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Optical properties of Ge-Se-In Amorphous Composites

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ABSTRACT

The effect on the optical and physical properties with the addition of In content viz. Constraint, heat of atomization, optical energy gap and the energetic parameter of $Ge_{10}Se_{90-x}In_x$ (x = 0, 5, 10, 15, 20 at %) glassy are theoretically. From heat of atomization data Optical gap has been determined. For the present glassy alloy it has been found that average coordination(<r>), no .of constraints(N), heat of atomization(H_s), glass forming ability, optical band gap(ΔE_g) and energetic parameter(A) are increases with increase of In content while lone-pair electrons(L) and the fraction of zero frequency mode(f) decreases.

Keywords: Chalcogenide Glasses, Optical gap, Heat of atomization, Energetic parameter.

INTRODUCTION

Ge-Se system is a widely studied system and it has been established that physical and optical properties in this system are highly composition dependent [1,2]. Chalcogenide glasses in Ge-Se system are used as switching memory elements and optoelectronic devices and are interesting materials for infrared optics too [3]. They have large range of transparency and very good mechanical properties low internal stress. Photoconductivity, thermal diffusivity and optical band gap of chalcogenide glasses can be considerably changed by allowing of third element to the Ge-Se [4-7], for example of In can increase the optical gap E_g.[5]

Ge-Se-In alloy are good glass formers over a wide compositional ranges reported by , Boncheva et al [8].Bakr[6] suggested that the main glass structure of Ge-Se is interrupted by bonding of In with the dangling Se atoms. It has also been suggested that the change in the glass structure upon addition of In to Ge-Se are associated with Se chains shortening and as increase in defect concentration. This result formation of new localized state in the band structure and a increase in the optical band gap.

In the present we reported and discussed the compositional dependence of the optical and physical properties in Ge-Se-In glass system.

RESULTS AND DISCUSSION

(A)Constraints and the fraction of zero frequency modes:-

The concept of the average coordination number <r> is useful in describing the cross linking in a covalently bonded solids. Phillips[15], Mott[9] and Flank et al[10] have shown that the coordination number of covalently bonded atoms in glass is given by the 8-N rulewhere N is the no. of the outer shell electrons. The average no. of coordination is calculated by the equation-

$$<r> = XZ_{Ge} + YZ_{Se} + ZZ_{In} \quad (1)$$

Where X, Y, Z are the mole fraction of Ge, Se, In. In a glassy system covalent networks can be mechanically constrained by interatomic valence force such as bond bending (N_α = <r>/2) and bond bending (N_β = 2<r>-3).Optimal glass formation are attained when the no. of constraints Ncon per atom is equal to the degree of freedom (N_d) per aton ,that is, for ideal glass N_{con} = N_d[11]. The average no. of constraints for compositions in our case = 3.5 and its expression is –

$$N_{con} = N_{\alpha +} N_\beta \quad (2)$$

The variation of <r> with In content is illustrated in fig.-(1).

We note that <r> gives a partial but very important description of the network. It has found to be the dominant determining parameter in describing many experimental results that relate to the structure, vibrations, hardness, the glass transition temperature (T_g) etc [12-15].This is sometimes referred to as the iso-coordinate rule.

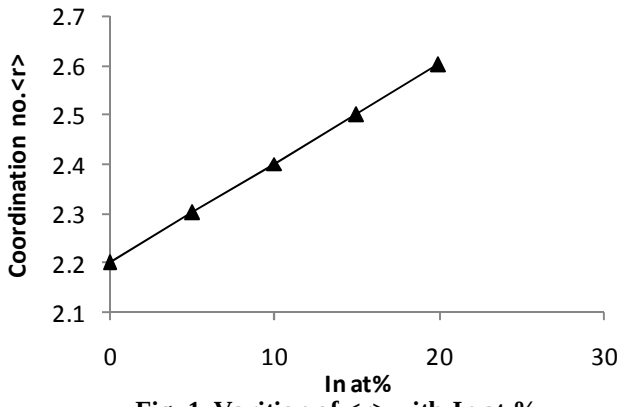

Fig.-1, Varition of <r> with In at %

If any eigen modes having zero frequency are present in the system then the smaller terms in the potential will give these modes a small finite frequency thus warranting the names floppy modes.

The total no. of zero frequency modes can be estimated by Maxwell [16] constraints counting was as first done by Thorpe [17], following the works of Phillips [18] on optical glass formation.

The fraction of zero frequency mode is given by-

$$f=2–5/6<r> \quad (3)$$

The variation of floppy modes with In content is illustrated in fig.-(2).

