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Advances in Applied Science Research, 2011, 2 (3): 127-133



Theoretical prediction of the optical properties of $(\text{Ge}_{0.20}\text{Se}_{0.80})_{100-x}\text{Ag}_x$ system

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ABSTRACT

The effect of silver (Ag) content on the optical and other physical characteristics of $(\text{Ge}_{0.20}\text{Se}_{0.80})_{100-x}\text{Ag}_x$ ($x = 0, 6, 11, 16, 20, 23$, at %) was investigated theoretically. The relation between the optical gap (E_g) and chemical composition has been discussed in terms of the average heat of atomization (H_s) and average coordination number (Z). In order to correlate the optical parameter (E_g) with film composition we used the energetic parameter (A). It was found that the magnitude of (E_g) and H_s decreases with increasing In content. The Arsova proposal is used to calculate the mean bond energy $\langle E_s \rangle$ for this system.

Keywords: Chalcogenide glasses, Optical gap, Energetic parameter, Mean bond energy.

INTRODUCTION

Impurity effect in chalcogenide glasses have importance in fabrication of glassy semiconductors. Several workers have reported the impurity effect in various chalcogenide glasses[1-4]. They are interesting as core materials for optical fibers and used for transmission especially when short length and flexibility are required [5-6].

The introduction of Ag in to chalcogenide glasses causes substitutional changes in the electrical and optical properties of the material [7-9]. Ag as an additive in chalcogenide glasses and particular thin film of such glasses have attracted wide interest in glass science[10-11]. The interest stems in part from light induced effect relevant to optical recording and information processing [6]. It also stems drastically increased electrical conductivity of Ag – chalcogenides some of which are solid electrolytes[12]. In this communication we report the compositional effect of Ag on the optical and physical properties of Ge-Se-Ag system. Ag is chosen as an additive material because it alloys with most of the metals and modified their physical properties [13].

2. Discussion of various theoretical parameters:-

Various parameters *viz* coordination number and constraints, number of lone pair electrons, heat of atomization, optical gap and energetic parameter has been theoretically predicted for Ge-Se-Ag glassy system.

2.1 Coordination Number and Constraints:-

For the given system of Ge-Se-Ag average coordination number $\langle r \rangle$ is calculated using the expression,

$$\langle r \rangle = Z_A X_A + Z_B X_B + Z_C X_C \quad (1)$$

where $Z_A = 4$, $Z_B = 2$, $Z_C = 4$, are the coordination numbers for Ge, Se, and Ag, respectively [14]. Fig.-(1) shows the variation of average coordination no. $\langle r \rangle$ with composition of Ag and the value of $\langle r \rangle$ is listed in table -(1)

2.2 Role of lone pair electrons:-

In order to calculate the no. of lone-pair electrons of a chalcogenide system, the average coordination no. proposed by Phillips [15] was introduced. 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.

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 [16].

2.3 Heat of Atomization and Optical gap :-

Heat of atomization $H_s(A-B)$ at standard temperature and pressure of a binary semiconductor formed from atoms A and B, as proposed by Pauling [17], is the sum of the heat of formation, ΔH , and the average of heat of atomization H_s^A and H_s^B , that corresponds to the average non polar bond energy of two atoms.

$$H_s(A-B) = \Delta H + (H_s^A + H_s^B)/2 \quad (2)$$

The first term in equation (4) is proportional to the square of the electro negativity difference of two atoms involved i.e.

$$\Delta H \propto (X^A - X^B)^2 \quad (3)$$

In order to extend this idea to ternary and higher order semiconductor compounds, the average heat of atomization H_s is defined for the compounds $A_\alpha B_\beta C_\gamma$ as a direct measure of cohesive energy and the average bond strength is given by

$$H_s = (\alpha H_s^A + \beta H_s^B + \gamma H_s^C) / (\alpha + \beta + \gamma) \quad (4)$$

Equation (4) is applicable to this ternary system. The value of H_s obtained by using the values of H_s for Ge, Se, and Ag (the H_s values in units of kJ/mol are 377 for Ge, 226.4 for Se and 284 for Ag) are listed in table-(2) As seen from table -(2) the value of H_s firstly decrease and then increases with the addition of Ag.

