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**Research Article**

# STUDY OF INFLUENCE OF Ge CONTENT ON PHYSICAL PARAMETER OF Ge-Se-Te SYSTEM

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## ABSTRACT

In the recent past, an adequate potential has been verified by so many distinguished researcher of germanium based and chalcogen enriched glassy alloys. In the present article, theoretical prediction of the effect of germanium on the physical parameters of $Ge_xSe_{50}Te_{50-x}$ (x = 10, 20, 30 and 40 at %) like, average coordination number, molecular weight, floppy mode, lone pair etc has been studied. It has been found that except the parameter R, molecular weight M, floppy mode f and lone pair L all other parameters are found to increase with the increase in Ge content.

## INTRODUCTION

Glasses are non-crystalline solids and described as a separate discipline in solid state physics. Non oxide glasses such as chalcogenide glasses are made up of one of the chalcogen elements (group VI elements) such as S, Se and (or) Te as a major constituent, in conjunction with more electropositive elements most commonly Ge and Ga.

Group VI elements S, Se, Te are most promising materials for various electronic, optoelectronic, optical memory switching devices, optical recording media and photonic applications. The chalcogenide glasses are studied by a number of researches, during the recent past. These materials can be used in reversible phase change optical recording devices (M. Abdel Rafea *et. al*, P. Sharma *et. al*, M.A. Majeed Khan *et al*, N. Mehta *et.al*.). These glasses are optically highly non-linear and useful for all optical switching, was reported by earlier researches (S.R. Ovinsky *et al*). The phase change material means we can reversibly switched the material between the amorphous and crystalline state and find application in rewritable optical recording (P.K.Jain *et al*, MHR Lankhorst *et al*, M. Saxena *et al*).

Se is widely used for various applications in many fields as optical recording media due to their excellent laser writer sensitivity, electrographic applications and xerography but short life time and low photo sensitivity are the some disadvantages of pure Selenium. To overcome this problem some impurity like Ge atoms is used to make alloys. This impurity enhances the sensitivity, crystallization temperature etc. which are more important for glass formation (R. Kumar *et al*, Sushil kumar *et al*, P. Boolchand *et al*).

The compositional dependence studies on glassy alloys were reported for binary element Ge-Se and ternary element Ge-Se-Te (J.C. Phillips *et al*, R. Ganesan *et al*, A. Sharma *et al*, S. Tiwari *et al*, S. S. Fouad *et al*, M. Saxena *et al*, A. George *et al*) In the present work we have incorporated the Ge in Se-Te alloy to form $Ge_xSe_{50}Te_{50-x}$ (x = 10, 20, 30 and 40 at %). Third elements generates compositional and configuration disorder in the material (S. Gupta *et al*).

This paper is concerned with the theoretical prediction of the physical parameters related to composition, viz. coordination number, constraints, cross-linking density, floppy mode, molecular weight, lone-pair electron, stoichiometry.

### *Average Coordination Number*

We know that coordination number of glasses varies with varying composition. Hence it is useful to calculate average coordination number <r>. Average coordination number <r> is

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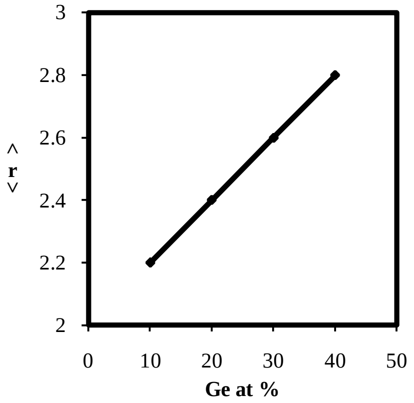
calculated by using the standard method (J.C. Phillips *et al*, P. Sharma *et al*). For the composition $Ge_xSe_{50}Te_{50-x}$ (x = 10, 20, 30 and 40 at %) average coordination number <r> is given by:

$$< r >= \frac{\alpha N_{Ge} + \beta N_{Se} + \gamma N_{Te}}{\alpha + \beta + \gamma}$$

where α, β, γ are concentrations (at %) of Ge, Se, Te respectively and $N_{Se} = 2$, $N_{Te} = 2$, $N_{Ge} = 4$ are their respective coordination number. The calculated values of average coordination number for $Ge_xSe_{50}Te_{50-x}$ (x = 10, 20, 30, 40 at %) lie in the range $2.2 < r < 2.8$ which inferred that <r> increases with Ge at % and system is compact as shown in Graph 1.



