WebLog Journal of Materials Science and Engineering

Research Article
Published: 22 Jan, 2026

Studies of Physical Parameters of $Se_{90-x}Te_5Sn_5In_x$ (0≤x≤9) Chalcogenide Glasses

*Dr. Sunil Kumar**

Department of Physics, Government Post Graduate College, Bisalpur, Pilibhit 262201 U.P. India

WebLog Open Access Publications
Article ID : wjmse.2026.a2204
Author : Dr. Sunil Kumar

Abstract

Chalcogenide glasses are of huge attention due to these intriguing optical and electrical characteristics. The physical parameters of $Se_{90-x}Te_5Sn_5In_x$ (0≤x≤9) glassy alloys have been thoroughly examined in this work. In this system I have theoretical evaluated density (ρ), molar volume (V_m), lone pair of electrons (LP), average coordination number <Z>, number of constraints (N_c) and mean bond energy <E> for this system. The evaluated values of V_m, LP, and stoichiometry (R) fall with increasing In content or average coordination number. Because indium has a larger atomic mass and stronger bonding properties than selenium, an increase in density was seen as the amount of indium increased. On the other hand, molar volume exhibited a declining trend, suggesting improved structural rearrangement and compactness within the glass network.

Keywords: Density; Molar Volume; Compactness; Mean Bond Energy

Introduction

Because of their unique thermal, electrical, and optical characteristics, chalcogenide glasses (ChGs) which are mostly made of chalcogen elements like Te and Se form a significant family of amorphous materials. These materials can be used in infrared optics, optical switching, and non-volatile memory systems due to their, high refractive index, wide infrared transparency, variable band gaps and low phonon energy [1, 2, 3]. These glasses presently used primarily in X-ray imaging (Se based semiconducting glasses) and in TV pickup tubes (as photoconductors) are mainly interesting. Applications in science and technology have recently focused on Se–Te-based glassy semiconducting alloys. ChGs presently significant challenges when utilized as a recording layer in optical phase change devices with compositional changes [6, 7]. Although pure selenium has poor mechanical strength, low thermal stability, and aging effects, selenium-based glasses are especially appealing due to their high photosensitivity and strong glass-forming ability [6]. Selenium is frequently alloyed with other elements to get around these restrictions. Because tellurium has a narrower band gap and is more polarizable than selenium, it improves electrical conductivity and infrared transmission. When the third element tin (Sn) is introducing into Se-Te system becomes compositional and configurational disordered. The electrical and optical properties of the Se-Te system may be considerably changed by the addition of Sn [8]. Establishing structure-property correlations and improving these materials for advanced optoelectronic and memory applications require a thorough grasp of these factors.

Additionally, the presence of metallic impurities induces instability in the arrangement and composition of the glassy alloys and expands glass-forming area. The temperature at which glass transition of the system is raised when the Indium is added beside with the stand-in of Se; each impurity atom of Indium attempts to adapt to the environment of its nearest neighbor in Se, thus it seems to have minimal influence of the glassy alloys [9]. Though, a new research reveals that the characteristics of ChGs are greatly impacted by the inclusion of metallic impurity [10]. There has been a consistent change in the physical properties as the chemical composition changes. The ordered bond network (OBN) model, sometimes referred to as the (CONM) chemically ordered network model, is typically used to explain how compositional variation affects the physical characteristics of ChGs. In order to clarify the function of indium in altering the glass network structure, the $Se_{90-x}Te_5Sn_5In_x$ (0≤x≤9) glassy alloys carefully examine the impact of indium content on their physical properties.

Preparation Technique for the Synthesis

Using an electronic microbalance with high-purity elemental selenium (Se), tellurium (Te),

OPEN ACCESS

Correspondence:
Dr. Sunil Kumar, Department of Physics, Government Post Graduate College, Bisalpur, Pilibhit 262201, Uttar Pradesh, India, Tel: +91 9454350485; E-mail: skcbhu07@gmail.com

Received Date: *31 Dec 2025*
Accepted Date: *20 Jan 2026*
Published Date: *22 Jan 2026*

Citation:
Sunil Kumar. Studies of Physical Parameters of $Se_{90-x}Te_5Sn_5In_x$ (0≤x≤9) Chalcogenide Glasses. WebLog J Materials Sci Eng. wjmse.2026.a2204. https://doi.org/10.5281/zenodo.18448256

Table 1: Different theoretical evaluated physicochemical parameters of multi-component $Se_{90-x}Te_5Sn_5In_x$ (0≤x≤9) chalcogenide glasses.

