International Journal of Pure and Applied Physics.
ISSN 0973-1776 Volume 14, Number 2 (2018), pp. 131-135
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A Study of Physical Parameters of $Ge_{10}Bi_xSe_{80-x}Sn_{10}$ Glasses

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ABSTRACT

Chalcogenide glasses show a wide range of applications in optoelectronic devices. These materials are amorphous in nature, but shows interesting feature of having properties similar to those of crystalline semiconductors and so they are very useful for phase change devices. A wide range of combinations with one or more chalcogen elements (S, Se, Te) have been fabricated and their properties have been studied. In the present work, the various properties of $Ge_{10}Bi_xSe_{80-x}Sn_{10}$ (x = 2, 4, 6, 8, 10, 12, 14, 16 at. %) chalcogenide glasses with variation in atomic % of Bi have been discussed.

Keywords*:* Chalcogenide Glasses, Average Coordination Number, Electro negativity, Average Heat of Atomization, Cohesive Energy.

1. INTRODUCTION

The fast growing need of usage of modern technology has revolutionized the study of chalcogenide glasses in present time. Although they were studied some fifty years ago, interest in chalcogenide glasses has emerged significantly as glasses, crystals, and alloys find new life in the wide range of optoelectronic devices. Investigators have worked significantly to find their applications in various fields. They may be very useful in the various infrared based applications such as IR remote chemical or temperature sensors. These materials find vast applications as memory devices, optical fibers, reversible phase change optical recording materials etc [1-2].

In the present work, we have taken a quaternary composition of Ge-Bi-Se-Sn. In this the atomic % of Ge and Sn is taken as 10 and the concentration of Bi is varying from 2 to 16 atomic %. Various parameters such as average coordination number, electro negativity, heat of atomization, cohesive energy etc. are studied for $Ge_{10}Bi_xSe_{80-x}Sn_{10}$ (x=2, 4, 6, 8, 10, 12, 14, 16 at. %) composition based on the theoretical prediction.

2. MATERIAL AND METHODS

2.1 Average Coordination Number and Deviation from the Stoichiometry of Composition

The average coordination number (Z) was calculated using standard method [3] for the composition $Ge_{10}Bi_xSe_{80-x}Sn_{10}$ and Z is given by

$$z = \frac{\alpha C(Ge) + \beta C(Bi) + \gamma C(Se) + \delta C(Sn)}{\alpha + \beta + \gamma + \delta}$$

where $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ are the atomic % of Ge, Bi, Se and Sn respectively and C(Ge), C(Bi), C(Se) and C(Sn) are their respective coordination number. The parameter R can be determined for $Ge_{10}Bi_xSe_{80-x}Sn_{10}$ system, by using the relation given by [4]

$$R = \frac{\gamma C(Se)}{\alpha C(Ge) + \beta C(Bi) + \delta C(Sn)}$$

where $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ are atomic fractions of Ge, Bi, Se and Sn respectively. On the basis of the values for R, the chalcogenide systems can be organized into three different categories. The threshold at R=1 marks the minimum chalcogen content at which a chemically ordered network is possible without metal–metal bond formation. If the value of R>1, the system is shifting towards chalcogen rich. If the value of R<1, the system is shifting towards chalcogen poor.

2.2 Electronegativity

Electro negativity is explained with the different approaches by various investigators. Pauling defined electro negativity as the power of an atom or molecule to attract electron to it. It is defined as the geometric mean of all the constituents forming a compound. The electro negativities for Ge, Bi, Se and Sn according to Pauling scale are 2.01, 2.02, 2.55 and 1.96 respectively [4].

2.2 Average Heat of Atomization and Cohesive Energy

Pauling proposed the interesting relation to determine the average heat of atomization H_s, in case of ternary and higher order semiconductor materials. This can be explained by relation given below for the compounds like $Ge_{\boldsymbol{\alpha}}Bi_{\boldsymbol{\beta}}Se_{\boldsymbol{\gamma}}Sn_{\boldsymbol{\delta}}$ [5]

$$H_s = \frac{\alpha H_s^{Ge} + \beta H_s^{Bi} + \gamma H_s^{Se} + \delta H_s^{Sn}}{\alpha + \beta + \gamma + \delta}$$

where $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ are the atomic percentages of Ge, Bi, Se and Sn respectively.

The cohesive energy is the measure of average bond strength of the system. In glassy system $Ge_{10}Bi_xSe_{80-x}Sn_{10}$ (x = 2, 4, 6, 8, 10, 12, 14, 16 at. %) the cohesive energy can be calculated by summing the bond energies over all bonds expected in the system by using the relation.

$$CE = \sum C_i D_i$$

where C_i and D_i are the number of expected chemical bonds and energy of each bond respectively.

