



Correlation of some opto-electrical properties of Se–Te–Sn glassy semiconductors with the average single bond energy and the average electronegativity



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ABSTRACT

Studies of some electrical and optical properties of $\text{Se}_{90}\text{Te}_{10-x}\text{Sn}_x$ ($x = 2, 4, 6$ and 8) glassy alloys, in bulk and thin film forms, were performed at room temperature. Pellets of a diameter ~ 1.3 cm and different thicknesses ranging from 0.04 cm to 0.06 cm of these compositions were obtained. Measurements of *I*–*V* characteristics of these pellets have been carried out at room temperature. Ohmic behavior was observed in low voltage range (0–5 V) while a deviation from ohmic towards non-ohmic behavior was observed at higher voltage range (6–20 V). This deviation can be interpreted in terms of space charge limited conduction (SCLC) mechanism whereas the plots of $\ln(I/V)$ vs. *V* were found to be straight lines. The room temperature DC electrical conductivity σ_{DC} has been calculated from the linear region of the *I*–*V* characteristic curves. In addition, thin films of a thickness ~ 1100 Å of the alloys under investigation were prepared and the optical band gap E_{opt} of these thin films is obtained from Tauc plot $(\alpha h\nu)^2 = B(h\nu - E_{opt})$ after the determination of the absorption coefficient α over a wavelengths range of 440–1100 nm. Analysis of the experimental data shows that σ_{DC} increases while E_{opt} decreases with increasing Sn content. These results are explained in terms of the decrease in the values of average single bond energy $H_S/\langle r \rangle$ and average electronegativity χ_m .

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1. Introduction

Electrical and optical properties of chalcogenide glasses have attracted a great deal of scientific attention since the discovery of the unique phenomenon of reversible switching in certain types of these glasses in 1968 [1]. Several efforts have been made, from that time, to develop suitable chalcogenide materials for electronic and optoelectronic applications. Chalcogenide glasses are generally semiconductors with band gap energies of 1–3 eV, opaque through the visible spectrum and to begin transmission from 2 to 14 μm . These properties make these materials suitable in several applications such as CO_2 laser (10.6 μm) radiation delivery for photovoltaics, infrared sensors, optical fiber communication systems over super long distances, industrial cutting/welding applications and also for microsurgery [2–5]. In addition, chalcogenide alloys have several applications in very exciting fields like x-ray imaging, photonics, acousto-optic devices, solid state optical limiters, solid state switching devices, optical memory devices, inorganic photo-

receptors, solar cells, bio-chemical sensing and holographic recording systems [6–9]. Wide window for improvement of chalcogenide glasses is still open and nowadays research focus has been shifted towards nano-sized chalcogenide materials.

Undoped a-Se usually suffers from thermal instability, aging effects, and low electrical conductivity, due to phase transformation and structural relaxations even in normal ambient conditions as it has a low glass transition temperature [10]. The addition of Te to Se overcomes some of these disadvantages and causes structural changes in the material which in turn modify band structure and hence electrical properties [11]. Moreover, addition of metallic or semi metallic elements (like Sn in this study) is used to improve the properties of pure chalcogen elements or chalcogenide compounds. The effect of an impurity in an amorphous semiconductor may be widely different, depending upon the conduction mechanism and the structure of the material. In crystalline semiconductors the effect of a suitable impurity is always to provide a new donor or acceptor state and this is not essential in amorphous semiconductors. Instead of providing a localized impurity level in the forbidden gap, an impurity may merely alter the mobility of the charge carriers or may introduce structural changes

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in amorphous material with or without modification of the localized states in the forbidden gap [12].

The current–voltage characteristic is an important tool for analyzing the different conduction processes operative in chalcogenide glasses. Several models were proposed to explain the non-linearity in the I – V curves of these materials such as Poole–Frenkel effect [13,14], small polaron conduction [15], tunneling conduction [16], hopping conduction [17] and space charge limited conduction [18,19]. Chalcogenide glasses generally exhibit p-type electrical conduction owing to the fact that the number of electrons excited above the conduction band mobility edge is smaller than the number of holes below the valence band mobility edge [20]. It has been observed [21–26] that when certain heavy metallic additives (like Bi or Pb) are added to Se–Ge or Se–In glasses, the number of holes decreases in these systems, while the number of electrons increases. These two effects together shift the Fermi level towards the conduction band and a remarkable change from p-to n-type conduction results.

