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Study of Energetic diffusion of Zn-modified Ge-Sb-Te Chalcogenide glasses

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Abstract

In the present study we have discussed, how the energetic parameter (A) influences by same amount of Zinc in the two different Ge-Sb-Te glassy systems like $(Ge_8Sb_2Te_{11})_{100-x}Zn_x$ and $(Ge_2Sb_2Te_5)_{100-x}Zn_x$ where X = 0, 1, 2, 5, 10, 25. The effect of Zn modified Ge-Sb-Te chalcogenide glasses have been studied by using bond constraint and rigidity percolation theory. By using topological theory which is exhibited by covalent network glasses, the finding results has been discussed. The optical gap diffusion of Zn modified Ge-Sb-Te glassy systems is also discussed on the basis of topological constraints theory.

Keywords: Ge-Sb-Te Chalcogenide glasses, mean coordination number and energetic parameter.

Introduction

Since the chalcogenide materials have unique characterization properties, so they have drawn growing and significant attention in different engineering and scientific applications during the past few years. These are superior materials to any other materials in different manner, including phase reversal property, high packing density, quick data rates, mass replication and their different technological applications.

The Chalcogenide glasses are covalently bonded and connected networks. In the periodic table, elements from the 14-15-16 groups containing chalcogenide glasses (such as Ge-Sb-S glasses) and these elements mostly follows the Mott-rule[1-5] because the total coordination number of these elements follows this rule.

According to the Mott rule[1-5], the total coordination number is equals to 8-N, where N is the total number of valence electrons of the element. Due to the ability of transmit infrared light and their customizable optical and physical characteristics, these chalcogenide materials are attributed to their wide-ranging propensity for glass formation.

A diverse range of compositions in glass-forming systems, combined with excellent resistance to crystallization, produce glasses that possess optical characteristics like nonlinearity, photosensitivity, and transparency to infrared light. These properties can be finely tuned to optimize their performance for photonic applications[6-9].

There are various compositional chalcogenide glasses like Ge-Se-Te, Ge-In-Te, Ge-Se-In ...etc but the composition like Ge-Sb-Te has great attention because this composition has phase reversal property, have unique optical properties like optical band gap, Urbach gap and different technological optical applications in the field of photonics. Ge-Sb-Te glassy systems exhibit many remarkable properties for non-volatile memories such as high speed, high scalability, and non-volatility. These glassy systems promising candidate for data storage device in next- generations[10-14].

For better performance and improving the various properties of Ge–Sb–Te chalcogenide glassy systems, a great effort has been made by different researchers[15]. Researchers either altered the stoichiometric composition of Ge-Sb Te or by doping the host composition[15].

Researchers[15] had been explored to tune the structural, chemical thermal and optical properties by doping a wide range of do pants from transition metal elements like Copper (Cu), Titanium (Ti), Zinc (Zn), Nickle (Ni)and Silver (Ag).

Transition metal element doping of the Ge-Sb-Te glassy system is of great interest since it greatly improves the host lattice's properties. We have taken Zinc (Zn) in our study as transition metal element Because Zn has a weak bonding strength with Te and can therefore result in a quick crystallization speed for phase transition[16].

In the present study, we have reported that how the concentration of small amount of Zn can affect the optical properties like theoretical optical gap and energetic diffusion parameter (A) in different compositions of Ge-Sb-Te chalcogenide glassy systems like:

$(Ge_8Sb_2Te_{11})_{100-x}Zn_x$ and $(Ge_2Sb_2Te_5)_{100-x}Zn_x$
(X = 0, 1, 2, 5, 10, 25) on the basis of covalent network theory and topological theory.

Theoretical predictions and Discussion

Average coordination number: An essential metric for estimating some of the physical-chemical and thermal characteristics of chalcogenide alloys is the average coordination number <r>. The average coordination number and local structural units have a strong correlation with the physical characteristics of chalcogenide glasses. Two topological or percolation thresholds, known as mechanical and chemical thresholds, exist at <r>=2.4 and <r>=2.67 respectively, according to Phillips[17], Thorpe[18], and Tanaka's constraint theories[19,20].