3. RESULT AND DISCUSSION

The value of Z varies from 2.42 to 2.56 and R varies from 1.81 to 1.00 for atomic % from 2 to 16. It is clear from the values so obtained that our system $Ge_{10}Bi_xSe_{80-x}Sn_{10}$ is chalcogen rich. The value of R at various atomic compositions of Bi is found to be greater than 1. The system is observed to be turning towards chalcogen poor with the increase in content of Bi in the system as it reduces overall chalcogen character.

The presence of Bi in the $Ge_{10}Bi_xSe_{80-x}Sn_{10}$ makes the system ionic in character. It is clear from the fig. 1 that values of electro negativity decreases with increase in concentration of Bi from 2 to 16 at %. This decrease in the electro negativity with increase in Bi is because the overall Se constituent decreases which has higher value of electro negativity.

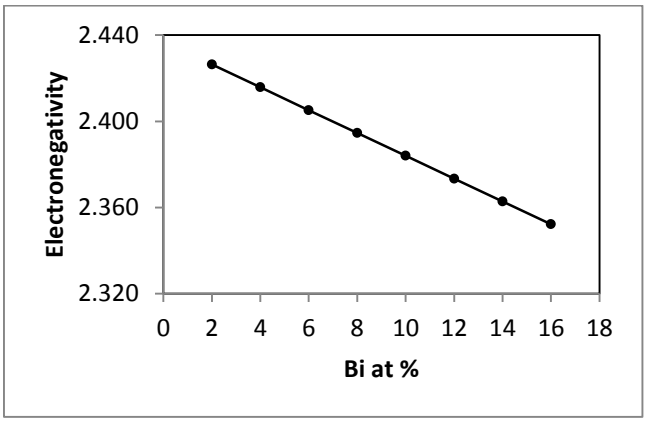

Fig. 1: Variation of electro negativity with Bi content

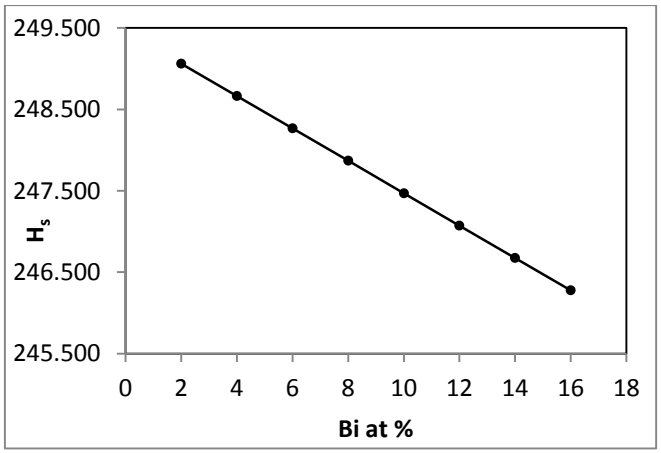

Fig. 2: Variation of heat of atomization H_s with Bi content

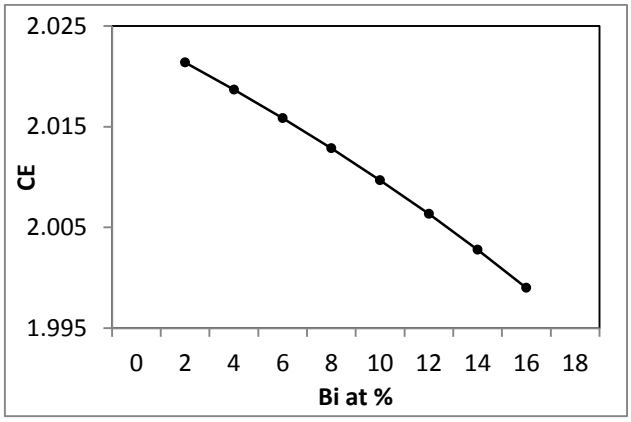

Fig. 3: Variation of CE with Bi content

Fig. 2 shows the graph of H_s with the increase in Bi content. The value of H_s is decreasing from 249.06 to 246.28 with the increase in the Bi atomic percentage. Fig. 3 shows that there is decrease in the value of cohesive energy with the increase in Bi content from 2 to 16 atomic %.

III. CONCLUSION

In the present work, we had studied a quaternary chalcogenide alloy comprising of Ge-Bi-Se-Sn. Here Ge and Sn have been fixed at 10 atomic %, and then studied the variation in various important physical parameters by varying the concentration of Bi from 2-16 atomic %. It has been established from the above results that physical properties in this system are highly composition dependent. The $Ge_{10}Bi_xSe_{80-x}Sn_{10}$ glass system is of special interest as it forms glasses over a wide domain of compositions. Adding Bi to this decreases the chalcogen concentration in this system. Here all the parameters were found to vary linearly with the variation in Bi content thus making this combination suitable for phase change optical recording.

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