**Graph 1** Variation of Average Coordination Number

The glassy network is greatly influenced by mechanical constraints (Nc) which is greatly associated with the an average coordination number < r > and atomic bonding (J.C. Phillips *et al*).

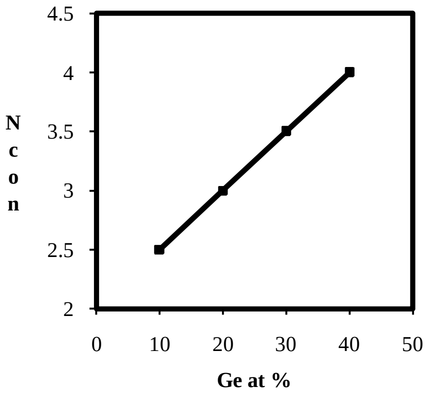
The number of Lagrangian bond-stretching constraints per atom is
$N_\alpha = < r >/2$
And, of bond-bending constraints is
$N_\beta = 2< r > - 3$
Hence the average number of constraints is given by
$N_c = N_\alpha + N_\beta$

For the case when all α and β constraints are intact and no dangling ends exist in the network, equation implies that the optimum mean coordination number is 2.40 which is known as the regiditty percolation threshold. Highly over coordinated or under-coordinated structures are not conducive to glass formation and, upon cooling, lead to crystalline solids.

In 1983, M. F. Thorpe (M.F.Thrope *et al*) pointed out that the number of floppy modes per atom, *f*, is found by the relation,
*f* = 3 – Nc (2)

When *f* → 0 then a glass network will become spontaneously rigid, defining a *floppy* to *rigid phase transition* (P.K. Gupta *et al*).

The calculated values of Nc with Z for $Ge_xSe_{50}Te_{50-x}$ (x = 10, 20, 30 and 40 at %) are given in. Graph 2 shows the variation of Nc with Ge at %. Here value of Nc increases from 2.5 to 4 with increase in Ge at.%, that indicates that Nc (The number of constraints) = Nd (number of degrees of freedom)

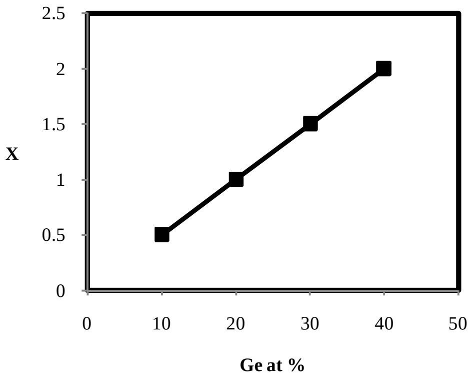


**Graph 2** Variation of number of constraints with Ge at. %

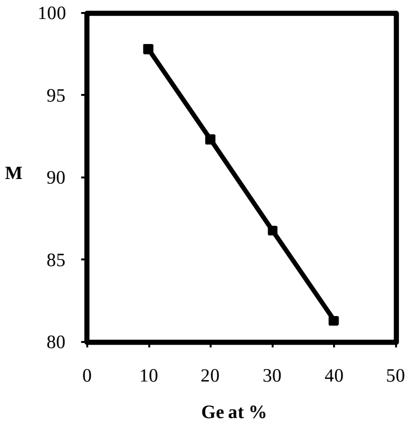
The cross-linking density(X) is given by (S.S.Foyad *et al*).

X = Nc – 2

The calculated values of cross linking density (X) and molecular weight (M) are shown in. From Graph 3 it is clear that the value X increase with increase in Ge content. Fig.4 shows the variation of M with Ge content.



**Graph 3** Variation of cross-linking density with Ge content at %



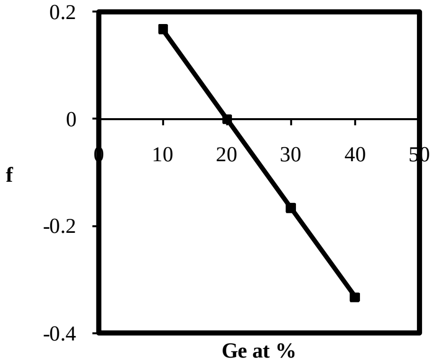
**Graph 4** Variation of Molecular weight with Ge content

According to Thorpe, the uncoordinated network having finite fraction of zero frequency normal vibrations modes termed as floppy modes in absence of weak long range forces. The fraction of floppy modes available in a network is given by

$$f = 2 - \frac{5 < r >}{6}$$

The values of f are listed in. It has been clear from the and Graph 5 that the value of f decreases and becomes more &

more negative (0.167 to -0.333) with increase in Ge content from 10 to 40 at. %. This rigidity of the system, which corresponds to a strong tendency for making glass (G. G. Naums *et al*).



