

## Theoretical Elastic Moduli of TeO<sub>2</sub> – B<sub>2</sub>O<sub>3</sub> – SiO<sub>2</sub> Glasses

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### Abstract

In this work, the elastic moduli of silica based borotellurite glass system with compositional formula; [(TeO<sub>2</sub>)<sub>0.7</sub>(B<sub>2</sub>O<sub>3</sub>)<sub>0.3</sub>]<sub>1-x</sub>(SiO<sub>2</sub>)<sub>x</sub> with x= 0.0, 0.1, 0.2, 0.3 and 0.4 was studied using theoretical models. Makishima and Mackenzie, bond compression, Rocherulle, and ring deformation models were employed in the calculation of the elastic moduli, Poisson ratio, packing density, dissociation energy, cross-link density, average stretching force constant and the glass network ring size of the studied glasses. The values of the elastic moduli obtained from the Makishima and Mackenzie model were found to be lower than those obtained from the Rocherulle model and the value from the bond compression model was reported to be highest among the three models. In all the models, the elastic moduli increased with an increase in the concentration of silica in the glass composition. Therefore, it satisfied the original intention of improving mechanical strength to achieve high Young modulus which is considered in glasses fiber drawing/manufacturing.

**Keywords:** Elastic moduli, packing density, Poisson ratio, Silica glasses.

### INTRODUCTION

Study of various properties (ranging from structural, elastic, mechanical, optical and spectroscopic properties) of tellurite glasses have been reported in many publications in the recent years due to their promising advantage over other glasses in many technological applications [1]–[4]. TeO<sub>2</sub> composition in glasses is utilized to provide a high refractive index, easy fabrication, good infrared region transmittance, high optical nonlinearity, and low phonon energies. With boron oxide combination, the borotellurite glass system is expected to possess high rare earth ion solubility, greater hardness, easier fabrication as well as improved optical transparency [5], [6]. To obtain greater thermal and chemical stability, and when optical transparency is required in excitation and lasing wavelengths in most glasses, SiO<sub>2</sub> combination is considered. In most glasses for special applications requiring mechanical strength, the SiO<sub>2</sub> composition is mostly considered [7].

Elastic and mechanical properties are essential in determining glass applicability in many technological applications [8], [9]. Glasses developed with high Young's modulus have been given much consideration in research and high strength glass fibers' manufacturing. This consideration has prompted glass scientists to begin to work on theoretical models for calculations of elastic moduli as well as the Poisson ratio of various glass compositions put under study.

Foremost of them all is the work of Makishima and Mackenzie which focusses on the elastic moduli and Poisson ratio determination using the packing density, dissociation energy per unit volume of oxide constituent as well as the chemical composition of the glasses under study [10]. Rocherulle and coworkers modified the Makishima and Mackenzie model by introducing some modifications to packing factor expression. The authors also introduced a thermodynamic factor through substitution of oxygen with nitrogen in the vitreous network of glasses and found good agreements between the calculated elastic moduli and their corresponding experimentally measured values [11]. Another theoretical model introduced mainly for the calculation of bulk modulus on the assumption that bond lengths in glass networks are changed by an isotropic deformation not bond angles [12]. The ring deformation model is an extension of the bond compression model which calculates the ring size in a 3-D network of atoms in the glass structure [13].

In this work, we employ the Makishima and Mackenzie model, the Rocherulle model, the bond compression model, and the ring deformation model in our calculations of elastic moduli, Poisson ratio, and other parameter explaining the nature and the structure of the glasses under study.

## MODELS

This section presents the four theoretical models adopted in this work for the study of the elastic properties of the studied glasses. The models used include the Makishima-Mackenzie model, the Rocherulle model, the bond compression model, and the ring deformation model.

### Makishima and Mackenzie model

The Makishima and Mackenzie model proposed a theoretical approach to determining the elastic moduli of oxide glasses with consideration to the chemical composition ( $x_i$ ) of the constituting oxide, individual oxides' packing densities ( $V_i$ ), and their corresponding dissociation energies ( $G_i$ ) [14]. The glass Young modulus is expressed in terms of the packing density ( $V_t$ ), and the dissociation energy ( $G_i$ ) as;

$$E_m = 2V_t \sum_i G_i x_i = 2V_t G_t \quad (1)$$

From the oxides' packing density,  $V_t$  can be determined by the next equation

$$V_t \left( \frac{\rho}{M} \right) \sum_i V_i x_i \quad (2)$$

Where  $M$  = glass molecular weight,  $\rho$  = glass density,  $x_i = i_{th}$  component's molar fraction (i), and  $V_i$  is calculated for an oxide ( $A_x O_y$ ) as:

$$V_i = N_A (4\pi/3) (xR_A^3 + yR_O^3) \quad (3)$$

where  $R_O$  and  $R_A$  represent the ionic radii of oxygen and cation respectively [15]. In the model of Makishima and Mackenzie, bulk modulus ( $K_m$ ), Shear modulus ( $G_m$ ) and Poisson ratio ( $\sigma_m$ ) for oxide glasses on any component are calculated as follows:

$$K_m = 1.2V_t E \quad (4)$$

$$G_m = (3EK/9K - E) \quad (5)$$

$$\sigma_m = (E/2G_m - 1) \quad (6)$$

### Rocherulle Model

Modified expression of the Makishima and Mackenzie model was proposed by Rocherulle et al. (1989). The packing density,  $V_i$  in the Makishima-Mackenzie model is replaced with  $C_i$  which is expressed as follows:

$$C_i = N_A(4\pi\rho/3M)(xR_A^3 + yR_O^3) \quad (7)$$

For glasses of poly component nature, the factor  $C_t$  is therefore expressed as follows:

$$C_t = \sum_i C_i x_i \quad (8)$$

$$C_t = \sum_i \frac{\rho_i}{M_i} V_i x_i \quad (9)$$

The Young Modulus ( $E_r$ ), bulk modulus ( $K_r$ ), and the shear modulus ( $G_r$ ) are calculated as in equations (1), (4), and (5) respectively. The basic difference between the two models is that the Makishima and Mackenzie model takes into consideration the bulk density and molecular weight of the glass, while the Rocherulle model considers the individual oxides' density and molecular weights into consideration [11].

### Bond Compression and Ring Deformation Models

The theoretical model of bond compression takes into consideration the atomic networking in a material and the bond stretching force constants between them to theoretically estimate the elastic characteristics of the material [16]. For single oxide glass systems, the bulk modulus is obtained as;

$$K_{bc} = \frac{n_b \bar{F} r^2}{9} \quad (10)$$

The expression for a multicomponent oxide glasses is given as;

$$K_{bc} = (\rho N_A / 9M) \sum_i (x n_f \bar{F} r^2)_i \quad (11)$$

Where  $\bar{F}$  the average stretching force constant, and  $n_b$  is the bond number per unit volume and  $r$  is the cation-anion bond length.