It is therefore interesting to relate the optical gap ΔE_g with the chemical bond energy, and the parameters we used to specify the bonding are H_s and $\langle r \rangle$. The relationship between the energy gap and average heat of atomization was discussed by Aigrain and Balkanski [18]. According to their study a linear correlation exists for semiconductors of the diamond and zinc blende structure.

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

Where a and b are characteristic constants. The value of ΔE_g for $(\text{Ge}_{0.20}\text{Se}_{0.80})_{100-x}\text{Ag}_x$ with $x = 0, 6, 11, 16, 20, 23$ are listed in table -(2). It can be seen that the addition of Ag leads to the increasing H_s 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 [19]. Fig.-(3) and (4) represents the dependence of H_s and ΔE_g on the composition. All these parameters are gradually increasing with x .

2.4 The Mean bond energy($\langle E_s \rangle$) and Optical gap(ΔE_g):

Arsova proposed that the optical band gap energy (ΔE_g) and the mean bond energy can be correlated as

$$E_g = a(\langle E_s \rangle - b) \quad (6)$$

and

$$\langle E_s \rangle = \sum C_i E_{s(i)} \quad (7)$$

Where C_i is a fraction of type (i) bond and $E_{s(i)}$ is the bond energy of that bond [20] Fig.-(6) represents the dependence of $\langle E_s \rangle$ on the composition. All these parameters are gradually decreasing with x .

2.5 The Energetic Parameter(A):-

In order to correlate the optical parameter (ΔE_g) with the film composition we used the energetic parameter (A) introduced by Angell [21,22].

$$A = \epsilon \Delta E_g / k \quad (8)$$

Where $\epsilon = \delta (Z-2)$ and $K =$ Boltzmann constant, δ an independent constant (0.55). Fig(5) shows the variation of A with % of composition. The value of A and $\langle E_s \rangle$ are listed in table-(3). Fig. - (5) & (6) Represent the dependence of A and $\langle E_s \rangle$ on the composition.

Table-(1) Values of $\langle r \rangle$ and L for the system $(\text{Ge}_{0.20}\text{Se}_{0.80})_{100-x}\text{Ag}_x$

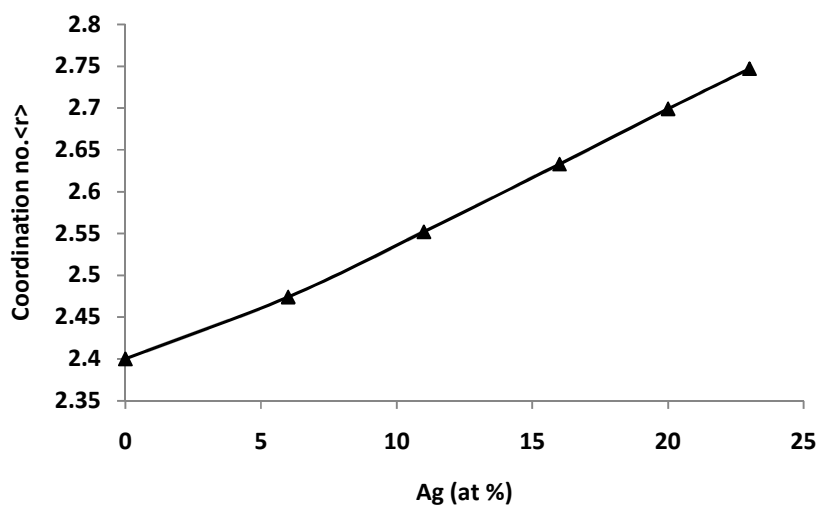
Composition(x)	$\langle r \rangle$	L
X = 0	2.4	3.2
X = 6	2.474	2.8754
X = 11	2.552	2.5653
X = 16	2.633	2.253
X = 20	2.699	2.002
X = 23	2.747	1.8152