Composition	<Z>	N_α	N_β	N_c	f	Density (g/cm³)	Molar Volume (cm³/mol)	<E> Kcal/mol	L= V-<Z>	δ	R
$Se_{90}Te_5Sn_5$	2.10	1.05	1.2	2.25	0.251	5.01	16.64	50.51	3.8	-0.002	9.5
$Se_{87}Te_5Sn_5In_3$	2.13	1.07	1.26	2.33	0.226	5.08	16.62	51.39	3.68	0.0021	6.34
$Se_{84}Te_5Sn_5In_6$	2.16	1.08	1.32	2.4	0.200	5.15	16.60	52.41	3.56	0.0023	4.68
$Se_{81}Te_5Sn_5In_9$	2.19	1.1	1.38	2.48	0.175	5.23	16.56	53.53	3.44	-0.001	3.66

tin (Sn), and indium (In) were weighed in accord with their atomic percentages with a purity of 99.999%. To avoid oxidation during melting, the weighed elements were properly mixed and sealed in evacuated quartz ampoules (inner diameter 8 mm, length 12 cm) at a vacuum of around 10^{-4} to 10^{-5} Torr. The ampoules were put in an electric furnace to progressively heat up to1098 K. The ampoules were kept at this temperature for ten to twelve hours in order to facilitate the melting and uniformity of the alloys. The ampoules were often shaken or rotated to guarantee uniform mixing and chemical homogeneity of the melt. Ice-cooled water was used to instantly quench ampoules. Quick quenching keeps the material amorphous and stops crystallization. The prepared material amorphous nature was demonstrated by X-ray diffraction (XRD) [11]. A Shimadzu DSC-60 Model differential scanning calorimetry (DSC) device was used to analyze the thermal behavior of each sample. For the observations, 10 mg of the crushed material was heated in standard aluminum pans at several rates (5 to 20 K/min). Both the observed glass transition speeds under non-isothermal circumstances and the heat that was collected or released during phase transitions were computed using a DSC. The DSC instrument was calibrated before to observations using high pureness standards for Sn, Pb, and In with defined melting points. The microprocessor of the thermal analyzer can measure heat runs with an accuracy of ±0.01 mW and temperatures with an accuracy of ±0.1 K.

Result and Discussion

The structural variations in the multi-component glasses may be described by using the idea of average coordination number. The formulas may be used to get the multi-component glasses' average coordination number [12, 13, 14, 15].

$$<Z>=\frac{\left(pM_{Se}+qM_{Te}+rM_{Sn}+sM_{In}\right)}{\left(p+q+r+s\right)}$$

According to the literature, the (CN) coordination numbers of Se, Te, Sn, and In are $M_{Se} = 2$, $M_{Te} = 2$, $M_{Sn} = 4$, and $M_{In} = 3$, respectively. The symbols p, q, r, and s represent the at. wt. % of the elements in the glassy matrix. From above equation may be used to get the <Z> for glassy $Se_{90-x}Te_5Sn_5In_x$ (0≤x≤9) systems with In = 0, 3, 6, and 9. The results are 2.1, 2.13, 2.16, and 2.19, respectively.

The structural variations in the multi-component glasses may be Covalent solids exhibit bond-stretching and bond-bending (α-forces and β-forces). For each atom, the Lagrangian bond-stretching constraints number is found using equation (1).

$$N_\alpha=\frac{<Z>}{2}\text{..........................(1)}$$

Equation (2) determines the bond bending constraints

$$N_\beta=2<Z>-3\text{..........................(2)}$$

The sum of the bond bending and bond stretching constraints is known as the number of constraints (N_c). The following formula [16] can be used to get the average coordination number (effective):