The bond number per unit volume is calculated as;

$$n_b = (n_f \rho N_A / M) \quad (12)$$

$n_f$  is the number of bonds per unit glass formula,  $N_A$  is Avogadro's number,  $\rho$  is the glass density, and  $M$  is the glass molecular weight [17]. The stretching force constant ( $f$ ) is deduced for multi-component glass using the expression as reported by [18] as;

$$\bar{F} = \frac{\sum_i (x n_f f)_i}{\sum_i (x n_f)_i} \quad (13)$$

The calculations of Poisson's ratio ( $\sigma_{bc}$ ) and the corresponding average crosslink density ( $\bar{n}_c$ ) of the glasses are deduced as in equations (3.64) and (3.65) respectively.

$$\sigma_{bc} = 0.28(\bar{n}_c)^{-0.25} \quad (14)$$

$$\bar{n}_c = \frac{1}{\eta} \sum_i (x n_c N_c)_i \quad (15)$$

where  $n_c =$  oxide ( $i$ ) cross-link number per cation and  $N_c =$  cation number per unit glass formula. The total number of cations per unit glass formula for a multicomponent glass system ( $\eta$ ) is obtained as;

$$\eta = \sum_i (x N_c)_i \quad (16)$$

$K_{bc}$  and  $\sigma_{bc}$  calculated is used to calculate the Young, shear, and longitudinal moduli. The ring deformation model is used to theoretically estimate the atomic ring size of the glass system. The model uses the experimental bulk modulus ( $K_e$ ) values and the bending force constant ( $F_b$ ) values to estimate the atomic ring size [19]. In the proximation process, the average stretching force constant is used in place of  $F_b$ . Equation (17) is used in the determination of the atomic ring size as;

$$K_e = 0.0106 F_b (l)^{-3.84} \quad (17)$$

The vale  $l$  represents the atomic ring size and is defined as the diameter of the external ring. The ring perimeter can be determined using  $l$  as bond number x bond length divide by  $\pi$  [20].

## RESULTS AND DISCUSSIONS

In this section the results and discussions of the elastic moduli, Poisson ratio, packing density, dissociation energy, packing factor, bond length, stretching force constant other parameters calculated theoretically using the Makishima-Mackenzie model, Rocherulle model, Bond compression model and Ring deformation model.

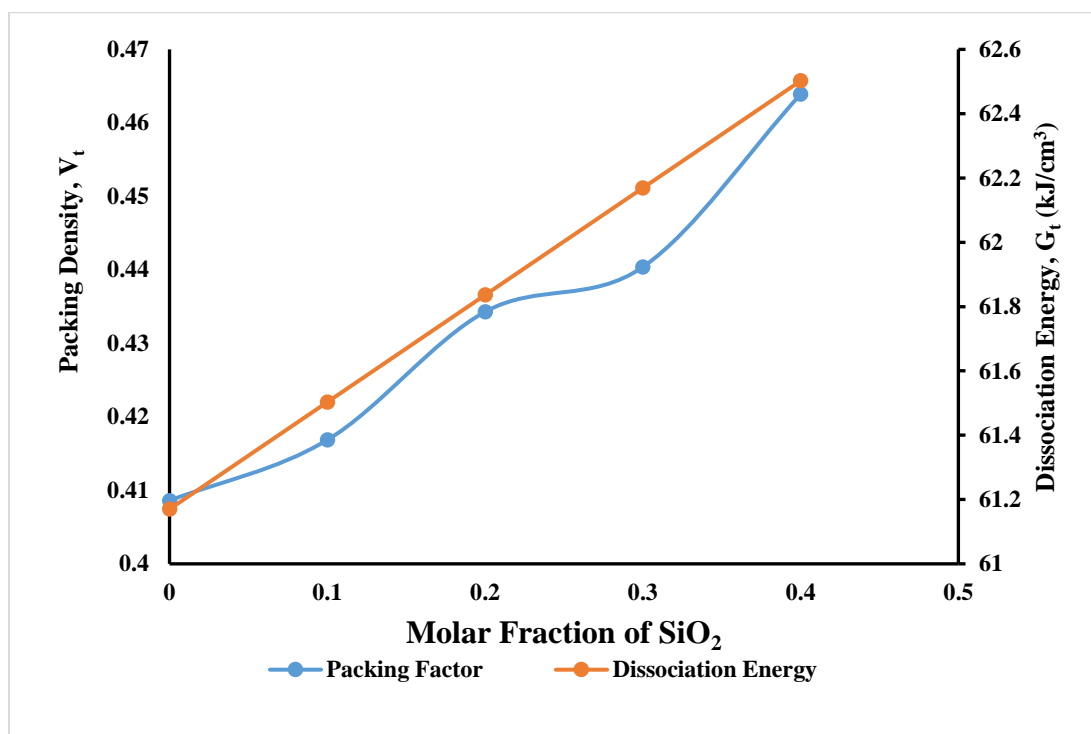
### Makishima-Mackenzie Model

The Makishima-Mackenzie model proposes a theoretical approach to determine the Young modulus of oxide glasses based on the oxides' atomic packing and their bond strengths. The model uses the bulk molecular weight and densities of the glasses [21]. The model proposed a correlation between the average dissociation energy and the packing density of the constituent atoms/oxides of glass material to its elastic moduli [15].

**Table 1:** Packing Density, Dissociation Energy, Young Modulus, Bulk modulus, Shear Modulus and Poisson Ratio for  $[(\text{TeO}_2)_{0.7} (\text{B}_2\text{O}_3)_{0.3}]_{1-x} (\text{SiO}_2)_x$  glass system

$x(\text{mol}\%)$	$V_t (\text{cm}^{-3})$	$G_t (\text{kJ}/\text{cm}^3)$	$E_m (\text{GPa})$	$K_m (\text{GPa})$	$G_m (\text{GPa})$	$\sigma_m$
0	0.4086	61.1700	49.9887	24.5108	21.5452	0.1601
0.1	0.4169	61.5030	51.2762	25.6499	21.9726	0.1668
0.2	0.4343	61.8360	53.7102	27.9913	22.7547	0.1802
0.3	0.4404	62.1690	54.7569	28.9371	23.1116	0.1846
0.4	0.4639	62.5020	57.9879	32.2799	24.1496	0.2006