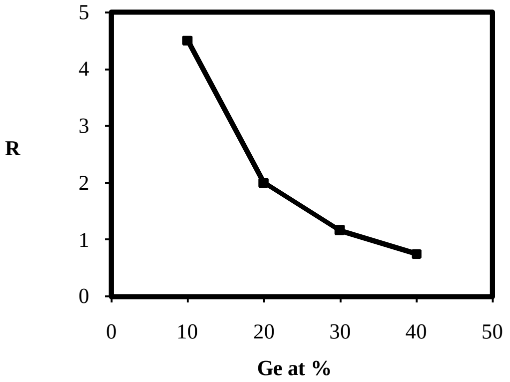
**Graph 5** Variation of floppy mode with Ge content at %

### *Deviation from the stoichiometry of composition*

The parameter R determines the deviation from stoichiometry and expressed as the ratio of content bond possibilities of total chalcogen atoms to that of non-chalcogen atoms. For $Ge_xSe_{50}Te_{40-x}$ (x = 10, 20, 30 and 40 at %) system, the parameter R is given by (S. Gupta *et al,* J. C. Mauro *et al*).

$$R = \frac{\beta Nse + \gamma N_{Te}}{\alpha N_{Ge}}$$

For R>1, the system is chalcogen rich, for R<1 system is chalcogen poor and R=1(point of existence of only hetropolar bonds) marks the minimum Selenium content at which a chemically network is possible without metal bond formation. From the Graph 6 it is clear that our system is turning from more chalcogen rich towards chalcogen poor with increase in content of Ge in system.



**Graph 6** Variation of Parameter R with Ge content

### *Role of lone pair electrons and glass forming ability*

The numbers of lone pair of electrons are calculated by using the relation:

L = V – <r>

Where L is the lone pair of the electrons, V is the valence electrons and <r> is the average coordination number. For the glassy system $Ge_xSe_{50}Te_{40-x}$ (x = 10, 20, 30 and 40 at %) the number of calculated lone pair of electrons are listed in.

It is observed that with increasing the Ge content the number of lone pairs of electrons goes on decreasing. This may be due to the interaction between Ge ion and lone pair electrons of bridging Se atom (A. Sharma *et al*). According to Zhenhua, the number of lone pair electrons for a binary number system must be greater than 2.6 and for a ternary system it must be greater than 1. In our system under investigation, the values of lone pair of electrons found to be greater than 1. So this explains the fact that the system can be obtained in glassy state.

The variation of L with Ge at % for $Ge_xSe_{50}Te_{40-x}$ (x = 10, 20, 30 and 40 at %) glassy system is shown in Graph 7 and calculated values are shown in.

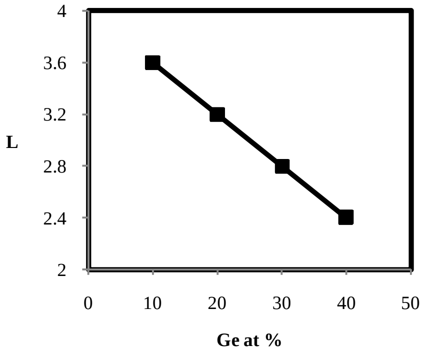


**Fig 7** Variation of lone-pair of electrons L with Ge content at %

## CONCLUSION

In the present work, important parameters viz. average coordination number, number of constraints, molecular weight, lone pair, stoichiometry, floppy mode etc., have been calculated theoretically for $Ge_xSe_{50}Te_{50-x}$ (x = 10, 20, 30 and 40 at %) system. It has been concluded from various figures given above that the values of almost all the parameters vary linearly with variation in concentration of Ge from 10 to 40 at. %. The value of parameter R shows that our system is more or less chalcogen rich for all at % of Ge. The results here clearly depict variations in almost all parameters with increasing the content of Ge from 10 to 40 at % and hence confirming the status of above mentioned combination good for optical recording.

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