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Study of Optical properties with compositional dependence in $(GeSe_3)_{1-x}Ag_x$ Glasses

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ABSTRACT

Optical and some physical properties of $(GeSe_3)_{1-x}Ag_x$ with $0<x>0.5$ glassy system has been predicted theoretically. Optical band gap has been determined from the average no. of coordination and the heat of atomization data. The correlation of optical gap with film composition(x) defines the spectral dependence of absorption coefficient this result is verified by energetic parameter relation Vs composition relation.From the theoretical prediction data it has been found that average coordination<r>, no. of constraint(N_{con}), heat of atomization (H_s), optical gap(ΔE_g) and the energetic parameter(A) increases with increase in Silver(Ag) concentration while all other parameters decreases with concentration.

Keywords:- Chalcogenide Glasses, Optical gap, Energetic parameter.

INTRODUCTION

For many years Chalcogenide glasses have been widely investigated since several of their properties make them very attractive materials. The Ge-Se-Ag glasses can be used as sensitive membranes for the development of chemical sensors for the detections of heavy ions in aqueous media[1]. They are

transparent in the infrared and have been used glasses for night vision [2], as optical fibers[3], and when prepared in a thin film form as components for integrated optics[4,5]. Ag as an additives in CG's and particularly thin films of such glasses has attracted wide spread interest in glass science [6-8]. In Ag-CG's Ag centered local structure apparently phase separated from the host network. The new structural results provide the new compositional properties in Ag chalcogenides glasses.

In the present work we have reported the theoretical prediction of optical and some physical parameters of $(GeSe_3)_{1-x}Ag_x$ glassy system .An attempt has been made to explain the varying trends of various parameters with increasing Ag content.

RESULTS AND DISCUSSION

Average coordination no<r> and No. of Constraints (Ncon):-

The average coordination number *r* for the system is calculated using the expression [9]

$$<r = Z_AX_A+Z_BX_B+Z_CX_C \quad (1)$$

where $Z_A = 4$, $Z_B = 2$, $Z_C = 4$, are the coordination numbers for Ge, Se, and Ag, respectively, the average coordination number being situated in the range $2.47 \leq r \geq 3.23$. In a glassy system covalent networks can be mechanically constrained by interatomic valence forces such as bond stretching and bond bending. Optimal glass formation is attained when the network is at a mechanically critical point. This point is reached when the number of constraints (N_{con}) per atom is equal to the degrees of freedom (N_d) per atom i.e. for ideal glass $N_{con} = N_d$. The enumeration of mechanical constraints in this system gives $<r>/2$ bond stretching constraints (N_α) and $2< r> - 3$ bond bending constraints (N_β) [10]. The average coordination number $< r>$ and the average number of constraints, given by $N_{con}= N_\alpha + N_\beta$ for various compositions with Ag are listed in table (1) and the variation of mean coordination no. with Ag at% is shown in fig.(1).

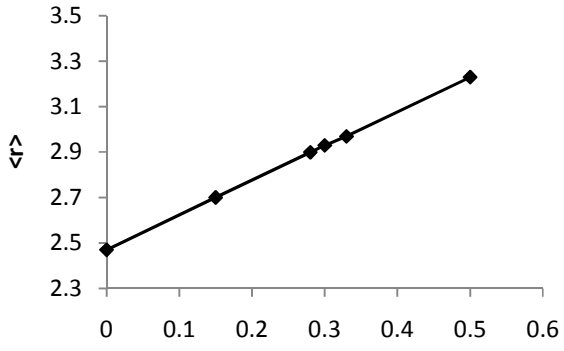

Fig.-1, Variation of average coordination <r> with x%

Role of lone pair electrons:-

In order to calculate the no. of role-pair electrons of a chalcogenide system, the average coordination no. proposed by Phillips [11] was introduced.

$$L = V - r \quad (2)$$

Where L and V are the lone pair electrons and valence electrons, respectively

The lone-pair electrons of the given glass system was obtained according to equation (2) and is listed in table-(1). It is seen from the above table and from the fig.-(2) that the no. of lone-pair electrons decreases continuously with the increase in Ag content.

Table-(1) Values of<r>, N_{con} and L for the system $(GeSe_3)_{1-x}Ag_x$

Composition	<r>	N_{con}	L
$(GeSe_3)$	2.47	3.175	3.0616
$(GeSe_3)_{0.85}Ag_{0.15}$	2.68	3.475	2.1529
$(GeSe_3)_{0.72}Ag_{0.28}$	2.88	4.242	1.3648
$(GeSe_3)_{0.70}Ag_{0.30}$	2.94	4.338	1.2129
$(GeSe_3)_{0.67}Ag_{0.33}$	2.97	4.435	1.0616
$(GeSe_3)_{0.50}Ag_{0.50}$	3.23	5.085	0.0313

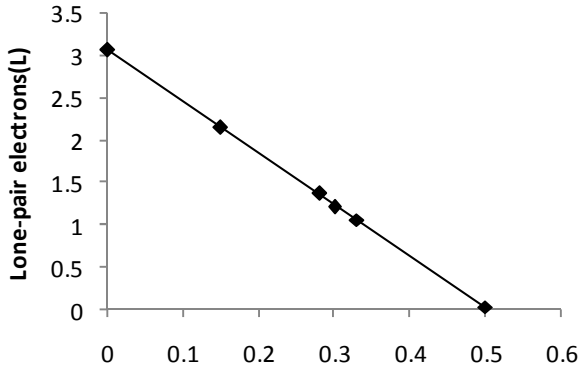

Fig.-2, Variation of L with Ag at %

We can conclude from the results above, 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>2.6 and, for a ternary system it must be >1 [9].

