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Effect of Ge Content on Physical Properties of Se-Te Chalcogenide Glasses

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Abstract: *Se based chalcogenides thin films have interesting physical properties which make them attractive for various optoelectronics, photonics, phase change memory alloys, and non-volatile memory applications. Chalcogenide thin films exhibit significant changes in their optical and electrical properties depending upon their composition and structure. This paper reports the change in the physical properties of* $Se_{70-x}Te_{30}Ge_x$ *(5≤x≤25) system with increase in Ge content. The coordination number, constraints and average heat of atomization increases, lone pair and parameter R decreases with Ge content which suggest that system is chalcogen rich and can form stable glasses.*

Keywords: Chalcogenide Glasses, Average Coordination Number, lone pair electron, parameter R, average heat of atomization

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1. Introduction

Chalcogenides are well known for their unique properties for broad transmission window, photo induced phenomena or high optical nonlinearities without free carriers [1-3]. These properties make them suitable for potential applications in several fields including, artificial neural networks, phase-change materials, non-linear photonics, mid-IR sources, and optical sensors, *etc*. [4-7].

Selenium and tellurium chalcogenides are intensively studied due to their wide transparency in the near-mid infrared region and favourable thermal stability. But as application point of view, they are not suitable in their pure form Se has lesser sensitivity, higher ageing effects, smaller lifetime. Same goes with Te, although glassy alloys based on Te offer the broadest range of IR-transmission and display optical phase recording, however, the "glass forming ability" of Te based glasses is not very noticeable. Therefore, Se is doped with Ge, Ga, Te, As, Pb, Bi, Sb, etc. to overcome this problem [8] and Se-Te binary alloy has been chosen as a base due to its more modified properties and vast industrial and scientific importance. However due to its relatively low crystallization temperature, limited reversibility and ageing effect, this binary glass alloy still has disadvantages which can be improved by adding suitable elements and synthesize the multi-component ternary matrix. Ge is chosen as third component of matrix as it cross-links with the selenium chain, modifies the bonds and strengthens the system's average bond and improves glass formation domain. Therefore produces a highly stable glassy matrix because of its electronegativity values and compatible size. The present system contain both selenium and tellurium elements, which are essential chalcogenide elements and having applications in the memory and switching devices [9].

The objective of the present work is to develop amorphous Ge doped Se-Te alloys and to analyse the various physical parameters theoretically viz. average coordination number (Z), total constraints (C_t), electron lone pairs (L), deviation from stoichiometry (R), and the heat of atomization (Hs) with the change in composition of Ge.

2. Results and Discussion

In the present investigation we have calculated the physical constants such as bonding constraints, average coordination number, lone pair electron, deviation from stoichiometry and heat of atomisation.

2.1 Bonding Constraints (C_t) & Average Coordination Number (Z)

The chalcogenide glassy materials having different compositions have varying average coordination number. The average coordination

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number is the number of nearest neighbors that bonded to a particular atom within a crystal. The average coordination number (r) provides the information about the dimensionality of the system [10, 11]. In constraint theory, Philips et al. [29] have stated the glass-forming conditions with interatomic fields. The total constraints or interatomic force field per atom plays an important role to understand the rigidity percolation in system. The average coordination number (Z) was calculated using standard method [12] for the composition $Se_{70-x}Te_{30}Ge_x$ ($5 \leq x \leq 25$):

$$Z = \frac{xN_{Se} + yN_{Te} + zN_{Ge}}{x + y + z}$$

Where x, y, z, are the atomic % of Se, Te and Ge respectively and N_x (N_{Se} (2), N_{Te} (2), N_{Ge} (4)) is the average coordination number [13, 14]. Fig. 1 shows that Z increases with the increase in concentration of Ge which shows that Se atom is forming more bonds with neighbouring atoms in the crystal structure. This could lead to changes in the physical and chemical properties as the increased coordination number can influence its structural stability, electronic properties, and reactivity. Bond-stretching (x-forces) and bond-bending (y- forces) are the two types of near-neighbour bonding forces in covalent bonds [10].