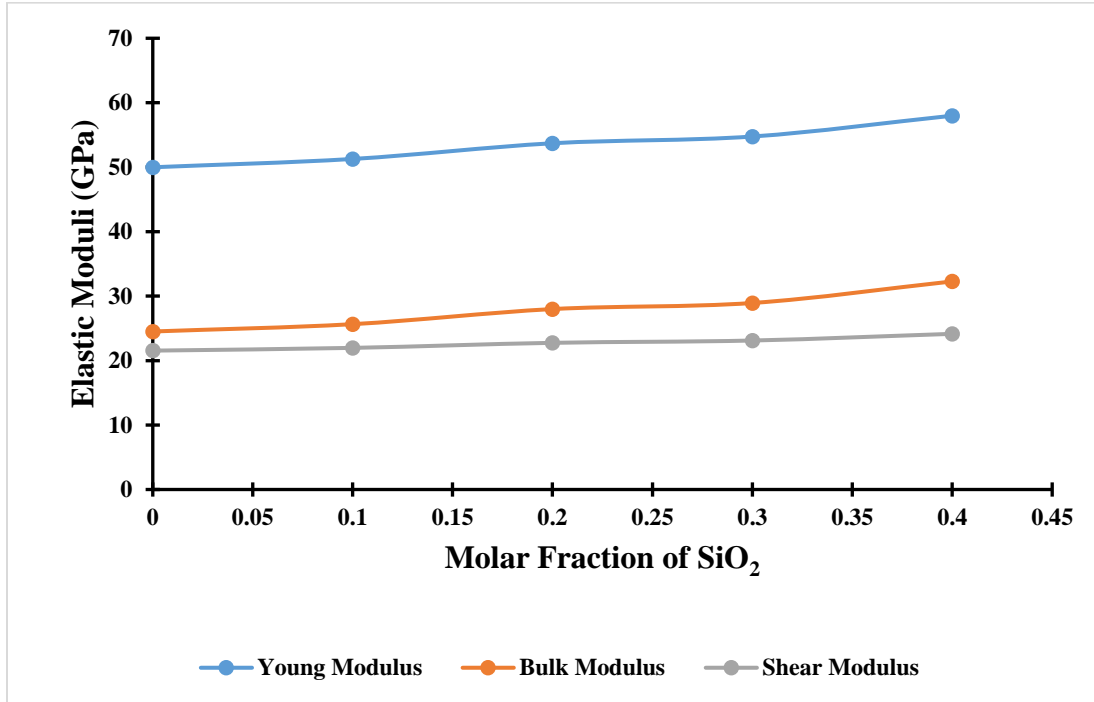
Table 1 presents the values of the packing density, dissociation energy, Young modulus, bulk modulus, shear modulus, and Poisson ratio obtained using the theoretical model proposed by Makishima and Mackenzie [10].



**Figure 1:** Variation of packing density and dissociation energy with molar fraction of SiO<sub>2</sub> for [(TeO<sub>2</sub>)<sub>0.7</sub> (B<sub>2</sub>O<sub>3</sub>)<sub>0.3</sub>]<sub>1-x</sub> (SiO<sub>2</sub>)<sub>x</sub> glass system

Figure 1 and Table 1 illustrate the variation of the packing density and the dissociation energy [(TeO<sub>2</sub>)<sub>0.7</sub> (B<sub>2</sub>O<sub>3</sub>)<sub>0.3</sub>]<sub>1-x</sub> (SiO<sub>2</sub>)<sub>x</sub> Glass system against the SiO<sub>2</sub> molar fraction. Both the packing density and the dissociation energy of the glasses were observed to have increased from 0.408605 to 0.463889 and 61.170 to 62.502 kJ/cm<sup>3</sup> respectively. Although the packing density depends on the glass's bulk density, the increase in the packing density observed in these glasses might not be associated with density increase. The packing density value increase with SiO<sub>2</sub> concentration might be mostly associated with the decrease in the molar volume [22]. The molar volume decrease leads to a decrease in the interstitial spaces between atoms of the glass network. This increases interatomic connectivity and glass rigidity (El-Moneim, 2012).

The increase in the dissociation energy [(TeO<sub>2</sub>)<sub>0.7</sub> (B<sub>2</sub>O<sub>3</sub>)<sub>0.3</sub>]<sub>1-x</sub> (SiO<sub>2</sub>)<sub>x</sub> Glass system with an increase in the SiO<sub>2</sub> concentration may be due to the higher dissociation energy of SiO<sub>2</sub> (64.5 kJ/cm<sup>3</sup>) introduced into the system. The SiO<sub>2</sub> substitutes are more TeO<sub>2</sub> with lower dissociation energy (54 kJ/cm<sup>3</sup>) than B<sub>2</sub>O<sub>3</sub> with higher dissociation energy (77.9 kJ/cm<sup>3</sup>) than SiO<sub>2</sub> [21]. The dissociation energy increase may also be associated with the increase in the TeO<sub>3</sub> conversion to TeO<sub>4</sub> with the higher energy of dissociation [24].



**Figure 2:** Elastic moduli for the  $[(\text{TeO}_2)_{0.7} (\text{B}_2\text{O}_3)_{0.3}]_{1-x} (\text{SiO}_2)_x$  glass system

Figure 2 illustrates the variation of elastic moduli with  $\text{SiO}_2$  concentration increase. The Young, bulk, and shear moduli increased from 49.9887 to 57.9879 GPa, 24.5108 to 32.2799 GPa, 21.5108 to 24.1496 GPa with increased  $\text{SiO}_2$  concentrations. The values of the theoretically calculated elastic moduli are higher compared to the experimentally obtained elastic moduli values. This might be due to the increase in both the average packing density and dissociation energy resulting from the substitution of lower dissociation energy of  $\text{TeO}_2$  ( $54 \text{ kJ/cm}^3$ ) molecule [25], with higher dissociation energy of  $\text{SiO}_2$  ( $64.5 \text{ kJ/cm}^3$ ) molecule [26]. Although the moduli values calculated using the Makishima and Mackenzie are higher than the experimentally obtained values, they presented the same value increase with an increase in the  $\text{SiO}_2$  concentration. The values' difference according to Makishima could reach up to 30% [11]. The Poisson ratio presented by the Makishima and Mackenzie model for the studied rice husk silicate borotellurite glass system have lower values than the experimentally obtained.

### Rocherulle Model

Rocherulle's model proposed a modification to the theoretical model presented by Makishima and Mackenzie. The model takes into consideration the individual oxide elastic properties in determining the overall elastic properties of oxide glasses. Individual oxide densities and molecular masses were considered instead of the bulk glass density and molecular weight used in the Makishima- Mackenzie model.

