

# Studies on Elastic Properties of Oxide Glass: A Theoretical Approach

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**Abstract:** *The present investigation discusses the elastic properties of oxide glasses, which can be measured by using theoretical models before the synthesis of glass. All the theoretical models are based on the chemical composition of the glass system. Evaluation of elastic moduli depending on the chemical composition was first time elaborated through Mackashima–Mackenzie Model. The semi-empirical formulation of this model is represented systematically. The calculation of essential parameters packing density and dissociation energy per unit volume is also discussed in the present investigation. Bond compression model based on the rigidity of the glass network and number bonds per unit volume is discussed with detailed formulation.*

**Index Terms -** Elastic moduli, Elastic properties, Mackashima–Mackenzie, Bond Compression

## I. INTRODUCTION

Amorphous state of the glass material is a fascinating property of supercooled liquids. When these supercooled liquids are cooled rapidly to avoid crystallization will form glassy state said to be the fourth state of matter [1, 2]. Due to the phenomenon of glass transformation connects the liquid and non-crystalline glassy state, which gives rise to a wide range of applications in daily life, electronic industry, materials preparation, laboratory wares, and a lot of natural phenomena. However, the exact and comprehensive physical understanding of the glass transition and glass natures is considered to be one of the most challenging problems in condensed matter physics and material science [3]. Due to the random disordered structure, the characterization of the glasses are very difficult, and this leads to problems for understanding the formation, deformation, fracture, nature, and the structure–properties relationship of the glasses [4].

Glass materials are having the characteristic property of highly transparent and brittle materials, which can be easily broken due to the impact of thermal or mechanical energy [5]. Thermal shock resistant and high fracture surface toughened glasses attained a great deal of interest by electronic industries [6]. These parameters are directly correlate with the elastic constants of materials such as Young's modulus, bulk modulus, shear modulus, hardness etc. The purpose of this research article is to focus on the investigation of theoretical models for calculating the elastic parameters based on chemical composition of oxide glasses.

## II. THEORETICAL BACKGROUND

The estimation of elastic moduli based on glass composition is very useful for the development of glass materials. The most widely used model is the one proposed by Mackashima and Mackenzie, which expresses elastic moduli as a function of packing density and dissociation energy per unit volume of the glass [4]. A considerable number of studies on the agreement between the experimentally measured elastic moduli and those theoretically calculated using Mackashima and Mackenzie model are available in the literature for different kinds of glasses [7-10]. It has been found that, although the theoretical prediction of elastic moduli, as well as their tendencies through series of silicate and tellurite glasses, is quite satisfactory, the elastic moduli of phosphate and borate glasses are greatly overestimated. In the case of phosphate glasses, this over-estimation originated from the presence of double P=O bonds which do not contribute to the network stiffness. In the case of borate glasses, the overestimation has been attributed to the weak bonds between BO<sub>3</sub> triangles [11].

### Mackashima–Mackenzie Model

According to Mackashima–Mackenzie model, the theoretical expression for the prediction of elastic constants of glasses in terms of a packing density of the atoms and the dissociation energy of the oxide glass constituents per unit volume [12]. Mackashima and Mackenzie (1973) considered that Young's modulus can be given by the product of the dissociation energy per unit volume ( $G$ ) and the packing density of ions ( $V_t$ ) [13]. For example, in a single-component glass such as silicate or multi-component glasses  $E$  can be expressed as:

$$E = 2V_t \sum G_i X_i \quad (1)$$

Where  $G_i$  is nothing but the dissociation energy per unit volume of the oxide which can be defined as the volume density of binding energy [14]. The packing density  $V_t$  can be defined as the ratio between the minimum theoretical volume occupied by the ions and the corresponding ionic volume of the glass which can be given by using the relation:

$$V_t = \left(\frac{1}{V_m}\right) \sum_i X_i V_i \quad (2)$$

Where,  $V_m$  is the molar volume of the oxide glass composition which is the ratio of the effective molecular weight ( $M$ ) and the density ( $\rho$ ).  $X_i$  is the mole fraction of oxide constituent atoms  $i$ , and  $V_i$  is a packing factor which can be obtained by using the following relation for oxide of the form  $A_xO_y$ :

$$V_i = 6.023 \times 10^{23} \left[ \left( \frac{4\pi}{3} \right) (xR_A^3 + yR_O^3) \right] \quad (3)$$

