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Bond Formation Perspective: Effect of Sn Addition in Se-Te-Sn Chalcogenide Glasses

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Article

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ABSTRACT

The aim of this study is to investigate the effect of Tin (Sn) addition on Band gap (Eg) and Dc conductivity of Se-Te-Sn semi-conducting glasses. This is an effort towards the understanding of physics of temperature dependence of dc electrical volume conductivity of Se$_{75}$Te$_{25-x}$Sn$_x$ (X= 2, 4, 6 & 8) glasses in bulk form. These Chalcogenide glasses were prepared by melt quenching (rapid cooling of melt) technique. The amorphous nature of as prepared glass was confirmed by XRD. Using Keithley Electrometer / High resistance Meter 6517 A, the I-V characteristics of these glasses have been recorded in a temperature range from room temperature to 100˚C. Additionally, the Poole-Frenkel conduction mechanism has also been verified in order to investigate the good agreement with the established fact that most of Chalcogenide glasses obey Poole-Frenkel conduction mechanism. To calculate the Band gap, with the help of Ocean Optics Spectrophotometer, absorption spectra has been recorded. Analysis of these absorption spectra using Tauc relation reveals that these glasses are semiconducting and direct band gap material.

INTRODUCTION

The most promising properties of chalcogenide glass have been found to deteriorate drastically during crystallization. The addition of Sn as third element in Se-Te system expands the glass forming area and also creates compositional and configurational disorder in the system. The lattice perfection and the energy band gap of the material play a major role in the preparation of the device for a particular wavelength, which can be modified by the addition of dopants [1, 2]. It has been reported that Sn may affect the density of states in a very effective way, if it is incorporated in parent binary Se-Te system during the preparation of ternary glasses [3,4,5].

EXPERIMENTAL TECHNIQUES AND METHODS

The glasses of desired composition i.e. Se$_{75}$Te$_{25-x}$Sn$_x$ (x = 2, 4, 6 & 8) [6]have been prepared by melt quenching technique. To confirm the amorphous nature of these samples, XRD characterizationhas been carried out using Bruker DX8 Advance machine with Cu K_α (λ = 1.5406 Ǻ) radiation. For I-V measurements in bulk, pellets of 12 mm diameter and thickness ≈ 1mm have been prepared under a load of 5 tons. These pellets (bulk) have been used in circuitry of Keithley Electrometer 6517A in order to record the I-V characteristics, in a temperature range from room temperature to 100°C. The thin films of Se-Te-Sn glasses have been prepared using Vacuum Coating Unit which is used for band gap calculation [7]. Using Tauc relation, the band gap has been calculated from absorption spectra, recorded by Ocean Optics Spectrophotometer.

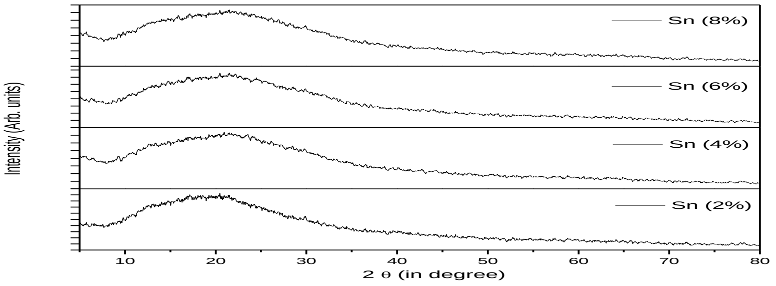
RESULTS AND DISSCUSSION

Absence of any sharp peak in XRD patterns of these samples, confirm their amorphous nature. Figure 1 shows the XRD patterns of these samples.A broad hump on lower angles confirms the presence of Short Range Ordering (SRO) in glasses.

I-V characteristics of Se$_{75}$Te$_{25-x}$Sn$_x$ (x = 2, 4, 6 & 8) glassy pellets were carried out in a temperature range from room temperature to 100 ˚C. These characteristics are shown in figure 2 at different temperatures for Se$_{75}$Te$_{19}$Sn$_6$glass, as representative case.

Semi-conducting nature of these samples has been confirmed in these I-V curves, as it is clearly evident in these curves that conductivity is increasing with the increasing temperature; a very basic fact. The dc conductivity was calculated using the slope of I-V curves of these samples at 0.1 volt. The variation in conductivity (in /Ω.mm) with respect to Sn content in the SeTeSn glassy system at different temperatures is shown in figure 3.

Figure 1: XRD patterns of $Se_{75}Te_{25-x}Sn_x$ (x = 2, 4, 6 & 8) glasses.