**Table 2:** The Packing Factor, Young Modulus, Bulk Modulus, Shear Modulus and Poisson Ratio for  $[(\text{TeO}_2)_{0.7} (\text{B}_2\text{O}_3)_{0.3}]_{1-x} (\text{SiO}_2)_x$  glass system

x(mol%)	$C_t (\text{cm}^{-3})$	$E_r (\text{GPa})$	$K_r (\text{GPa})$	$G_r (\text{GPa})$	$\sigma_r$
0	0.5940	72.6700	51.7992	28.6965	0.2662
0.1	0.5963	73.3485	52.4852	28.9439	0.2671
0.2	0.5986	74.0301	53.1773	29.1922	0.2

0.3	0.6009	74.7147	53.8753	29.4415	0.2689
0.4	0.6032	75.4024	54.5793	29.6919	0.2697

Table 2 presents the packing density, elastic moduli and the Poisson ratio values for  $[(\text{TeO}_2)_{0.7} (\text{B}_2\text{O}_3)_{0.3}]_{1-x} (\text{SiO}_2)_x$  Glass system. The packing density of the glasses increased from 0.5940 to 0.6032 as the concentration of  $\text{SiO}_2$  increased from 0 to 40%. The increase in the values of the packing density may be attributed to a higher packing factor ( $C_i$ ) of  $\text{SiO}_2$  (0.617) compared to the substituted  $\text{TeO}_2$  (0.522) [27]. The increase may be due to an increase in network connectivity and rigidity [28]. The Poisson ratio value increased from 0.2662 to 0.2697 with  $\text{SiO}_2$  concentration increase from 0 to 40%. The Poisson ratio increase is associated with an increase in glass connectivity and rigidity. The increase can also be associated with an increase in the concentration of  $\text{TeO}_4$  in the network [29].

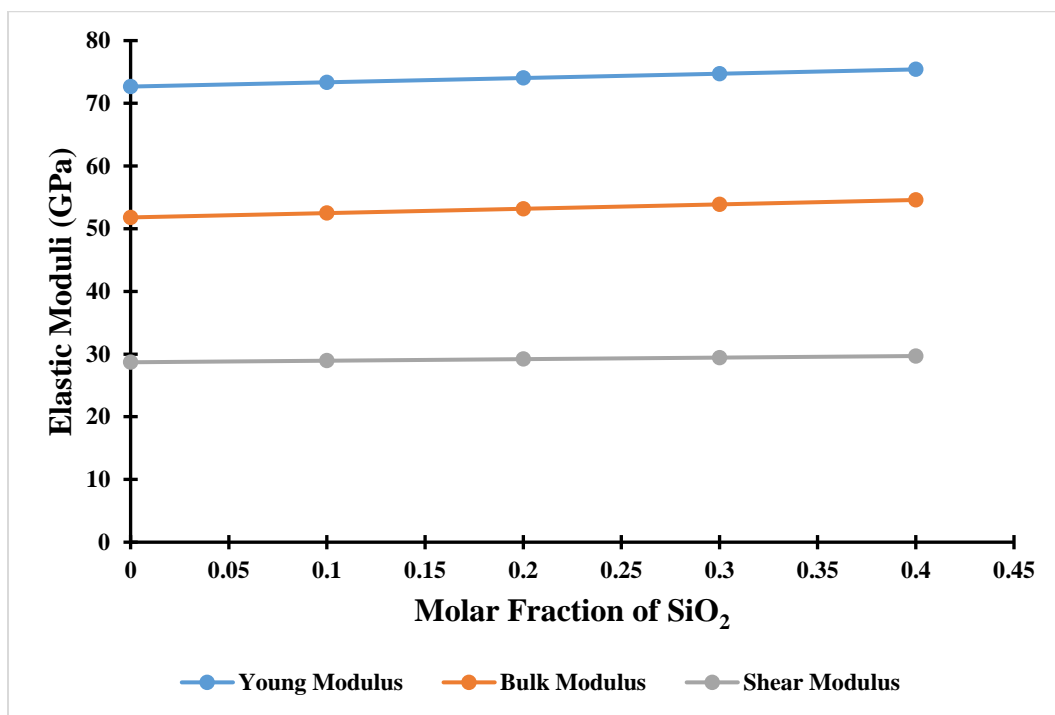


Figure 3: Elastic moduli for the  $[(\text{TeO}_2)_{0.7} (\text{B}_2\text{O}_3)_{0.3}]_{1-x} (\text{SiO}_2)_x$  glass system

Table 3: Oxides' Coordination numbers, packing densities ( $V_i$  and  $C_i$ ), Dissociation Energies ( $G_i$ ), Bond Length ( $r$ ), and Stretching Force constant ( $F$ )

Oxide	CN	$V_i$ ( $\text{cm}^3/\text{mol}$ )	$G_i$ ( $\text{kJ}/\text{cm}^3$ )	$C_i$	$r$ (nm)	$F$ ( $\text{Nm}^{-1}$ )
$\text{SiO}_2$	4	14.000	64.500	0.617	0.161	432
$\text{B}_2\text{O}_3$	4	20.800	77.900	0.762	0.138	660
$\text{TeO}_2$	4	14.700	54.000	0.522	0.199	216
$\text{Er}_2\text{O}_3$	6	38.276	27.319	0.815	0.225	149

Figure 3 and Table 3 presents the variation of the elastic moduli of  $[(\text{TeO}_2)_{0.7} (\text{B}_2\text{O}_3)_{0.3}]_{1-x} (\text{SiO}_2)_x$  Glass system with a molar fraction of  $\text{SiO}_2$ . The Young, bulk and shear moduli increased from 72.6700 to 75.4024 GPa, 51.7992 to 54.5793 GPa and 28.6965 to 29.6919 GPa respectively as the  $\text{SiO}_2$  concentration was increased from 0 to 40%. The increase in the elastic moduli reflects the experimental trend of the elastic moduli increase with  $\text{SiO}_2$  concentration, although the Rocherulle model data presented higher values of the elastic moduli compared to the experimental data. The increase in the elastic moduli is associated with an increase in the glass rigidity in the glass network as confirmed by the increased packing density and decreased molar volume of the glass system [30], [31]. The moduli of elasticity are structural configuration dependent parameters [22].