Where,  $R_A$  and  $R_O$  are the respective standard ionic radii e.g. Pauling's or Shannon's ionic radii of metal and oxygen atoms of oxides. Thus, the elastic moduli (e.g. Young's modulus  $E$ , Bulk modulus  $K$ , Shear modulus  $S$  etc.) and Poisson's ratio of oxide glass composition can be obtained with theoretical formulae as given below.

$$E = 83.6 V_t \sum_i G_i X_i \quad (4)$$

$$K = \gamma V_t E = 100 V_t^2 \sum_i G_i X_i \quad (5)$$

$$S = \frac{3EK}{9k-E} \quad (6)$$

$$\mu = \left( 0.5 - \frac{1}{7.2V_t} \right) = \left( \frac{E}{2S} - 1 \right) \quad (7)$$

In this expression, all the parameters are given in SI units then the elastic moduli are measured in GPa. If the units of dissociation energy per unit volume  $G_i$  is given in kilocalories per cubic centimeter. All theoretical expressions of elastic moduli are found to be in good agreement with the experimentally calculated one except the non-boron containing glasses [15]. Since borate glasses are having variable coordinated boron with ( $B_2O_3$ ) glass former composition. Hence, the glass former boron changes its coordination number from 3 to 4 with the addition of the network modifier producing trigonal [ $BO_3$ ] to tetragonal [ $BO_4$ ] groups [7]. To avoid this problem of different borate group formation the dissociation energy per unit volume should be calculated by considering the exact fraction of 3-coordinated  $N_3$  and 4-coordinated  $N_4$  borate units.

### Bond Compression Model

According to the bond compression model, the rigidity of glass networks can be described by high cross-link density and number of network bonds per unit volume apparently glass composition will have high bulk moduli. It was assumed that isotropic deformation can change the network bond length ( $l$ ). Based on this assumption, Bridge and Higazy [16] successfully attempt for theoretical computation of bulk moduli ( $K_{bc}$ ). Furthermore, the bond compression model was extended and derived the expressions for bulk modulus and a number of network covalent bonds per unit volume ( $n_b$ ) of multi-component oxide glasses which can be given as:

$$K_{bc} = \left( \sum_i x_i n_i r_i^2 f_i \right) \frac{N_A}{9V_m} \quad (8)$$

$$n_b = \frac{nN_A}{V_m} \quad (9)$$

Where  $n_i$  is the coordination of the cation,  $r$  is the bond length and  $f_i$  be the bond stretching force constant of a covalent bond between the cation and oxygen atom of glass former oxide e.g. Si-O, B-O, Ge-O, P-O etc. which depends on the crosslink density of constituent oxides. The bulk modulus  $K_{bc}$  is directly proportional to a number of network covalent bonds per unit volume. Another theoretical model named as ring deformation model was proposed by Bride B.[17] and later extended by Abd El-Moneim [5]. Ring deformation model is mainly based on the crosslink density and ring diameter of the glass network.

In this way, one can determine the elastic constants theoretically by using above discussed models for the study of structural defects and improvement of mechanical properties prior to synthesis of glass system. The theoretical results obtained should be cross verified by using the experimental techniques such as pulse-echo technique or superposition method for ultrasonic velocity measurement through the glass samples. By using the longitudinal and shear velocity all the elastic constants (e.g. Longitudinal  $L$ , shear  $G$ , Young's  $E$ , bulk modulus  $K$  and Poisson's ratio  $\mu$ , Debye temperature  $\theta_D$ , glass softening temperature  $T_s$  etc.) can be determined [18].

### III. CONCLUSION

Elastic moduli and the parameters can be obtained from the theoretical calculation given by Makishima–Mackenzie and the bond compression model. The results of elastic properties are found to be very useful to get the information about the structure, stability and mechanical properties of glasses. There is no need to go for the direct experimental synthesis of glass system. Prediction of all the essential structure and elastic property details can be derived prior to preparation of glass by using the theoretical approach of present study.

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