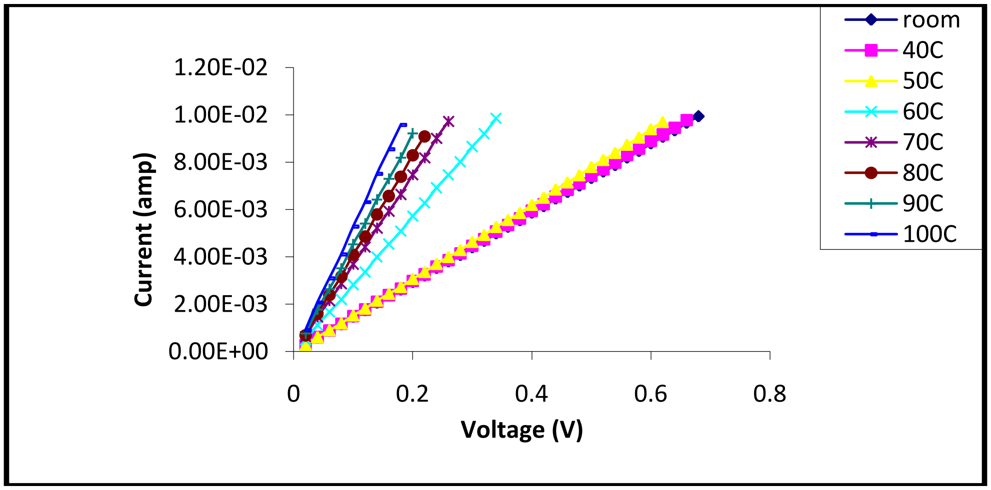


Figure 2:I-V Characteristics of $Se_{75}Te_{19}Sn_6$ glass at different temperatures, a representative case.

It can be inferred from figure 3 that $Se_{75}Te_{19}Sn_6$ glass has the maximum conductivity in comparison to the other counterparts of the series i.e. it offers minimum resistance to the current compared to other candidates under test. This variation in conductivity with respect to the composition can be explained on the basis of formation of bonds between Se-Sn and Te-Sn.

The structure of Se-Te binary glasses is a mixture of Se_8 member rings (having strong covalent bond), Se_6Te_2 mixed rings and Se-Te co-polymeric chain [8]. The addition of Sn in Se-Te system changes the configuration by forming Sn-Te cubic and $SnSe_2$ tetrahedral phase and decreases the concentration of Se_8 member rings resulting the increase in conductivity. When Sn is added to the Se-Te system, it makes the bonds with both Se and Te. The bond energy of Sn-Se bond is 402.8 kJ/mol and of Sn-Te bond is 320.5 kJ/mol[9]. The effect of increasing concentration of Sn-Se bonds, having higher bond energy than Sn-Te bonds, is reflected as the increase in conductivity of these glasses as we increase Sn content from 2 at. Wt.% to 6 at. wt.% in Se-Te-Sn system, as shown in figure 3.

Plots of Ln (I) with respect to $V^{1/2}$ were taken into account in order to verify the Poole-Frenkel (P-F) conduction mechanism in these glasses.

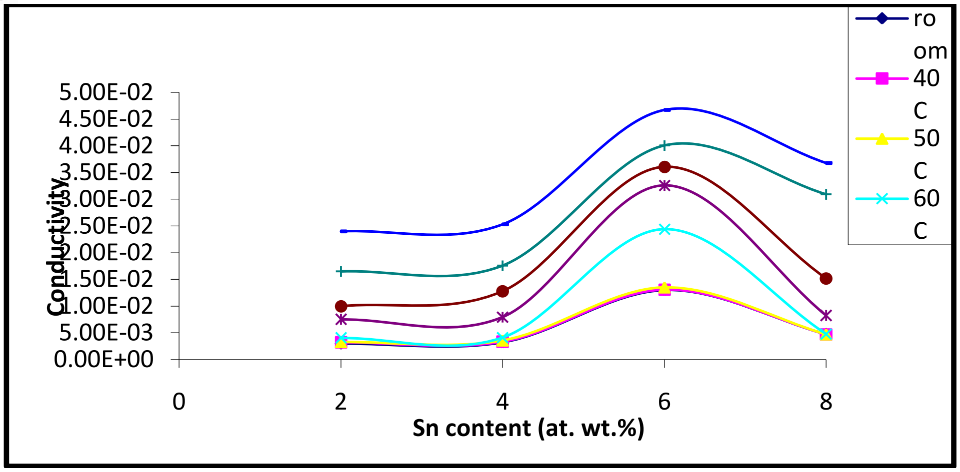


Figure 3:Variation of Conductivity (/Ω.mm) against composition at different temperatures.