### Bond Compression and Ring Deformation Models

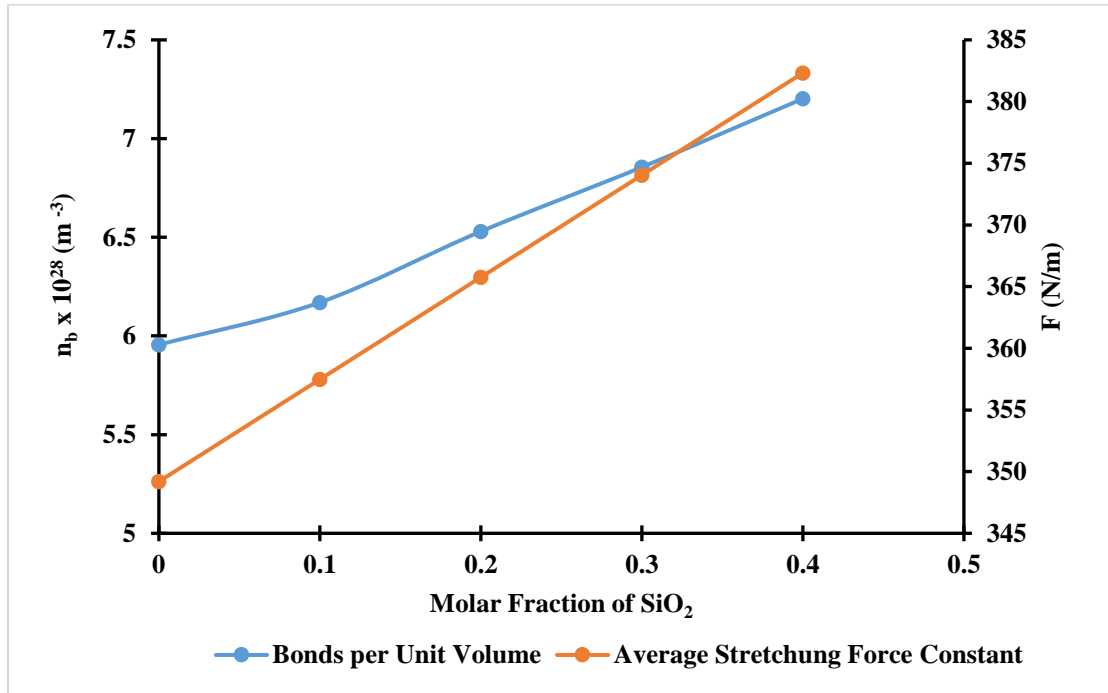
The bond compression model presents a theoretical approach to the determination of the bulk modulus of oxide glasses. The model proposes a dependence of material's bulk modulus on the average stretching force constant and the bond per unit volume number of the glass system under study. The bulk modulus dependence on the average ring size of the glass network is also presented in this model.

**Table 4:** Bond per unit volume number ( $n_b$ ), Bulk modulus, Bulk modulus ratio ( $K_{bc}/K_e$ ), Atomic ring size ( $\ell$ ) and Stretching Force Constant ( $F$ ) for  $[(\text{TeO}_2)_{0.7} (\text{B}_2\text{O}_3)_{0.3}]_{1-x} (\text{SiO}_2)_x$  glass system

$x$	$n_b \times 10^{28} (\text{m}^{-3})$	$K_{bc} (\text{GPa})$	$K_{bc}/K_e$	$\ell (\text{nm})$	$F (\text{N/m})$	$n_c$
0	5.9553	64.5712	3.0026	0.6329	349.2	2.4615
0.1	6.1700	66.8996	3.0326	0.6325	357.48	2.4252
0.2	6.5296	70.7982	3.1719	0.6344	365.76	2.3871
0.3	6.8552	74.3286	3.2875	0.6360	374.04	2.3471
0.4	7.2020	78.0883	3.3166	0.6329	382.32	2.3051

Figure 4 and Table 4 illustrate the variation of the bond number per unit volume ( $n_b$ ) and the average stretching force constant of the  $[(\text{TeO}_2)_{0.7} (\text{B}_2\text{O}_3)_{0.3}]_{1-x} (\text{SiO}_2)_x$  Glass system. The value of the  $n_b$  increased from  $5.9553 \times 10^{28}$  to  $7.2020 \times 10^{28} \text{ m}^{-3}$  with  $\text{SiO}_2$  concentration increase from 0 to 40% in the glass system. The increase may be associated with atomic close packing observed in the molar volume decrease. This is also confirmed with the observed increase in the packing density of the glasses. The increase may also be attributed to the increase  $\text{TeO}_3$  to  $\text{TeO}_4$  units' conversion with increasing concentration of  $\text{SiO}_2$  in the network [15], [32], [33].

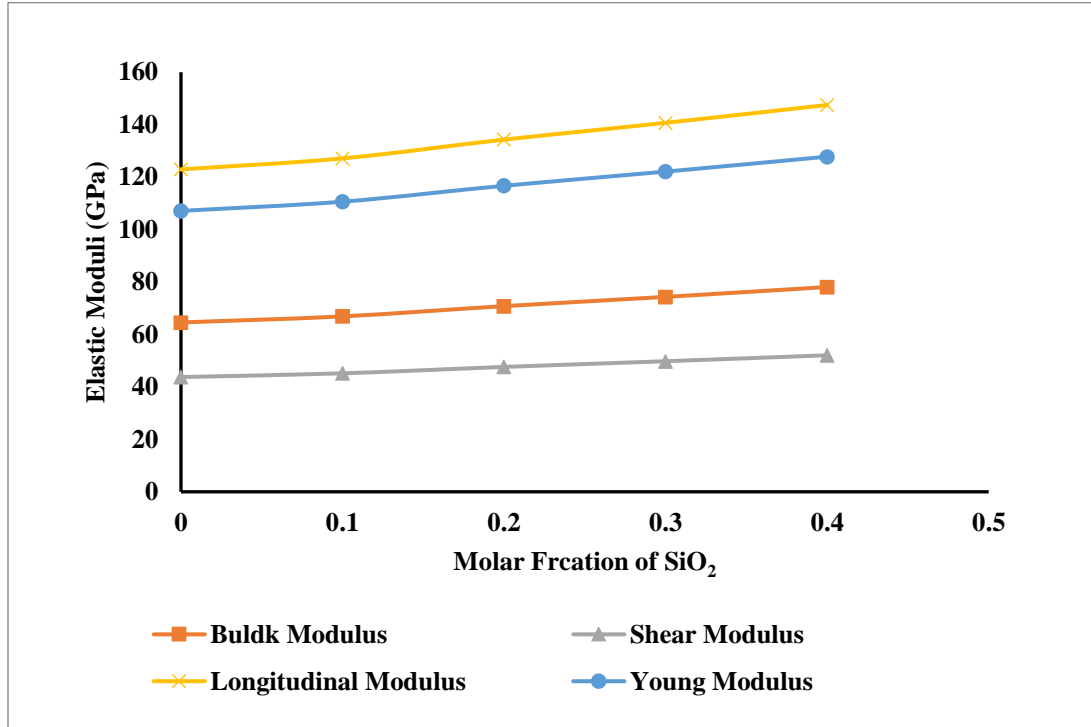




**Figure 5:** Bond per unit volume and the average stretching force constant variation with the molar fraction of SiO<sub>2</sub> for [(TeO<sub>2</sub>)<sub>0.7</sub> (B<sub>2</sub>O<sub>3</sub>)<sub>0.3</sub>]<sub>1-x</sub> (SiO<sub>2</sub>)<sub>x</sub> glass system