The number of Lagrangian bond-stretching constraints per atom [15] is,

$$C_x = Z/2$$

and, of bond-bending constraints is:

$$C_y = 2Z - 3$$

Total numbers of constraints are:

$$C_t = C_x + C_y$$

Therefore the cross-linking density is given by,

$$Y = C_t - 2$$

The calculated values of average coordination number (Z) (figure 1), constraints ($\mathbf{C_x}$, $\mathbf{C_y}$, $\mathbf{C_t}$), and cross linking density (Y) are given in the Table 1. The increase in Z and constraints with Ge content suggests that the system is thermally stable with higher glass transition temperature [8].

Table 1. Values of average coordination number (Z), constraints ($\mathbf{C_x}$, $\mathbf{C_y}$, $\mathbf{C_t}$), and cross linking density (Y).

x	Z	C_x	C_y	C_t	Y
5	2.10	1.05	1.20	2.25	0.25
10	2.20	1.10	1.40	2.50	0.50
15	2.30	1.15	1.60	2.75	0.75
20	2.40	1.20	1.80	3.00	1.00
25	2.50	1.25	2.00	3.25	1.25

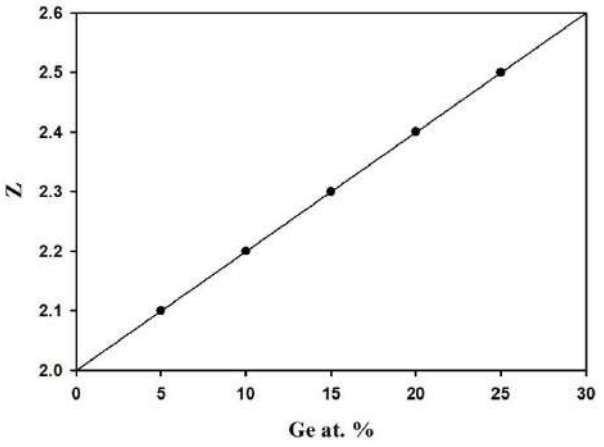

Fig. 1.: Variation of Average Coordination number of $Se_{70-x}Te_{30}Ge_x$ ($5 \leq x \leq 25$) system.

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2.2 Lone Pair Electrons (L) & Glass Forming Ability

The glass forming ability of Se-Te system is obtained by calculating the electron lone pair with Ge content. The increase in lone pair of electron indicates the development of stable glasses. If L, V, and Z are the number of lone pair electrons, valance electrons and average coordination number respectively then the lone–pair of electrons is calculated by using the relation [16]:

$$L = V - Z$$

Zhenhua's stated that, the glass formation ability in chalcogenide, i.e. electron lone pairs for binary system L > 2.6 and for ternary system L >1. The variation of lone-pair electron with Ge content is shown in Fig. 2. The decreasing behaviour is caused by the interaction between the Ge ion and lone-pair electrons of bridging Te atom. From table 2 it may be concluded that the present system under study is exhibiting good glass forming ability [17].

2.3 Deviation from Stoichiometry of Composition

R parameter determines the deviation from stoichiometry and is expressed by the ratio of content bond possibilities of chalcogen atoms to that of non-chalcogen atoms. For the present system:

$$R = \frac{xN_{Se} + yN_{Te}}{zN_{Ge}}$$

where x, y, z are atomic frictions of Se, Te and Ge respectively [18]. The values of R are mentioned in table 2. The analysis of the results can be done from the parameter R. If R = 1, the system reaches the stoichiometric composition, for R > 1, the system is chalcogen-rich and if R < 1, the system is chalcogen-poor. From fig. 3 and Table 2, it is clear that our system is chalcogen rich and may turn towards chalcogen poor with the increase in content of Ge in the system.

Table 2. Values of average coordination number (Z), Valence electrons **(V)**, lone pair electron (L), and parameter R

x	Z	V	L	R
5	2.10	5.90	3.80	9.50
10	2.20	5.80	3.60	4.50
15	2.30	5.70	3.40	2.83
20	2.40	5.60	3.20	2.00
25	2.50	5.50	3.00	1.50

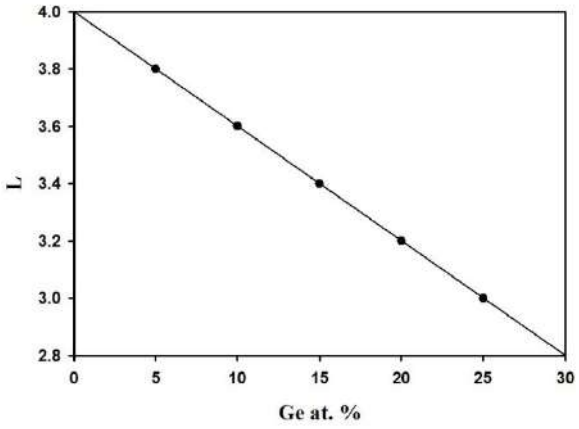

Fig. 2.: Variation of Lone Pair of electron of $Se_{70-x}Te_{30}Ge_x$ (5≤x≤25) system.