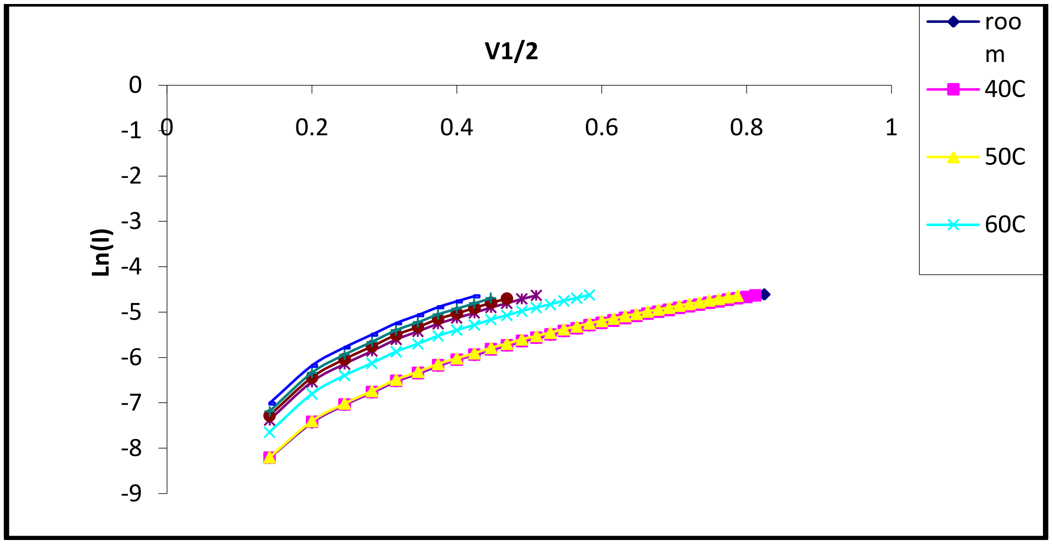


Figure 4: Verification of P-F conduction in $Se_{75}Te_{19}Sn_6$ glass at different temperatures.

The linearity of Ln(I) vs $V^{1/2}$ curves in figures 4 (a representative case) is suggestive of the fact that the conduction in these glasses is also of Poole-Frenkel type i.e. localized states produced by addition of Sn in these Se-Te-Sn glasses play an important role in conduction.

The band gap of Se-Te-Sn films has been calculated from the absorption spectra, recorded by Ocean Optics Spectrophotometer, using Tauc relation[10]. Figure 5 shows the absorption spectra, for $Se_{75}Te_{25-x}Sn_x$ glassy films.

When content of Sn is increased in the Se-Te-Sn system, Sn makes bonds with both Se and Te. Since Sn is added at the cost of Te hence the concentration of Sn-Se bonds (bond energy 402 kJ/mol) increases as compared to Sn-Te bonds (bond energy 320.5 kJ/mol) [9] causing the decrease in band gap uptoSn 6 at. wt.% in the sample. At Sn 8 at. wt. % band gap increases and this increase in band gap can be attributed to the changes occurred during the film preparation. Figure 6 shows the band gap calculation using Tauc relation, as $(\alpha h\nu)^2$ is plotted against hν (energy) for $Se_{75}Te_{25-x}Sn_x$ glassy films. Table 1 lists the calculated band gap of $Se_{75}Te_{25-x}Sn_x$ glasses.

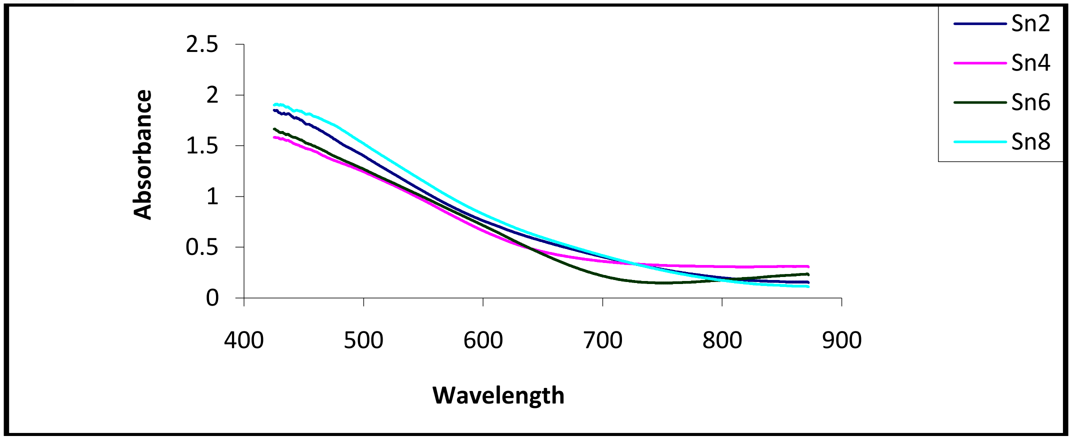


Figure 5:Absorption spectra of $Se_{75}Te_{25-x}Sn_x$ (x = 2, 4, 6 & 8) glasses.