Table-(2) Values of Hs and ΔE_g for the system $(\text{Ge}_{0.20}\text{Se}_{0.80})_{100-x}\text{Ag}_x$

Composition(x)	Hs(kj/mol)	$\Delta E_g(\text{eV})$
X = 0	256.52	2.653
X = 6	256.311	2.6498
X = 11	257.7843	2.6639
X = 16	259.2571	2.6779
X = 20	260.4353	2.689
X = 23	261.319	2.6973

Table-(3) Values of $\langle E_s \rangle$ and A for the system $(\text{Ge}_{0.20}\text{Se}_{0.80})_{100-x}\text{Ag}_x$

Composition(x)	$\langle E_s \rangle$	$A \times 10^4 (\text{kel})$
X = 0	2.669	1.6917
X = 6	2.658	2.002
X = 11	2.685	2.344
X = 16	2.701	2.7021
X = 20	2.715	2.9964
X = 23	2.725	3.212

Fig. 1. Coordination no. $\langle r \rangle$ versus Ag content (at %)

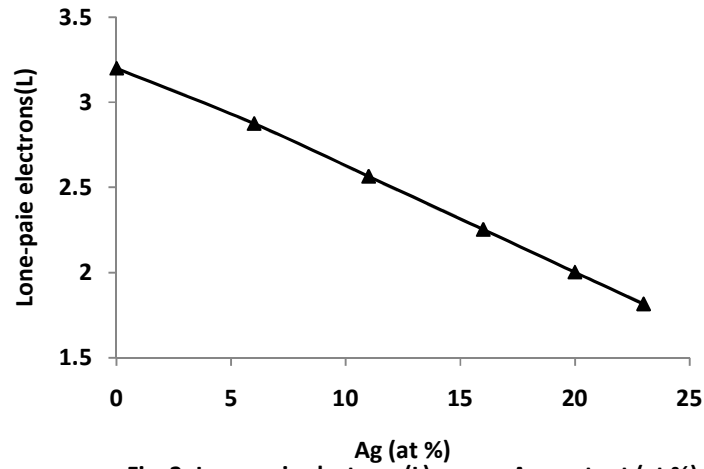


Fig. 2. Lone-pair electrons(L) versus Ag content (at %)

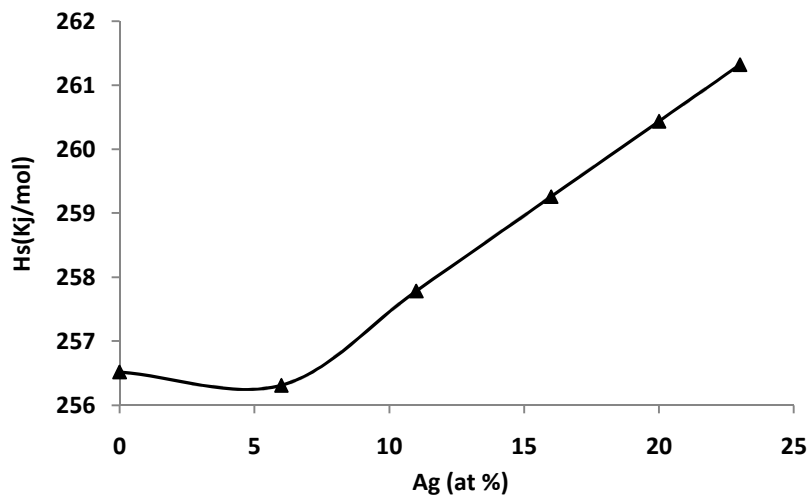


Fig. 3. Variation of Hs(Kj/mol) with Ag content (at %)

