprehensive and consistent

1. INTRODUCTION

Se-Sb binary chalcogenide Thin Films due to the large absorption coefficient and compositional dependence of absorption. These materials may be suitable for solid state memory devices like Solar cells, photoconductors, alloys, glass production etc. Both have an indirect energy band gap varies between 2.50 eV to 1.753 eV. Literature shows so many methods for deposition of thin films such as thermal evaporation deposition, molecular beam epitaxial, organ-metallic, chemical vapour deposition, solution growth etc. The choice of the deposition method may be based on quality of the films required for specific applications [1-4]. Stoichiometry ratio of $Se_{(1-x)}Sb_x$ Thin Films with (x = 0.25, 0.50, 0.80) of different composition of Se_{75} $–Sb_{25}$, Se_{50} $–Sb_{50}$, Se_{20}– Sb_{80} deposited onto a glass substrate by thermal evaporation method under the vacuum of about 10^{-5} torr by the pallets using vacuum coating unit.

2. EXPERIMENTAL DETAILS

2.1 Materials & Methods

Selenium (Se) was purchased from Koch-Light laboratories LTD, Colebrook Berks England. Antimony (Sb) was purchased from Sigma Aldrich laboratories. Both the material has (99.99%) purity as powder form. For deposition the Se:Sb thin films on Glass substrate the powder was converted into small pallets with different stoichiometry ratio.

2.2 Synthesis

Thin film of $Se_{(1-x)}Sb_x$ has deposited using thermal evaporation method on a properly cleaned Glass plate as substrate of 1x1 cm^2 dimension. Initially clean the tungsten boat and chamber by acetone. The exact proportions of high purity (99.999%) Se and Sb elements powder in accordance with their atomic percentages were weighed using an electronic balance (LIBROR, -120) with the least count of 10^{-4} gm and made the pallets of Se:Sb Nano crystalline thin films with different stoichiometry ratio. The materials as a pallet form were placed in high resistive tungsten boat which was heated indirectly by passing high current through the electrodes. The temperature of the furnace was raised slowly at a rate of 3 - 4°C/minute. The Deposition rate was maintained at 4.4 – 7.6 Å/sec. The rate of thickness and evaporation rate of the as-deposited films was monitored using quartz crystal monitor which work as sensor. To achieve the metastable equilibrium the deposited thin films were kept inside the vacuum deposition chamber for 2- 3 hours. Thickness of the Se and Sb layer on glass substrate were controlled using quartz crystal monitor (“Hind Hivac” Digital Thickness Monitor Model–DTM–101).

2.3 Characterization

Structural characterization was done using Panalytical (Xpert-Pro) manufactured X-ray diffraction (XRD) unit & The surface morphology of thin films was analyzed by Nova Nano SEM 450 make scanning electron microscopy (SEM). Optical properties of the prepared thin films were studied by measuring the optical absorption spectra using by an ultra violet visible range UV-VIS spectrometer (Shimadzu Corporation make Probe 1800). The output absorbance can be recorded and printed out.

3. RESULT AND DISCUSSION

3.1 Optical Properties

The optical absorption of prepared Se/Sb thin films shown in Figure 1 for different Stoichiometry ratio of Se: Sb at different annealing temperature. By Fig.1. It was observed that absorption coefficient in Optical Band Gap decreases exponentially with increases wavelength of Photon (λ nm). The absorption edge of Se/Sb Nano Crystalline thin film is located in visible range i.e. from 580 nm to 620 nm. It may be due to increase in energy density because of higher concentration of Stoichiometry ratio of Se: Sb was further increases with annealing temperature. The band gap of the Se:Sb prepared thin film was calculated using Tauc's relation shown in Figure 2 and Table 1 for different stoichiometry ratio at different annealing temperature which shows that optical band gap decreases exponentially with Increases the Photon Energy (E_g).

Absorption is defined as $\log_{10}(I_0/I)$, where I_0 is the incident wavelength intensity and I is the transmitted wavelength intensity. So absorption coefficient (α) can be written as

$$\alpha = (1/d)\log_{10}(I_0/I) \quad (1)$$

Where d is the absorption path length [5, 6].