Heat of atomization (Hs) and Optical gap(ΔEg):-

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-

$$Hs = (\alpha Hs^a + \beta Hs^b + \gamma Hs^c) / (\alpha+\beta+\gamma) \qquad (3)$$

Eq.(3) is applicable to this ternary system. From eq.(3) it is clear that Hs decreases with the partial substitution of Ge and Se. The variation of H_s with composition is shown in fig.(3).The value of H_s is listed in table-(2).

Loffe and Regel [12] 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

$$\Delta E_g = a(H_s\text{-})b \qquad (4)$$

It is suggested from the above equation that average heat of atomization is a measure of H_s which in terms are correlated with energy of iso- structural system. Where a and b are characteristic constants. The value of H_s and ΔE_g for $(GeSe_3)_{1-x}Ag_x$ with $0<x>0.5$ are listed in table –(2). It can be seen that the addition of Ag 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[13].Fig.-(3) and (4) represents the dependence of H_s and ΔE_g on the composition. All these parameters are gradually increasing with x.

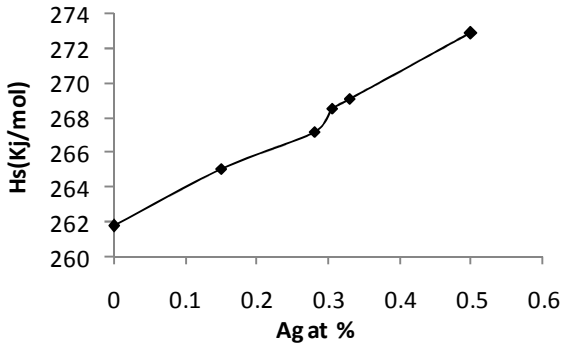

Fig.-3, Variation of Hs(Kj/mol) with Ag at%

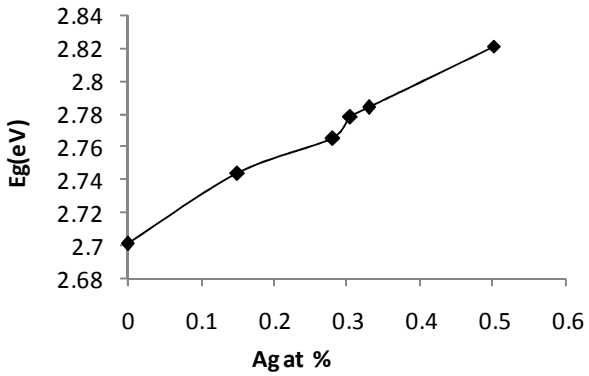

Fig.-4, Variation of Eg(eV) with Ag at%

Correlation of Optical gap with film composition:-

The correlation of optical gap with film composition(x) defines the spectral dependence of absorption coefficient which indicates an indirect allowed transition. The result is verified by energetic parameter relation Vs composition [14,15] which is given by-

$$A = \epsilon\Delta E_g/k \qquad (5)$$

Where $\epsilon = \delta(Z-2)$ and K = Boltzmann constant, δ an independent constant(0.55).The value of A are listed in table-(2).The variation of energetic parameter(A) with composition is illustrated in Fig.-(5).

Table-(2) Values ofHs, ΔE_g and A for the system $(GeSe_3)_{1-x}Ag_x$

Composition	Hs(kj/mol)	ΔE_g (eV)	A X 10^4/ ^{0}K
$(GeSe_3)$	261.724	2.709	5.9266
$(GeSe_3)_{0.85}Ag_{0.15}$	265.043	2.743	7.0135
$(GeSe_3)_{0.72}Ag_{0.28}$	267.094	2.765	7.948
$(GeSe_3)_{0.70}Ag_{0.30}$	268.518	2.778	8.1559
$(GeSe_3)_{0.67}Ag_{0.33}$	269.075	2.783	8.3460
$(GeSe_3)_{0.50}Ag_{0.50}$	272.862	2.822	9.6344

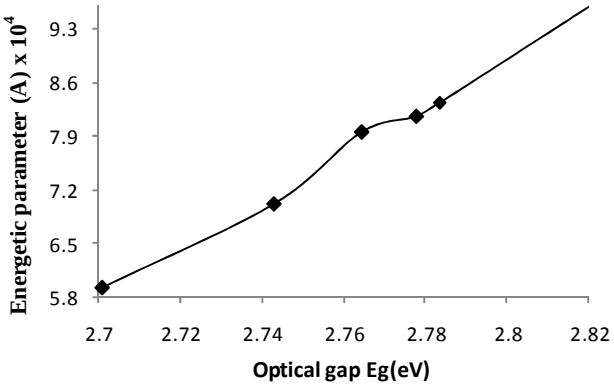

Fig.- 5, Variation of Energetic parameter A x 10^4 /K

CONCLUSION

The result from the theoretical prediction of $(GeSe_3)_{1-x}Ag_{x\ glass}$ system can be summarized as follows-

- The average coordination number<r> increases with increase in Ag content which gives an indication that N_{con} increases hence the value of ΔE_g will strongly depends upon H_s.
- With addition of Ag content lone-pair electrons (L) decreases continuously.
- The correlation of optical gap with film composition(x) defines the spectral dependence of absorption coefficient which indicates an indirect allowed transition. This result is verified by energetic parameter relation Vs composition.

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