The study of the optical absorption spectra in chalcogenide glasses provides essential information about band structure and band gap energy [27]. The optical band gap (E_{opt}) of amorphous semiconductors is usually determined using the Tauc plot $\alpha hv = B(hv - E_{opt})^m$ [28,29]. In addition, conductivity (DC or AC) measurements have been widely used to investigate the nature of defect centers in disordered systems since it is assumed that they are responsible for the type of conduction. This in turn determines the field in which a particular glass can be used. It is well known [20] that the dependence of band tail on the absorption spectra of amorphous materials is usually related to the distribution of localized states in the valance band tail which is sensitive to the structure and disorder level in the material. In addition, the electrical properties of amorphous materials are sensitive to charge defects with energy levels inside the forbidden gap which can be affected by doping. Therefore, the dependence of the optical band gap and the electrical conductivity on the structure of chalcogenide glasses is very important for better understanding of transport mechanisms. The average coordination number and the heat of atomization have been conducted to characterize the glassy network. There were lots of investigations [30–37] that related the optical band gap and the electrical conductivity with chemical composition using these two parameters. Moreover, the optical band gap and the electrical conductivity are found to be correlated with the average electronegativity of the glassy alloy. In the present work, the DC conductivity at room temperature and the optical band gap (E_{opt}) of some Se–Te–Sn glassy alloys were measured. The composition dependence of these parameters was investigated through the correlation with the average coordination number, the average heat of atomization, and the average electronegativity.

2. Experimental details

Glassy alloys of $Se_{90}Te_{10-x}Sn_x$ ($x = 2, 4, 6$ and 8) were prepared by the conventional melt quenching technique that described elsewhere [38]. To ensure the glassy nature, X-ray diffraction of the prepared samples were done and given in Fig. 1.

Disc shaped samples (pellets) of a diameter ~ 1.3 cm and different thicknesses ranging from 0.04 to 0.06 cm were obtained by grinding the alloy to a fine powder and then compressing it in a die at a load of about 5 tons. For measurement of the DC electrical conductivity, pellets were mounted in between a specially designed sample holder consists of two copper electrodes of identical size and shape. The pellets were coated with silver paint to ensure good electrical contact between the samples and the electrodes. DC voltage, ranging from 0 to 20 V, was applied across the samples at room temperature and the resultant current was measured by a

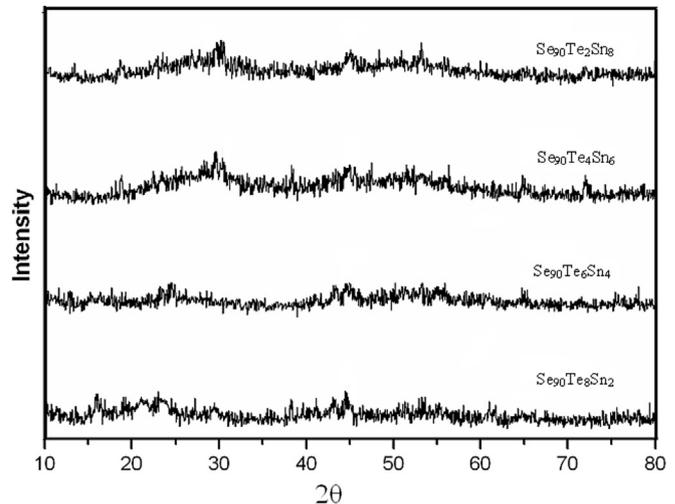


Fig. 1. XRD patterns of $Se_{90}Te_{10-x}Sn_x$ ($x = 2, 4, 6$ and 8) glasses.

digital electrometer (Keithley 6430) in order to obtain the I – V characteristic curves. For optical measurements, thin films of a thickness ~ 1100 Å of glassy alloys of bulk $Se_{90}Te_{10-x}Sn_x$ ($x = 2, 4, 6$ and 8) were deposited on a well cleaned glass substrate, at a rate of 4 nm/s, by vacuum evaporation technique, keeping the substrate at room temperature and in a vacuum of 2×10^{-5} Torr using a molybdenum boat. The film thickness was accurately controlled using a single crystal thickness monitor. A double beam (Cintra-10) UV–VIS spectrophotometer, coupled with personal computer, was used to find the variation of the reflectance and transmittance with wavelength, which in turn were used to calculate the absorption coefficient and the optical band gap of the prepared films. The measurements were carried out at room temperature, with wavelength in the range 440–1100 nm.

3. Results and discussion

3.1. Room temperature I – V characteristics and DC electrical conductivity

The resultant current–voltage (I – V) curves for $Se_{90}Te_{10-x}Sn_x$ ($x = 2, 4, 6$ and 8) glassy samples in the voltage range (0–20 V), recorded at room temperature ($T = 300$ K) are shown in Fig. 2 and Fig. 3. It is observed, from these figures, that the studied samples showed linear (ohmic) behavior in low voltage range (0–5 V). However, at higher voltage range (6–20 V), they deviate from linearity (i.e. a non-ohmic behavior is observed). In order to understand qualitatively this trend, the whole mechanism will be divided into two parts. First one is related to the linear region from which the room temperature DC electrical conductivity of the studied samples can be calculated. The second one is related to the non-linear region of the I – V characteristics at higher applied voltages (higher electric field). Here, this non-linearity will be explained according to a suitable model.

DC electrical conductivity can be found, at a given temperature, using the following well known relation:

$$\sigma_{DC} = \frac{1}{\rho_{DC}} = \frac{L}{RA} \quad (1)$$

where R is the resistance, L is the thickness, A is the cross-sectional area and ρ_{DC} is the resistivity of the studied sample. The room temperature (R) for all samples was calculated from the slopes of

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