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Atomic-Scale Observation of Room and Low-Temperature Ultrasonic Properties of Tellurite Glasses

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Abstract

Theoretical analysis of room temperature bulk modulus and low-temperature ultrasonic attenuation coefficient in the glass system (1-x)TeO2-xV2O5, x= 20, 25, 30, 35, 40 mol % was achieved. The bond compression (BC) and Makishima-Mackenzie (MM) models were used to interpret room-temperature bulk modulus K. The main parameters used were: average cross-link density, number of network bonds per unit volume, and average atomic ring size (λ). Analyses of low-temperature (300-150 K) ultrasonic attenuation (α) at 2, 4, 5, and 6 MHz were achieved by calculating: potential energy, centers of energy loss, elongation, and contraction of the two-well potential. Also, the deformation potential is found to be sensitive to the variations of the modifier content. The analysis revealed a sensitive effect of variation of modifier contents for elongation or contraction of the dual-well potential. The number of centers of energy loss is related to the elastic moduli as a function of the modifier content. Correlation between room temperature bulk modulus and ultrasonic attenuation coefficient has been achieved.

1-Introduction:

The advanced glass materials or ‘functional glasses’ are new glasses used for new technological purposes. New tellurite glasses containing transition metal oxides (TMO) or rare earth oxides (REO) have been prepared by the melt quenching technique [1, 2]. Technological applications of tellurite glasses had been started in 1992 [2] when the DC electrical conductivity of tellurite glasses, in the temperature range of 300-150 K, increased by increasing the γ-irradiation dose. Moreover, a broad emission spectrum of the width of 121 nm peaked at a wavelength of 1550 nm had been measured for erbium titanium-tungsten tellurite glasses [3]. From 2018 to 2022 gamma-ray and neutron shielding features of tellurite glasses were achieved to be used in nuclear shielding areas [4]. Besides that, borotellurite glass systems doped with erbium and erbium nanoparticles have been achieved and glasses with erbium nanoparticles got a higher refractive index to be a candidate for photonic applications [5]. Moreover, in 2022, Tm3+/Er3+/Sm3+ tri-doped TeO2-Li2O-ZnO glasses...
have been achieved for temperature sensors using color emissions and for generating white light sources were investigated and these glasses are promising platforms for optical temperature sensing [6].

The elastic properties of glasses are of great importance. The investigation of the elastic properties of glasses as a function of composition is very informative about the structure of glasses and they are directly related to the interatomic potentials. An extensive number of publications on the measurement of elastic properties of glasses, by using the ultrasonic non-destructive pulse-echo technique have been achieved [7-9]. The impact of the above finding is clear in the international scientific attention paid to tellurite glasses and the uses of these glasses in multifunctional applications like; visible to infrared down conversion of Er$^{3+}$ doped tellurite glass for luminescent solar converters and float, borosilicate, and tellurites as cover glasses in Si photovoltaics optical properties and performances under sunlight [10-14].

The objective of the present work is to analyze and correlate between room temperature elastic moduli [15] and low-temperature ultrasonic attenuation [16] for the semiconducting tellurite glasses in the form (1-x) TeO$_2$-xV$_2$O$_5$, where x = 20, 25, 30, 35, and 40 mole %.

2-Analysis and Discussions:

2-1 Room Temperature Elastic Moduli

Table. 1 collected the selected room temperature experimental values of density, molar volume, bulk modus, and Poisson's ratio of the investigated binary (1-x)TeO$_2$-xV$_2$O$_5$ glasses [15]. A gradual decrease in density of the studied TeO$_2$–V$_2$O$_5$ glasses is observed as TeO$_2$ is replaced by V$_2$O$_5$. At first sight, the variation of density with composition is well understandable from the variation of density of the oxide constituents. The respective densities of TeO$_2$ and V$_2$O$_5$ are 5.670 and 3.357 g/cm$^3$. It is clear from Table 1 that the, by increasing vanadium oxide content, the bulk modulus increased from 27.2 to 39.40 GPa and Poisson’s ratio decreased from 0.360 to 0.346. Values for the theoretical bulk modulus (K$_{bc}$), Poisson’s ratio ($\sigma_{bc}$), and ring diameter ($\bar{\ell}$) were calculated according to the bond compression model and ring deformation models [17-20] by using the next relations:

$$K_{bc} = \frac{n_b r^2 F}{9}, \quad \sigma_{bc} = 0.28 (\bar{n}_c)^{0.25}, \quad K=0.0106 F (\bar{\ell})^{3.84}$$

(1)