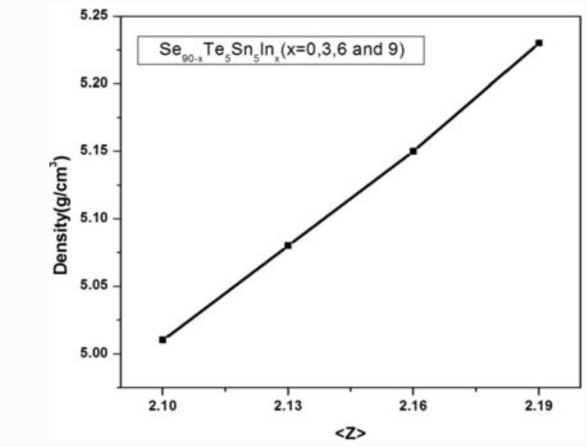

Figure 1: Density against average coordination number of $Se_{90-x}Te_5Sn_5In_x$ (0≤x≤9) glassy system.

$$<Z_{eff}>=\frac{2(N_c+3)}{5}\text{.............................(3)}$$

Maxwell and Thorpe [12] used counting to estimation the amount of restrictions. The calculation for the degree of freedom (*f*) results from taking this counting into account [16]:

$$f=2-\frac{5<Z>}{6}\text{...............................(4)}$$

Table 1 lists the calculation of *f* for changing In composition at the expense of Se, Te, and Sn. With increasing In content in the STSI system, the value of *f are* decreasing, indicating that the system becomes more stiff at 9 at.wt% of Indium

Evaluation of density (ρ), molar volume (V_m) and compactness (δ)

Density is a physical parameter that evaluates the system's stiffness. This is also related to the system <Z>. The following relation [17] can be used to compute it:

$$\rho=\left(\sum\frac{m_i}{d_i}\right)^{-1}\text{.....................(5)}$$

where m_i and d_i denote mass and density of i^{th} structural unit.

Tables 1 show the density (ρ) values for several glassy alloys of $Se_{90-x}Te_5Sn_5In_x$ (0≤x≤9) multi-component systems. Figure 1 represents the variation of density for STSI glassy alloys. The molar volume is computed using the relation [17] and the density value found in Eq. (5):

$$V_m=\frac{\sum x_iM_i}{\rho}\text{......................(6)}$$

Here, M_i and x_i is the atomic mass and atomic fraction of i^{th} component respectively. Tables 1 provide the calculated values of V_m for $Se_{90-x}Te_5Sn_5In_x$ (0≤x≤9) multi-component glasses. Figure 2 displays molar volume graphs vs average coordination number for STSI glassy system. This image makes it evident that the growing

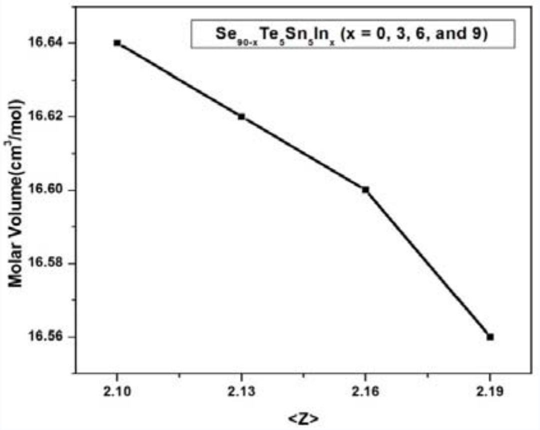

Figure 2: Molar Volume against average coordination number of $Se_{90-x}Te_5Sn_5In_x$ (0≤x≤9) glassy system.

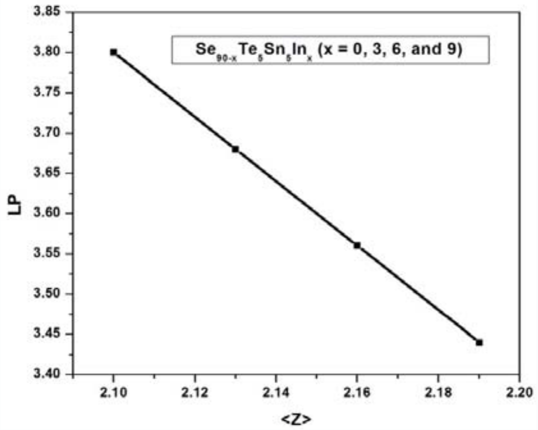

Figure 3: Loan pair electrons against average coordination number of $Se_{90-x}Te_5Sn_5In_x$ (0≤x≤9) glassy system.

molar volume sequence is exactly the reverse of the density sequence (From Figure 1). In theory, density and volume are inversely related. This fact is evident from the graphs displayed in Figure 2. Compactness (δ) can be used to determine the given formula [18, 19]:

$$\delta = \frac{\sum \frac{c_i A_i}{\rho_i} - \sum \frac{c_i A_i}{\rho_i}}{\sum \frac{c_i A_i}{\rho_i}} ....(7)$$

Here, ρ_i, c_i, and A_i represent the atomic density, atomic fraction, and atomic weight of the ith element for glassy alloys. Tables 1 list the computed values of δ. The compactness of glasses have resolute by measure the normalized change in mean atomic volume, that is an indication of the chemical relations between the elements that make up the glassy system [7].