The characteristics of the involved atoms are summarized as –

Elements	Ge	Se	In
Atomic number	32	34	49
Atomic configuration	[Ar] $3d^{10}4s^24p^2$	[Ar] $3d^{10}4s^24p^4$	[Kr] $4d^{10}5s^25p^1$
Valence electrons	4	6	3
Coordination no.	4	2	4

The values of average coordination no.<r>, no. of constraints N_{con} and the no. of floppy modes are listed in table-(1).

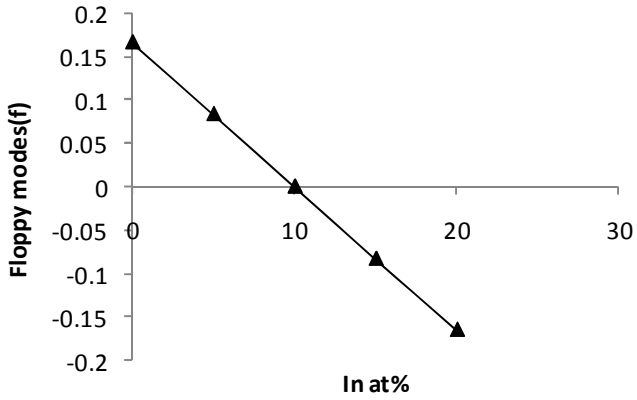

Fig.-2, Vasriation of f with In at%

Table-(1) Values of<r>, Nr and L for the system $Ge_{10}Se_{90-x}In_x$

Composition(x)	<r>	n_r	f	L	ability
X = 0	2.20	2.5	0.1667	3.599	+
X = 5	2.30	2.75	0.0834	3.356	+
X = 10	2.40	3.0	0	3.100	+
X = 15	2.50	3.25	-0.0864	2.850	+
X= 20	2.60	3.50	-0.166	2.600	+

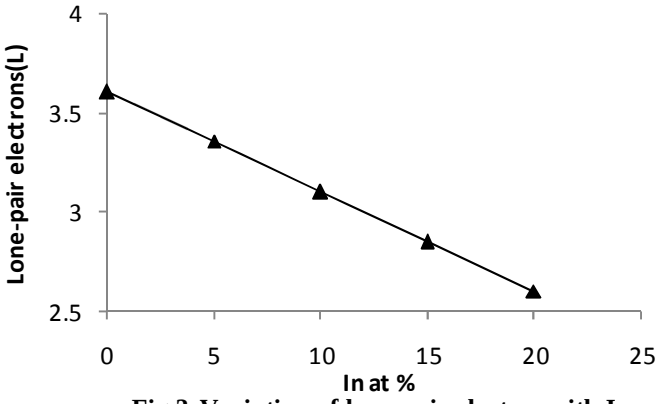

Fig.3, Variation of lone-pair electros with In at%

(B)Role of lone pair electrons:-

The number of lone pair electrons in a chalcogenide glass system can be calculated by using the relation [19]

$$L = V - r \qquad (4)$$

where L and V are the lone pair electrons and valence electrons, respectively. We can conclude from these results that some lone pair electrons in the structure of a system are a necessary condition for obtaining the system in vitreous state. For a binary system the value of L must be larger than 2.6 and for a ternary system it must be larger than 1. The value L for the present glass system lies between 2.6 to 3.99, concludes that the present system is a good glass former and has good glass forming ability. The value of lone-pair electrons (L) is listed in table-(1) and variation with In content is shown in fig.-(3).

(C) Heat of Atomization and Optical gap :-

For ternary compounds the Hs is defined for the compounds $A_\alpha B_\beta C_\gamma$ as a direct measure of cohesive energy and average bond strength is given by-

$$Hs = (\alpha Hs^a + \beta Hs^b + \gamma Hs^c) / (\alpha+\beta+\gamma) \qquad (5)$$

Eq.(5) is applicable to this ternary system.It is clear from eq. (5) that heat of atomization increases with In content and is illustrated in Fig.-(4).

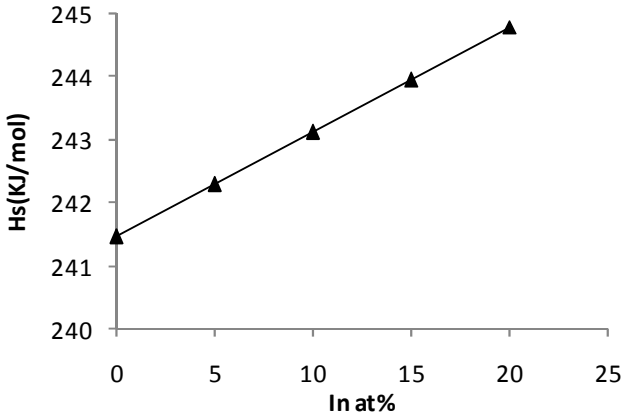

Fig.-4, Variation of Hs(KJ/mol) with In at%

Loffe and Regel [20] suggested that the bonding character in nearest neighbor region which means the coordination no. N_{con} characterized the electronic and optical properties of semiconductor materials. The N_{con} in terms of optical energy is defined by –