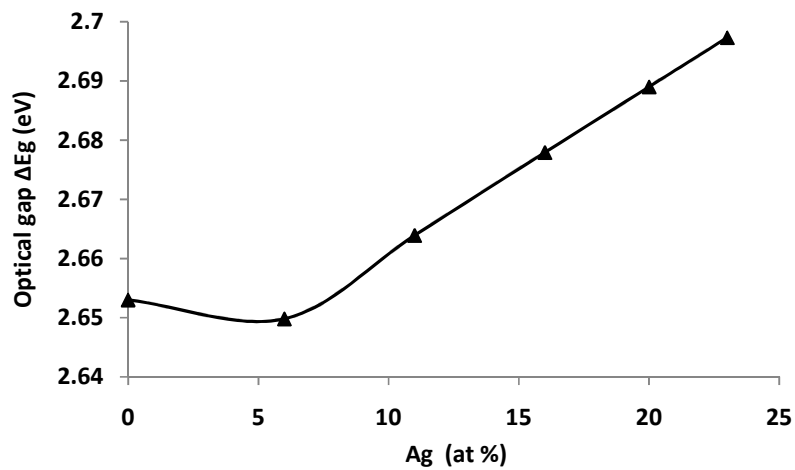
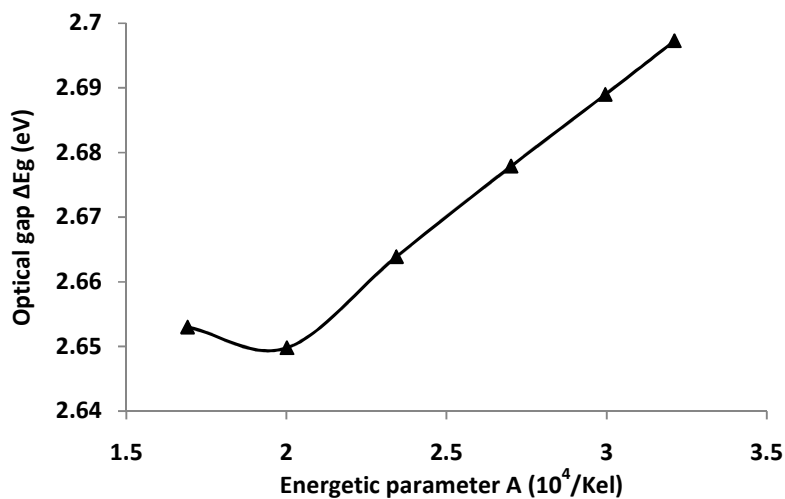
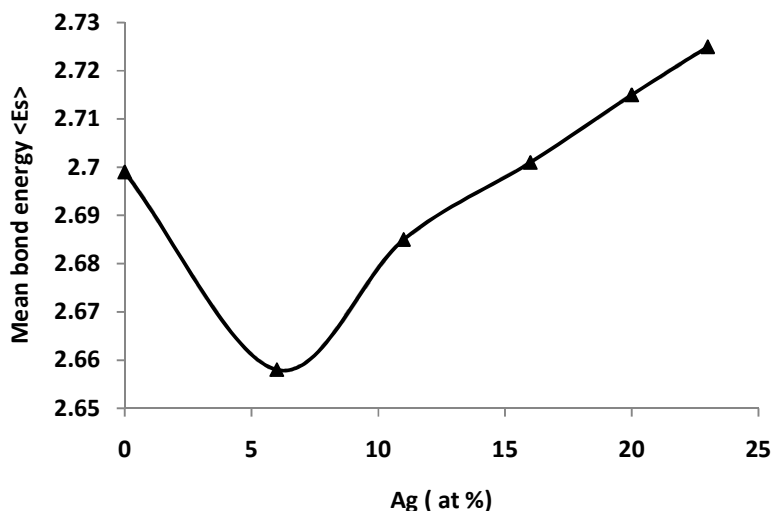


Fig. 4. Variation of Optical gap ΔEg with Ag content (at %)

Fig. 5. Variation of Energetic parameter (A) with Optical gap ΔE_g Fig. 6. Variatio of $\langle E_s \rangle$ with Ag content (at %)

CONCLUSION

It is seen that the average coordination no., number of constraints and the energetic parameter heat of atomization Optical gap and mean bond energy increases with increasing the Silver (Ag) content whereas lone-pair of electrons decrease with increasing In content. According to optical gap with composition approach of B.Angell the energetic parameter is proportional to the optical gap and increases with increasing Ag content.

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