Calculation of Lone pair electron (LP)

The lone-pair electron (LP) has been intended by given formula [17]:

$$LP = V - \langle Z \rangle ....(8)$$

In this case, V denotes the valence electrons that are equivalent to unshared lone-pair electrons. Table 1 lists the assessed LP values for multi-component glasses. Figure 3 shows variation of LP vs average coordination number for STSI glassy alloys.

Stoichiometry deviation R and Mean Bond Energy <E>

The stoichiometry deviation is made known by the parameter R. It is determined by comparing the chalcogen atom's covalent bonding capabilities to those of a non-chalcogen atom. The method for determining the R values of $Se_aTe_bSn_cIn_d$ quaternary alloys has been explained in [20].

$$R = \frac{bN_{Te} + dN_{In}}{aN_{Se} + cN_{Sn}} ....(9)$$

Here, a, b, c, and d stand for the atomic fractions of Se, Te, Sn, and In, respectively. When In is substituted for Se, the value of R rises, indicating that the system is more in chalcogen (Table 1). Figure 3 shows variation of R against <Z> for STSI glassy system.

Bond type, network bond energy, average coordination number, and cross-linking all affect mean bond energy [20]. The mean bond energy is equal to the average cross-linking per atom (heteropolar bonds) plus the average bond energy per atom of the remaining matrix.

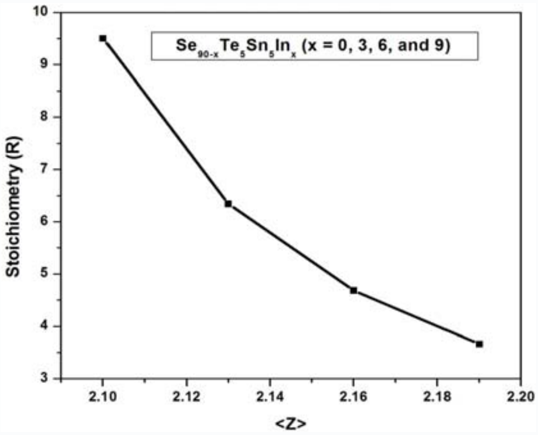

Figure 4: R parameter against average coordination number of $Se_{90-x}Te_5Sn_5In_x$ (0≤x≤9) glassy system.

$$\langle E \rangle = \langle E_c \rangle + \langle E_{rm} \rangle ....(10)$$

For present semiconductors, may be expressed as

$$\langle E \rangle = aN_{Se}E_{Se-Te} + cN_{Sn}E_{Sn-Te} + dN_{In}E_{Te-In} ....(11)$$

Above relation is used to compute the bond energy values of heteropolar bonds. Se-Te, Sn-Te, and Te-In bond values were determined to be 170 kJ/mol, 320.5 kJ/mol, and 218 kJ/mol, respectively [21]. The contribution resulting from weaker links, or , can be computed as follows: The contribution resulting from weaker links, or , can be computed as follows:

$$\langle E_{rm} \rangle = \frac{\left[bN_{Te} - aN_{Se} - cN_{Sn} - dN_{In}\right]E_{Te-Te}}{m} ....(12)$$

and $E_{Sn\text{-}Sn}$ = 125.4 kJ/mol, $E_{Se\text{-}Se}$ = 184.9 kJ/mol, $E_{Te\text{-}Te}$= 138 kJ/mol and $E_{In\text{-}In}$ = 143 kJ/mol. Figure 4 shows variation of <E> with <Z> for different In contents. The values of <E> increases with increases values of Indium, shows more rigidity of glass alloys. We have published a paper which shows same trends for stability of glasses [11].