These models predict a threshold at <r> = 2.4 and characterize the compositional dependence in terms of the average coordination number <r>. The network is rigid above <r> = 2.4 and floppy below it. The following formula has been used to determine the value of <r> for the compositions $(Ge_8Sb_2Te_{11})_{100-x}Zn_x$ and $(Ge_2Sb_2Te_5)_{100-x}Zn_x$(x = 0, 1, 2, 5, 10, 25).

$$<r>= \frac{\alpha X+\beta Y+\gamma Z+\delta W}{\alpha+\beta+\gamma+\delta}$$

Where: α, β, γ and δ are the atomic % of elements present in the chalcogenide alloy and X, Y, Z and W are their respective co-ordination numbers of a pure element. Ge, Sb, Te, and Zn are considered to have values of <r>as 4, 3, 2, and 4, respectively. According to topological models, the composition range is the threshold composition. Tables-1 and 2 list the values of <r>for the two sets of Zn-modified Ge-Se-Te chalcogenide glasses.

The Energetic Parameter: An indirect permitted transition is indicated by the absorption coefficient's spectral dependency, which can be confirmed by the energetic parameter Vs composition relation. The Angell suggestion[21] states that the energy parameter (A), which is determined by the following equation, correlates the compositional changes in the optical energy gap.

$$A=\frac{\varepsilon\Delta Eg}{k}$$

Where: ε = δ(<r> - 2), k = Boltzmann constant (1.38 x 10^{-23}J/Kel.), δ = an independent constant (0.55).

For the two glassy systems $(Ge_8Sb_2Te_{11})_{100-x}Zn_x$ and $(Ge_2Sb_2Te_5)_{100-x}Zn_x$, Figure-1 shows how the parameter (A) varies as a function of mean coordination number<r>. The trajectories of these two glassy systems reveal identical tendencies in the <r> dependency. The energetic parameter (A) grows as <r> increases initially, reaching a local maximum at <r> = 2.67.

For the $(Ge_8Sb_2Te_{11})_{100-x}Zn_x$ and $(Ge_2Sb_2Te_5)_{100-x}Zn_x$ (x = 0, 1, 2, 5, 10, 25) chalcogenide glassy systems, the computed values of theoretical energy gap Eg and energetic parameter (A) are reported in Table-1 and 2. As the value of <r> increases, the value of Eg drops. The proportional quantity of Ge-Zn, Zn-Sb, and Zn-Te bonds is what causes this decline in Eg[22-23].

The band gap is determined more by the GeSb2 structural unit than by the Zn-Se and Zn-Te links. All of these compositions seem to have the Ge-Sb, Ge-Te, and Ge-Ge bonds. Under the action of Zn, the number of Ge-Ge and Ge-Sb bonds decreases, resulting in a constant drop in Eg. Since The crystallization temperature dramatically changed to a higher value with a progressive rise in Zn doping concentration, giving the amorphous phase considerable thermal stability. High Zn concentration doping limited the fcc to hcp phase transition because Zn–Te and Zn–Sb bonds took the role of the Sb–Te link, which is primarily responsible for the phase transition from fcc to hcp phase. This resulted in a one-step crystallization between amorphous and fcc phases. Therefore, we get a diffused state that illustrates the relative sensitivity of the energetic parameter (A) when we add Zn to the varied ternary composition of Ge-Sb-Te with the same concentration[24].

Table-1: Calculated parameter values for $(Ge_8Sb_2Te_{11})_{100-x}Zn_x$ for X = 0, 1, 2, 5, 10, 25.

Glassy system	Average coordination no. <r>	Optical energy gap E_g(eV)	Energetic parameter (A X 10^3/Kel.)
$(Ge_8Sb_2Te_{11})_{100}$	2.90	0.6685	3.821
$(Ge_8Sb_2Te_{11})_{99}Zn_1$	2.91	0.6619	3.841
$(Ge_8Sb_2Te_{11})_{98}Zn_2$	2.92	0.6606	3.875
$(Ge_8Sb_2Te_{11})_{95}Zn_5$	2.95	0.6468	3.919
$(Ge_8Sb_2Te_{11})_{90}Zn_{10}$	3.01	0.6277	4.042
$(Ge_8Sb_2Te_{11})_{75}Zn_{25}$	3.17	0.5704	4.256

Table-2: Calculated parameter values for $(Ge_2Sb_2Te_5)_{100-x}Zn_x$ for X = 0, 1, 2, 5, 10, 25.