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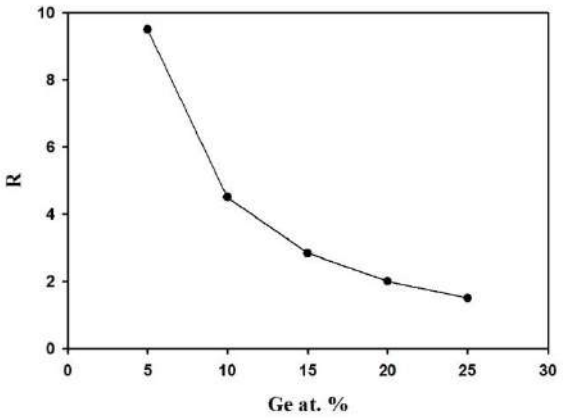

Figure 3. Variation of Parameter R of $Se_{70-x}Te_{30}Ge_x$ ($5 \leq x \leq 25$) system.

2.4 Average Heat of Atomization

The energy essential to split one mole from a particular material into atoms is heat of atomization.The average atomization heat is the strength to break one mole into atoms of a given element. The atomization heat gives information regarding the bond strength of atoms. The larger is the atomization heat, the stronger the bond strength and better would be the separation among bonding and anti-bonding atomic orbitals. CE is also the measure of the material's relative bond strength. The heat of atomization H_s (A-B) at standard temperature and presence of a binary semiconductor formed from atom A and B is a sum of heats of formation ΔH and average of heats of atomization H_s^A and H_s^B that correspond to the average non-polar energies of the two atoms, is given by the relation [19, 20]

$$H_s = \frac{xH_s^A + yH_s^B + zH_s^C}{x + y + z}$$

where x, y, z are the ratios of A(Se), B(Te), and C(Ge) respectively. From Table 3, it is clear that average heat of atomization (H_s), increases with increase in Ge content. The graphical representation of average heat of atomization H_s with the variation in Ge content is shown in figure 4.

Table 3: Values of average heat of atomization (H_s).

x	H_s (KJmol^{-1})
5	225.5
10	233.0
15	240.5
20	248.0
25	255.5

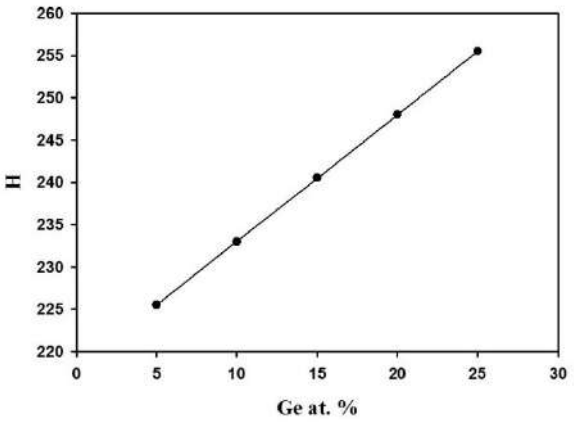

Fig. 4.: Variation of Heat of Atomization$Se_{70-x}Te_{30}Ge_x$ ($5 \leq x \leq 25$) system.

3. CONCLUSION

The physical properties of Ge-Se-Te glassy alloys investigated theoretically and discussed in detail. It has been found that the co-ordination number (Z) increases with Ge content which shows that Se atom is forming more bonds with neighbouring atoms in the crystal structure and system is thermally stable. The higher values of lone pair electron for all samples suggest that the system is a good glass former. The variation in the values of R parameter and heat of atomization shows that the $Se_{70-x}Te_{30}Ge_x$ ($5 \leq x \leq 25$) system is chalcogen rich and is having stronger bond strength.

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