Conclusions

The physical parameters of $Se_{90-x}Te_5Sn_5In_x$ (0≤x≤9) glassy system have been theoretical investigated. The density and molar volume with Indium contents shows inverse trends. Total number of constraints (N_c) and degree of freedom with <Z> are also shows opposite behaviors for this system, but LP and mean bond energy decreases with the increase of in content

Acknowledgement

I would like thanks to Prof. Kedar Singh SPS JNU New Delhi for providing research facilities.

References

1. Feltz A. Amorphous inorganic materials and glasses. Weinheim, Germany: VCH Publishers. 1993.
2. Popescu M. Non-crystalline chalcogenides. Dordrecht, Netherlands: Kluwer Academic Publishers. 2000.
3. Singh J, Shimakawa K. Advances in amorphous semiconductors. London, UK: Taylor & Francis. 2003.
4. Weiser K, Gambino R J, Reinhold J. A. Optical properties of amorphous materials. Applied Physics Letters. 1973, 22, 48–49. https://doi.org/10.1063/1.1654469
5. Brown B. R. Optical absorption in amorphous semiconductors. Applied Optics. 1974, 13, 761–764.
6. Elliott S. R. Physics of amorphous materials (2nd ed.). London, UK: Longman 1990.
7. Mott N. F & Davis E. A. Electronic processes in non-crystalline materials. Oxford, UK: Oxford University Press. 1979.
8. Chander R,Thangaraj R. Structural and thermal properties of chalcogenide glasses. Chalcogenide Letters. 2008, 5, 229–234.
9. Saffarini G, Schlieper A. Optical and structural studies of chalcogenide thin films. Applied Physics A. 1995, 61, 29–34. https://doi.org/10.1007/BF01577665
10. El-Samanoudy M. M. Optical properties of chalcogenide thin films. Thin Solid Films. 2003, 423, 201–206.
11. Kumar S, Singh K. Glass transition, thermal stability, and glass-forming tendency of Se–Te–Sn–In chalcogenide glasses. Thermochimica Acta. 2012, 528, 32–37. https://doi.org/10.1016/j.tca.2011.11.005
12. Thorpe M. F. Continuous deformations in random networks. Journal of Non-Crystalline Solids. 1983, 57, 355–370. https://doi.org/10.1016/0022-3093(83)90424-6
13. Phillips J. C Thorpe M. F. Constraint theory, vector percolation, and glass formation. Solid State Communications. 1985, 53, 699–702. https://doi.org/10.1016/0038-1098(85)90381-3
14. Tichy L & Ticha H. On the chemical threshold in chalcogenide glasses. Materials Letters. 1994, 21, 313–319. https://doi.org/10.1016/0167-577X(94)90196-1
15. Tichy L, Ticha H. Covalent bond approach to the glass transition temperature of chalcogenide glasses. Journal of Non-Crystalline Solids. 1995. 189, 141–146. https://doi.org/10.1016/0022-3093(95)00202-2
16. Fadel M. Physical properties and chemical bond approach for Se–Ge–As amorphous chalcogenide glasses. Vacuum. 1997, 48, 73–83. https://doi.org/10.1016/S0042-207X(96)00229-1
17. Sharma A, Barman P. B. Effect of Bi incorporation on the glass transition kinetics of $Se_{85}Te_{15}$ glassy alloy. Journal of Thermal Analysis and Calorimetry. 2009, 96, 413–417. https://doi.org/10.1007/s10973-008-9312-8
18. Savova E, Skordeva E, Vateva E, Topological phase transition in Ge–Sb–S glasses and thin films. Journal of Physics and Chemistry of Solids. 1994, 55, 575–578. https://doi.org/10.1016/0022-3697(94)90055-8
19. Skordeva E, Arsova D, Topological phase transition in ternary chalcogenide films. Journal of Non-Crystalline Solids, 1995, 192–193, 665–668. https://doi.org/10.1016/0022-3093(95)00422-X
20. Lafi O. A, Imran M. M. A & Abdullah M. K. Chemical bond approach to glass transition temperature and crystallization activation energy in $Se_{90}In_{10-X}Sn_x$ ($2 \le x \le 8$) semiconducting glasses. Materials Chemistry and Physics. 2008, 108, 109–114. https://doi.org/10.1016/j.matchemphys.2007.09.011
21. Aly K. A, Othman A. A, Abousehly A. M. Physical properties of chalcogenide alloys. Journal of Alloys and Compounds. 2009, 467, 417–423. https://doi.org/10.1016/j.jallcom.2007.12.009