The absorption coefficient (α) [7] of the thin films was calculated by the absorbance data [8] at different photon energies (hv) and different temperature.

Table 1: Band gap calculated values of Se: Sb for different stichiometric ratio at various temperature

Stichiometric ratio	Optical Bandgap (eV)		
	RT	150^{o}C	200^{o}C
75:25	2.04	2.06	2.07
50:50	2.04	2.07	2.07
20:80	2.01	2.06	2.08

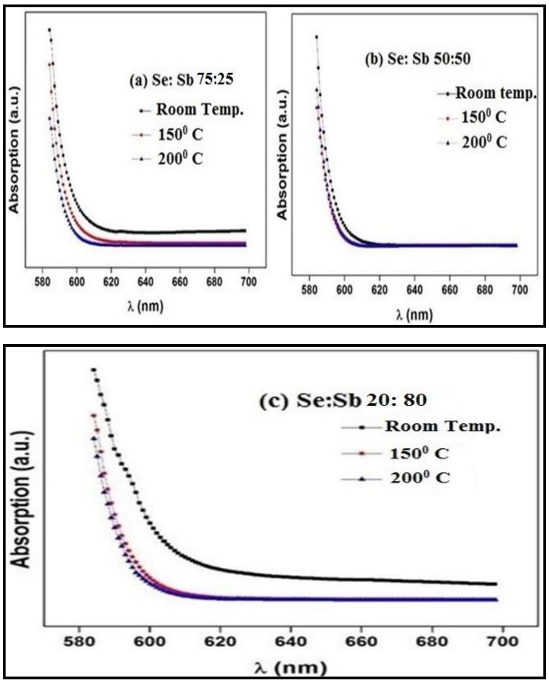

Figure 1: Optical absorption curves for different stichiometric ratio of Se:Sb hetero-structure thin films (a) 75:25 (b) 50:50 (c) 20:80

3.2 Structural Properties of the thin films

To identify the structure of the deposited thin films, X-ray diffraction method is used. The XRD patterns of the deposited and annealed $Se_{(1-x)}\ Sb_x$ thin films shown in Fig.3. The XRD spectrum exhibits the multiple characteristics peaks at 2θ. Further, no additional peak was observed for the annealed sample as compared to the as-deposited thin films, that indicating that no new interfacial phase was formed after annealing. It has also been observed that peak intensity increases with increase the annealing temperature. It is also observed that no crystallize phase appeared in without annealed thin films at room temperature which show amorphous nature of thin films. But after annealing crystallization phase appeared as the peak of Antimony Tri Selenide (Sb_2Se_3) at 150^{o} C and 200^{o} C and grain particles arrange in more crystalline form on surface of substrate which shows polycrystalline nature of thin films.

The SEM images of $Se_{(1-x)}\ Sb_x$ thin films at magnification 10 um shown in fig. 4 for (a) Without annealed thin films (b) Annealed thin films at 150^{0} C (c) Annealed thin films at 200^{0} C.

Without annealed thin films shows amorphous nature of thin films which indicate that granular particles grow on Glass plate substrate as spherical granular manner which show smoothness of the surface with polycrystalline nature of thin films. At without annealing granular particle connected to each other by covalent bonding between inter atomic particles due to this surface shows the smoothness of thin films [9]. But After annealing the surface morphology of thin films changed considerably which shows that big cluster and uneven lumps have appeared in spherical shape and are distributed on the entire surface [10]. These clusters may be formed due to the agglomeration of particles during to heat treatment. After annealing the covalent bonding between inter atomic particles respites and Selenium (Se) deposited into Antimony (Sb) and make compound of Antimony Tri Selenide (Sb_2Se_3). After annealing thermal vibration between inter atomic molecules increases due to it there observed lamped gaps between granular particles. According to these SEM images we may conclude that as-deposited thin films have partially amorphous structure while after annealing the thin films become polycrystalline in nature.