$$\Delta E_g = a(H_s - b) \qquad (5)$$

It is suggested from the above equation that average heat of atomization is a measure of Hs which in terms are correlated with energy of iso- structural system. Where a and b(= 0.89 N^2_{con}) are characteristic constants. The value of ΔE_g for $Ge_{10}Se_{90-x}In_x$ with x = 0,5, 10, 15, 20 are listed in table –(2). It can be seen that the addition of In leads to the increasing Hs as well as ΔE_g. It is suggested by the above equation that the average heats of atomization are a measure of the cohesive energy and represent the relative bond strength, that in turn are correlated with properties like energy gap[21].Fig.-(4) and (5) represents the dependence of H_s and ΔE_g on the composition. All these parameters are gradually increasing with x..The value of Hs and ΔE_g are listed in table-(2).

Table-(2) Values of H and ΔEg for the system $Ge_{10}Se_{90-x}In_x$

Composition(x)	Hs(kj/mol)	ΔEg(eV)	$Ax10^4$(/kel)
X = 0	241.460	2.497	1.4385
X = 5	242.290	2.506	1.6524
X = 10	243.120	2.514	1.9953
X = 15	243.950	2.521	2.3367
X= 20	244.780	2.529	2.4180

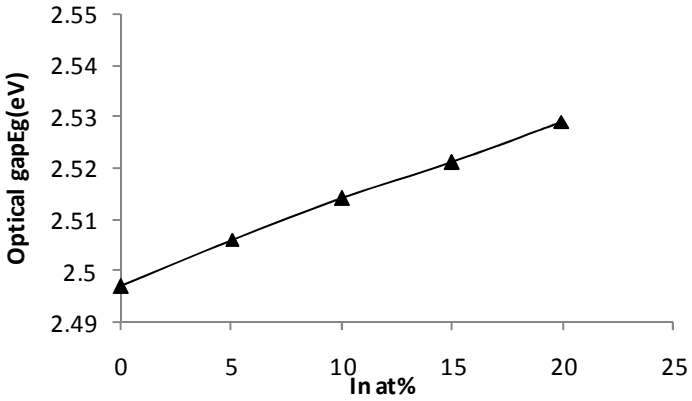

Fig.-5, Variation of Optical gap Eg(eV) with In at%

(D)The Energetic distribution of Absorption coefficient:-

The spectral dependence of the absorption coefficient indicates an indirect allowed transition. The result is verified by energetic parameter relation vs. composition. According to Angell proposal [22], the compositional changes in the optical gap is correlated by energetic parameter (A) which is given by the equation-

$$A = \epsilon \Delta E_g / k \qquad (6)$$

Where $\epsilon = \delta (Z-2)$ and K = Boltzmann constant, δ an independent constant (0.55). Fig (6) shows the variation of A with % of composition.

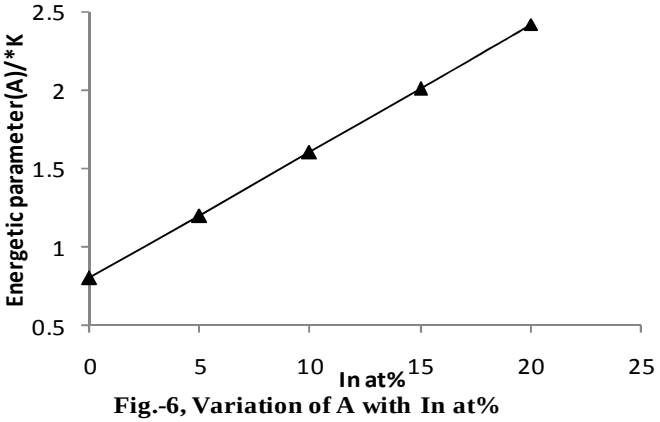

Fig.-6, Variation of A with In at%

CONCLUSION

The influence of In content on the optical and physical parameters of Ge-Se glassy alloy is investigated .With the addition of In, Ge-Se system changes from floppy to intermediate or rigid region. Average no. of constraints per atom (Ncon) exceeds the no. of degree of freedom for all

composition and shows non-monatomic behavior and increases with In content. With addition of In no. of lone-pair electrons decreases continuously which is caused by the interaction between the In ion and lone-pair electrons of bridge Se atoms. In general the optical parameter investigated in this work shows a tendency of increasing with increase of In content as it is shown from the optical band gap, heat of atomization and energetic parameter.

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