The average stretching force constant increased from 349.2 to 382.32 N/m as the SiO<sub>2</sub> molar fraction in the [(TeO<sub>2</sub>)<sub>0.7</sub> (B<sub>2</sub>O<sub>3</sub>)<sub>0.3</sub>]<sub>1-x</sub> (SiO<sub>2</sub>)<sub>x</sub> Glass system increased from 0 to 40%. The increase in the value may be attributed to the substitution of TeO<sub>2</sub> with a lower stretching force constant (216 N/m) with SiO<sub>2</sub> (432 N/m). The increase might also be due to shorter bond length of Si-O in SiO<sub>2</sub> (161 nm) as compared to that of Te-O in TeO<sub>2</sub> (199 nm) [15], [25], [34].

The elastic moduli variation of [(TeO<sub>2</sub>)<sub>0.7</sub> (B<sub>2</sub>O<sub>3</sub>)<sub>0.3</sub>]<sub>1-x</sub> (SiO<sub>2</sub>)<sub>x</sub> glass system with SiO<sub>2</sub> molar fraction is presented in Figure 6 and Table 6. The bulk, shear, longitudinal and Young moduli increased from 64.5712 to 78.0882 GPa, 43.7697 to 52.0663 GPa, 122.9308 to 147.51.01 GPa, 107.1079 to 127.7959 GPa respectively. The increase in the elastic moduli might be associated with increased connectivity and rigidity of the glasses. It may also be attributed to the increasing concentration of TeO<sub>4</sub> in the glass network with the introduction of more SiO<sub>2</sub> [16], [35].

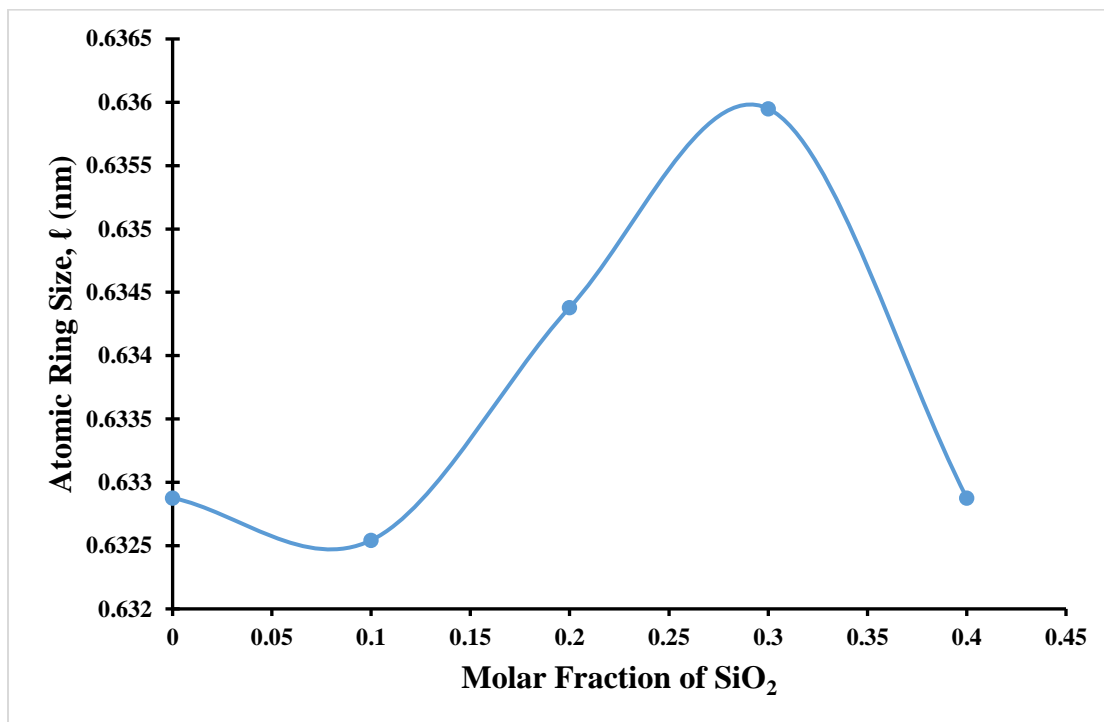


**Figure 6:** Elastic moduli variation with the molar fraction of  $\text{SiO}_2$  for the  $[(\text{TeO}_2)_{0.7} (\text{B}_2\text{O}_3)_{0.3}]_{1-x} (\text{SiO}_2)_x$  glass system

**Table 6:** The Elastic Moduli and Poisson for  $[(\text{TeO}_2)_{0.7} (\text{B}_2\text{O}_3)_{0.3}]_{1-x} (\text{SiO}_2)_x$  glass system

$x$	$K_{bc}$ (GPa)	$G_{bc}$ (GPa)	$L_{bc}$ (GPa)	$E_{bc}$ (GPa)	$\sigma_{bc}$
0	64.5712	43.7697	122.9308	107.1079	0.2235
0.1	66.8996	45.1806	127.1403	110.6358	0.2244
0.2	70.7982	47.6245	134.2976	116.7052	0.2252
0.3	74.3286	49.7871	140.7114	122.0996	0.2262
0.4	78.0883	52.0663	147.5101	127.7959	0.2272

The Poisson ratio value for the  $[(\text{TeO}_2)_{0.7} (\text{B}_2\text{O}_3)_{0.3}]_{1-x} (\text{SiO}_2)_x$  glass system as shown in Table 6 increased from 0.2235 to 0.2272 with the increase in the  $\text{SiO}_2$  concentration. The increase in the Poisson ratio is always connected to glass rigidity and network connectivity. Hence, the increase may be attributed to an increase in material (atomic) packing with an increase in the  $\text{SiO}_2$  concentration [33].