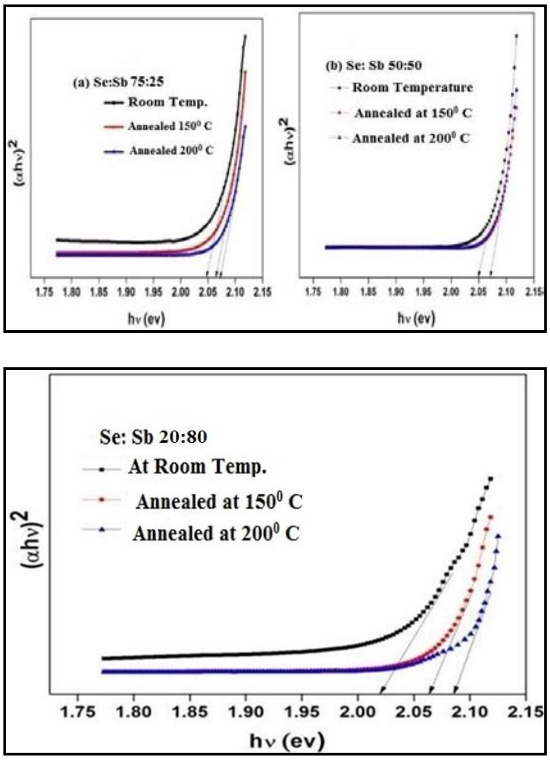

Figure 2: $(\alpha h\nu)^2$ vs hν (eV) curves for different stichiometric ratio of Se:Sb heterostructure thin films (a) 25:75 (b) 50:50 (c) 20:80

4. CONCLUSION

Thin films of Se $_{(1-x)}$ Sb_x of thickness 200 nm with different stoichiometry ratio were prepared on Glass substrate by thermal evaporation method under the vacuum of about 10^{-5} torr, using vacuum coating unit. A direct optical band gap between 2.04 eV to 2.01 eV is obtained at without annealing which shows that optical band gap decreases exponentially with Increases the photon energy (E_g) It was also observed that absorption coefficient in optical bandgap decreases exponentially with increase in wavelength of photon (λ nm). To find out the effect of recrystallization thin films of Se $_{(1-x)}$ Sb_x were annealed at 150^{o}C and 200^{o}C. The decrease in optical band gap with increase in Sb concentration may be due to the increase in the amount of disorder in the materials and increase in the density of defect states. Samples were studied by X-ray diffraction (XRD) and scanning electron microscopy (SEM) to obtain comprehensive and consistent micro structural information.

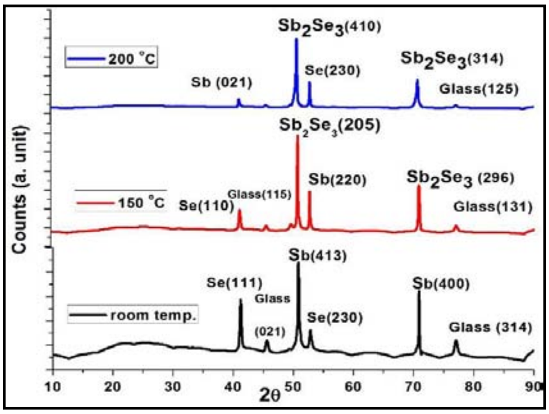

Figure 3: XRD spectra of thin films for 200 nm

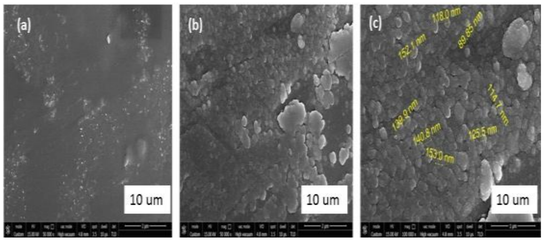

Figure 4: SEM analysis (a) For without annealed (b) Annealed at 150^{0}C (C) Annealed at 200^{0}C

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