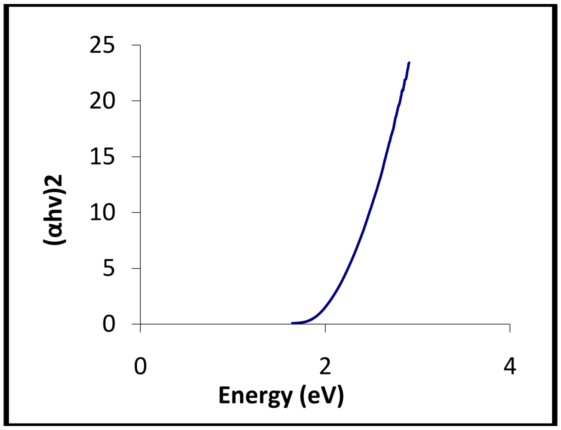


Figure 6: Band gap calculation for $Se_{75}Te_{19}Sn_6$ glass.

Table 1: Band gap of $Se_{75}Te_{25-x}Sn_x$ (x = 2, 4, 6 & 8) glasses.

S. No.	Composition of glass	Band gap (eV)
1.	$Se_{75}Te_{23}Sn_2$	2.175
2.	$Se_{75}Te_{21}Sn_4$	2.171
3.	$Se_{75}Te_{19}Sn_6$	2.108
4.	$Se_{75}Te_{17}Sn_8$	2.112

CONCLUSION

The detailed discussions in the paper can conclude the facts that the presented series of Chalcogenide glasses (Se-Te-Sn) is semi-conducting in nature, which can be observed from I-V characteristics. The effect of increasing concentration of Sn-Se bonds, having higher bond energy than Sn-Te bonds, is reflected as the increase in conductivity of these glasses as we increase Sn content from 2 at. wt. % to 6 at.wt. % in Se-Te-Sn system. The composition $Se_{75}Te_{19}Sn_6$ can be considered as the most chemically ordered critical composition at which the system possesses the highest concentration of Sn-Se bonds. As we go beyond 6 at. wt. % ofSn in the system, there may be a possibility of small clustering of Sn in the system that can act as scattering centers for carriers resulting the decrease in conductivity. The linearity of Ln (I) vs $V^{1/2}$ curves is in good agreement with the fact that these glasses obey Poole-Frenkel conduction mechanism. The variation in band gap of these glassy films can be explained on the basis of bond formation between Se &Sn and Te&Sn. The observed value of the band gap supports the dc conductivity data.

REFERENCES

1. Marquez E, Wagner T, Leal -Gonzalez, Bernal-Olive AM, Prieto-Alion R, Jimenez-Garay R, Ewen PJS. J Non-Cryst Solids.2000; 274:62.
2. Tripathi SK, Sharma V, Thakur A, Sharma J, Saini GSS, Goyal N. Effect of Sb additive on the electrical properties of Se-Te Alloy. J Non-Cryst Solids.2005; 351:2468.
3. Calventus Y, Surinach S, BaroMD. Crystallization mechanisms of a $Se_{85}Te_{15}$ glassy alloy. J Phys Cond Matter. 1996; 8:927.
4. Hagen SH, Derks PJA. Photogeneration and optical absorption in amorphous Se-Te alloys. J Non-Cryst Solids. 1984; 65:241.
5. Parthasarathy G, Gopal ESR. Electrical conduction in bulk $Se_{1-x}Te_x$ glasses at high pressure and at low temperature.Bull Mater Sci.1984;6:231.
6. Maharjan NB, Singh K, Saxena NS. Calorimatric studies in $Se_{75}Te_{25-x}Sn_x$Chalcogenide glasses. Phys Stat Sol (a). 2003; 195:305.
7. Hata David M. Introduction to Vacuum technology, Prentice Hall, (2008)
8. Mehra RM, Kaur Gurinder, Mathur RC. Crystallization kinetics of bulk amorphous $Se_{80-x}Sb_xTe_{20}$J Mater Sci1991; 26:3433.
9. LideDR.70th edition: CRC Handbook of Chemistry and Physics, (1995-1996).
10. Stephen Brunauer. Volume 1: Physical absorption, Princeton University Press, (1943).