**Figure 7:** Atomic ring size variation with molar fraction of SiO<sub>2</sub> for [(TeO<sub>2</sub>)<sub>0.7</sub> (B<sub>2</sub>O<sub>3</sub>)<sub>0.3</sub>]<sub>1-x</sub> (SiO<sub>2</sub>)<sub>x</sub> glass system

Figure 7 presents the value of the atomic ring size for [(TeO<sub>2</sub>)<sub>0.7</sub> (B<sub>2</sub>O<sub>3</sub>)<sub>0.3</sub>]<sub>1-x</sub> (SiO<sub>2</sub>)<sub>x</sub> glass system. The value has not shown any uniformity with an increase in the SiO<sub>2</sub> concentration. A decrease in the atomic ring size is usually attributed to an increase in network connectivity and rigidity. It is associated with an increase in the close packing of atoms in the glass system. This may be due to the conversion of TeO<sub>3</sub> to TeO<sub>4</sub> and the formation of more BO<sub>3</sub> with non-bridging oxygen [25], [30].

## CONCLUSION

Makishima and Mackenzie, bond compression, Rocherulle's, and ring deformation models were employed in this work for the theoretical study of the elastic moduli of [(TeO<sub>2</sub>)<sub>0.7</sub> (B<sub>2</sub>O<sub>3</sub>)<sub>0.3</sub>]<sub>1-x</sub> (SiO<sub>2</sub>)<sub>x</sub> glass system. The values of the Young, bulk, and shear moduli calculated using the Makishima and Mackenzie model increased from 49.9887 to 57.9879 GPa, 24.5708 to 32.2799 Gpa, and 21.5452 to 24.1496 Gpa respectively with an increase in SiO<sub>2</sub> concentration. On the Rocherulle model, the moduli increased respectively from 72.6700 to 75.4024 Gpa, 51.7992 to 54.5793 Gpa, and 28.6965 to 29.6919 Gpa. Also, the values on the bond compression model increased respectively from 107.1079 to 127.7959 Gpa, 64.5712 to 78.0883 Gpa, and 43.7697 to 52.0663 Gpa, in addition to the calculated longitudinal modulus which increased from 122.9308 to 147.5101 Gpa. The Poisson ratio value ranged from 0.1601 to 0.2006, 0.2000 to 0.2697, and 0.2235 to 0.2272 respectively for Makishima and Mackenzie, Rocherulle, and bond compression models. The atomic ring size was also calculated using the ring deformation model and the ring size values indicated non-uniformity with SiO<sub>2</sub> concentration. Increase in the elastic moduli shown by all the models suggested that the addition of SiO<sub>2</sub> improved moduli of elasticity in glasses and the observed wide variation in the values of the moduli of elasticity suggested that only one of the models can be used for the study of the elastic moduli of the studied glasses.

## REFERENCES

- [1] S. A. A. Umar, M. K. K. Halimah, K. T. T. Chan, and A. A. A. Latif, "Physical, structural and optical properties of erbium doped rice husk silicate borotellurite (Er-doped RHSBT) glasses," *J. Non. Cryst. Solids*, vol. 472, no. July, pp. 31–38, 2017, doi: 10.1016/j.jnoncrysol.2017.07.013.
- [2] M. K. H. A. A. Awshah, A. M. Hamza, K. T. C. S. A. Umar, and S. H. Alazoumi, "Effect of neodymium nanoparticles on optical properties of zinc tellurite glass system," *J. Mater. Sci. Mater. Electron.*, vol. 31, no. 2020, pp. 3785–3794, 2020, doi: 10.1007/s10854-020-02907-9.
- [3] S. H. Alazoumi *et al.*, "Optical properties of zinc lead tellurite glasses," *Results Phys.*, vol. 9, no. March, pp. 1371–1376, 2018, doi: 10.1016/j.rinp.2018.04.041.
- [4] M. N. Azlan, M. K. Halimah, S. S. Hajer, A. B. Suraini, Y. Azlina, and S. A. Umar, "Enhanced Optical Performance of Tellurite Glass Doped with Samarium Nanoparticles for Fiber Optics Application," *Chalcogenide Lett.*, vol. 5, no. May, pp. 215–229, 2019.
- [5] M. K. Halimah *et al.*, "Effect of erbium nanoparticles on structural and spectroscopic properties of bio-silica borotellurite glasses containing silver oxide," *Mater. Chem. Phys.*, vol. 236, no. June, p. 121795, 2019, doi: 10.1016/j.matchemphys.2019.121795.
- [6] S. A. Umar, M. K. Halimah, A. M. Hamza, and A. A. Abdulbaset, "The Structural, Physical and Optical Properties of Borotellurite Glasses Incorporated with Silica from Rice Husk," *J. Sci. Math. Lett.*, vol. 6, no. 2018, pp. 32–46, 2018.
- [7] S. A. Umar *et al.*, "Optical and structural properties of rice husk silicate incorporated borotellurite glasses doped with erbium oxide nanoparticles," *J. Mater. Sci. Mater. Electron.*, vol. 30, no. 2019, pp. 18606–18616, 2019, doi: 10.1007/s10854-019-02213-z.
- [8] S. A. Umar, M. K. H. M. N. Azlan, L. U. G. G. Ibrahim, and A. F. A. A. M. Hamza, "Structural, elastic and thermo-physical properties of - Er 2 O 3 nanoparticles doped bio-silicate borotellurite glasses," *SN Appl. Sci.*, vol. 291, no. 2, pp. 1–10, 2020, doi: 10.1007/s42452-020-2112-x.
- [9] H. A. A. Sidek, R. El-Mallawany, K. A. Matori, and M. K. Halimah, "Effect of PbO on the elastic behavior of ZnO–P2O5 glass systems," *Results Phys.*, vol. 6, pp. 449–455, 2016, doi: 10.1016/j.rinp.2016.07.014.
- [10] A. Makishima and J. D. Mackenzie, "Direct calculation of Young's modulus of glass," *J. Non. Cryst. Solids*, vol. 12, no. 1, pp. 35–45, 1973, doi: 10.1016/0022-3093(73)90053-7.
- [11] J. Rocherulle, C. Ecolivet, M. Poulain, P. Verdier, and Y. Laurent, "Elastic moduli of oxynitride glasses. Extension of Makishima and Mackenzie's theory," *J. Non. Cryst. Solids*, vol. 108, no. 2, pp. 187–193, 1989, doi: 10.1016/0022-3093(89)90582-6.
- [12] H. A. A. Sidek, R. El-Mallawany, K. A. Matori, and M. K. Halimah, "Effect of PbO on the elastic behavior of ZnO-P2O5 glass systems," *Results Phys.*, vol. 6, no. August, pp. 449–455, 2016, doi: 10.1016/j.rinp.2016.07.014.
- [13] R. El-mallawany and A. Abd El-Moneim, "Comparison between the Elastic Moduli of Tellurite and Phosphate glasses," *Phys. Stat. Sol.*, vol. 62, no. 166, pp. 829–834, 1998.
- [14] Y. B. Saddeek, "Ultrasonic study and physical properties of some borate glasses," *Mater. Chem. Phys.*, vol. 83, no. 2004, pp. 222–228, 2004, doi: 10.1016/j.matchemphys.2003.09.051.
- [15] S. H. Alazoumi, H. A. A. Sidek, M. K. Halimah, K. A. Matori, M. H. M. Zaid, and A. A. Abdulbaset, "Synthesis and elastic properties of ternary ZnO-PbO-TeO2 glasses," *Chalcogenide Lett.*, vol. 14, no. 8, pp. 303–320, 2017.
- [16] A. A. El-Moneim and A. Abd El-Moneim, "Bond compression bulk modulus and Poisson's ratio of the polycomponent silicate glasses," *Mater. Chem. Phys.*, vol. 70, no. 3, pp. 340–343, 2001, doi: 10.1016/S0254-0584(00)00519-8.
- [17] R. Laopaiboon and C. Bootjomchai, "Physical properties and thermoluminescence of glasses designed for radiation dosimetry measurements," *Mater. Des.*, vol. 80, pp. 20–27, 2015, doi: 10.1016/j.matdes.2015.05.002.
- [18] Y. B. Saddeek, "Structural analysis of alkali borate glasses," *Phys. B*, vol. 344, pp. 163–175, 2004, doi: 10.1016/j.physb.2003.09.254.
- [19] H. Afifi, S. Marzouk, A. Hesham, and M. Samier, "Ultrasonic velocity and elastic moduli of heavy metal tellurite glasses," vol. 80, no. 2, pp. 517–523, 2003, doi: 10.1016/S0254-0584(03)00099-3.
- [20] M. S. Gaafar, S. Y. Marzouk, H. A. Zayed, L. I. Soliman, and A. H. S. El-deen, "Structural studies and mechanical properties of some borate glasses doped with different alkali and cobalt oxides," *Curr. Appl. Phys.*, vol. 13, no. 1, pp. 152–158, 2013, doi: 10.1016/j.cap.2012.07.007.
- [21] A. Abd El-Moneim, H. Y. Alfifi, A. A. El-Moneim, and Y. A. Hassan, "Approach to dissociation energy and elastic properties of vanadate and V2O5-contained glasses from single bond strength: Part I," *Mater. Chem. Phys.*, vol. 207, pp. 271–281, 2018, doi: 10.1016/j.matchemphys.2017.12.057.
- [22] Y. B. Saddeek, "Study of elastic moduli of lithium borobismuthate glasses using ultrasonic technique," *J. Non. Cryst. Solids*, vol. 357, no. 15, pp. 2920–2925, 2011, doi: 10.1016/j.jnoncrysol.2011.03.034.