Glassy system	Average coordination no. <r>	Optical energy gap E_g(eV)	Energetic parameter (A X 10^3/Kel.)
$(Ge_2Sb_2Te_5)_{100}$	2.66	0.6092	2.564
$(Ge_2Sb_2Te_5)_{99}$Zn1	2.67	0.6059	2.589
$(Ge_2Sb_2Te_5)_{98}Zn_2$	2.68	0.6028	2.614
$(Ge_2Sb_2Te_5)_{95}Zn_5$	2.72	0.5931	2.723
$(Ge_2Sb_2Te_5)_{90}Zn_{10}$	2.79	0.5771	2.907
$(Ge_2Sb_2Te_5)_{75}Zn_{25}$	2.99	0.5286	3.337

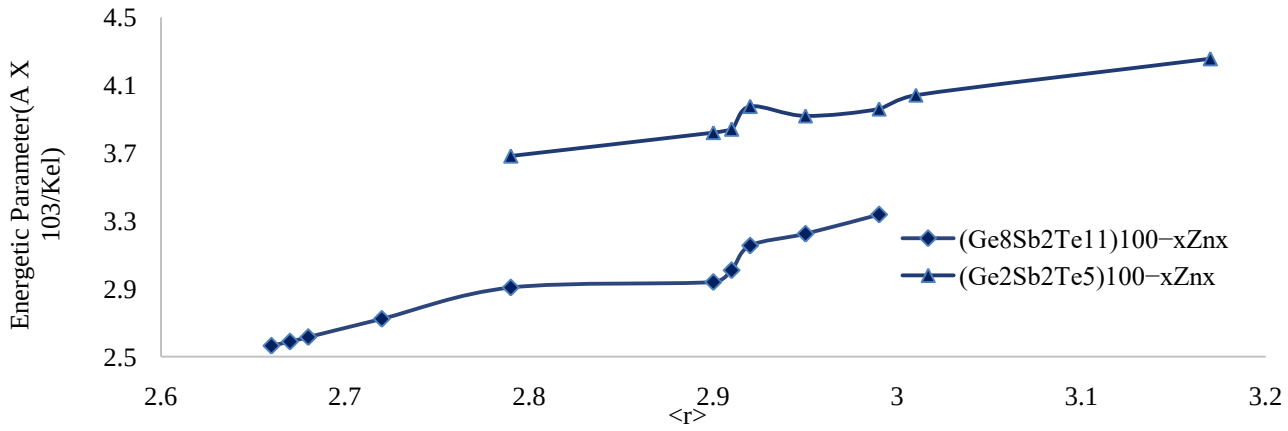

Figure-1: Variation of Energetic parameter (A) with <r> for the two sets of Zn doped Ge-Sb-Te Glasses.

Conclusion

From the calculated value of optical gap E_g and energetic parameter (A) for the two glassy systems $(Ge_8Sb_2Te_{11})_{100-x}Zn_x$ and $(Ge_2Sb_2Te_5)_{100-x}Zn_x$ as listed in Table-1 and Table-2, it is clear that the glassy system $(Ge_2Sb_2Te_5)_{100-x}Zn_x$ have less value of E_g and A than for $(Ge_8Sb_2Te_{11})_{100-x}Zn_x$ with the same concentration of Zn. This is due to the higher affinity/ coordination of Zn reorganizes the chemical environment, replacing weak, flexible Sb–Te links with Zn–Te and Zn–Sb bonds. These bonds produce the diffused state. So, both of them the glassy system $(Ge_2Sb_2Te_5)_{100-x}Zn_x$ is more preferable than $(Ge_8Sb_2Te_{11})_{100-x}Zn_x$ in different practical applications.

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