- [23] A. A. El-Moneim, "Correlation between acoustical and compositional parameters of borate and tellurite glasses," *Mater. Chem. Phys.*, vol. 135, no. 2–3, pp. 653–657, 2012, doi: 10.1016/j.matchemphys.2012.05.040.
- [24] A. A. El-Moneim and A. Abd El-Moneim, "Correlation between acoustical and compositional parameters of borate and tellurite glasses," *Mater. Chem. Phys.*, vol. 135, no. 2–3, pp. 653–657, 2012, doi: 10.1016/j.matchemphys.2012.05.040.
- [25] R. A. H. A. H. El-mallawany, *Tellurite Glasses Handbook: Physical Properties and Data*. Florida: CRC Press LLC, 2002.
- [26] Y. B. Saddeek, L. Abd, and E. Latif, "Effect of TeO<sub>2</sub> on the elastic moduli of sodium borate glasses," *Phys. B*, vol. 348, pp. 475–484, 2004, doi: 10.1016/j.physb.2004.02.001.
- [27] A. Makishima and J. D. Mackenzie, "Calculation of bulk modulus, shear modulus and Poisson's ratio of glass," *J. Non. Cryst. Solids*, vol. 17, no. 2, pp. 147–157, 1975, doi: 10.1016/0022-3093(75)90047-2.
- [28] T. Rouxel and E. Properties, "Elastic Properties and Short-to Medium-Range Order in Glasses," *J. Am. Ceram. Soc.*, vol. 90, no. 10, pp. 3019–3039, 2007, doi: 10.1111/j.1551-2916.2007.01945.x.
- [29] L.-G. G. Hwa, C. L. Lu, and L.-C. C. Liu, "Elastic moduli of calcium alumino-silicate glasses studied by Brillouin scattering," *Mater. Res. Bull.*, vol. 35, no. 8, pp. 1285–1292, 2000, doi: 10.1016/S0025-5408(00)00317-2.
- [30] Y. B. Saddeek, "Elastic properties of Gd<sup>3+</sup>-doped tellurovanadate glasses using pulse-echo technique," *Mater. Chem. Phys.*, vol. 91, pp. 146–153, 2005, doi: 10.1016/j.matchemphys.2004.11.005.
- [31] R. A. Tafida *et al.*, "Structural, optical and elastic properties of silver oxide incorporated zinc tellurite glass system doped with Sm<sup>3+</sup> ions," *Mater. Chem. Phys.*, vol. 246, no. February, p. 122801, 2020, doi: 10.1016/j.matchemphys.2020.122801.
- [32] Y. B. Saddeek and L. A. El Latif, "Effect of TeO<sub>2</sub> on the elastic moduli of sodium borate glasses," *Phys. B Condens. Matter*, vol. 348, no. 1–4, pp. 475–484, May 2004, doi: 10.1016/j.physb.2004.02.001.
- [33] L. Hasnimulyati, M. K. Halimah, A. Zakaria, S. A. Halim, and M. Ishak, "A comparative study of the experimental and the theoretical elastic data of Tm<sup>3+</sup>-doped zinc borotellurite glass," *Mater. Chem. Phys.*, vol. 192, pp. 228–234, 2017, doi: 10.1016/j.matchemphys.2017.01.086.
- [34] A. Abd El-Moneim, "Bond compression bulk modulus and Poisson's ratio of the polycomponent silicate glasses," *Mater. Chem. Phys.*, vol. 70, no. 3, pp. 340–343, 2001, doi: 10.1016/S0254-0584(00)00519-8.
- [35] Y. B. Saddeek, "Structural and acoustical studies of lead sodium borate glasses," *J. Alloys Compd.*, vol. 467, pp. 14–21, 2009, doi: 10.1016/j.jallcom.2007.11.126.