Where, $n_b$ is the number of network bonds per unit volume, $r$ is the cation-anion bond length =1.99 nm for TeO$_2$ and 0.1196 nm for V$_2$O$_5$ [15, 21], $F$ is the average first-order stretching force constant = 216 N/m for TeO$_2$ and 277 N/m for V$_2$O$_5$, respectively [15, 21], and $\bar{n}_c$ is the average crosslink density. The calculated $K_{bc}$ and $\sigma_{bc}$ values are given in Table 2. As can be seen from this table $K_{bc}$ decreased from 73.3 to 64.2 GPa as the V$_2$Os increased from 20 to 45 mol%. These values are higher than the experimentally measured bulk modulus K. Also, the number of bonds per unit
volume \( n_b \) decreased from \( 7.56 \times 10^{28} \) to \( 6.48 \times 10^{28} \) m\(^{-3}\) in the same composition range. Theoretically, the decrease in the experimental Poisson’s ratio with an increase in V\(_2\)O\(_5\) content is attributed to increasing the average cross-link density. The crosslink density is shown in Fig.1. In the present case, the average crosslink density increased from 2.33 to 2.62. As a result, the calculated Poisson ratio \( \sigma_{bc} \) decreased from 0.227 to 0.222. Besides the above, the \( (K_{bc}/K) \) ratio decreased from 2.7 to 1.7. When \( (K_{bc}/K) \) is \( \approx 1 \) this means that the interaction between neighboring bonds is neglected [17-20]. On the other hand, \( (K_{bc}/K) > 1 \) and less than 3, indicates a relatively open three-dimensional network [17]. In the present case, all TeO\(_2\)-V\(_2\)O\(_5\) glasses have \( (K_{bc}/K) \) values greater than 1, which are attributed to the open 3D structure [17-20]. The average atomic ring size \( l \) values, which have been calculated from Eq.1 changed from 5.00 nm for pure TeO\(_2\) glass [21] to 0.535 nm for 80TeO\(_2\)-20V\(_2\)O\(_5\) glass sample and 0.499 nm for 40TeO\(_2\)-60V\(_2\)O\(_5\) glass sample. The increase in \( (K_{bc}/K) \) ratio is attributed to the higher the atomic ring size \( l \) (nm) as shown in Fig.2. If the experimental bulk modulus \( K < K_{bc} \), compression requires much less energy than that is that required for pure compression of network bonds.

Makishima-Mackenzie's model [22, 23] was used for more interpretation of the elastic moduli according to the following equations:

\[
<< K_m = 1.2 \, V_t \, E_m >>, << E_m = 8.3V_t \, G_t >>, << \sigma_m = (E / 2S_m) - 1 >> \quad (2)
\]

The packing density, \( V_t \) for the used oxides, TeO\(_2\), V\(_2\)O\(_5\); 14.7, 35.4 (cm\(^3\)/mol) and dissociation energy, \( G_t \); 54 and 69.5 (kJ/cm\(^3\)) [24], respectively. The calculated elastic moduli according to (MM) are shown in Table 3. Moreover, Fig.3 shows the experimental bulk modulus, calculated bulk modulus according to the bond compression model and Makishima-Mackenzie's model. The calculated dissociation energy per unit volume \( G_t \) increased from 13.66 to 14.77 (kcal/cm\(^3\)). Also, the mean atomic volume \( \overline{V} \) decreased from 8.81 to 8.54 (cm\(^3\)/mole). Moreover, both bulk modules \( K_m \) and Poisson’s ratio \( \sigma_m \) increased from 43.44 to 51.18 GPa and from 0.2537 to 0.2640, respectively.

### 2-2 Ultrasonic attenuation at low Temperature

The central force model [17-20] suggested oscillations of the light atoms in the glass structure in asymmetric two-well potential. These atoms are considered oxygen atoms. These atoms aim to surpass the wall elevation (activation energy). This aim is a result of the effect of ultrasonic energy on these atoms. The ultrasonic energy increases as the frequency \( (f) \) of these waves increase with the increment of the temperature as shown in Table 4 and Table 5. The increment of the ultrasonic energy formed extra oscillating oxygen atoms in a potential well. Therefore, the transmission of ultrasonic waves into the amorphous structure changes the equilibrium of the
vibrating oxygen atom around the bottom of the well. This procedure created an energy change ($\Delta E$) between the minima of the well. This energy shift can be presented by the deformation potential ($D$).

The last parameter means the energy motion of the relaxing states in a strain field, so, it presents the interaction between ultrasonic waves within the asymmetric dual-well potential. The central force model [17-20] suggested an equation that represents the internal friction ($Q^{-1}$) of a set of oxygen atoms/volume ($n$) proceeding in comparable dual-well potential with a wall height $E_h$. When $\omega \tau(E) = 1$, the ultrasonic attenuation is maximum, and in this case, there is a distribution of both the activation energies and the relaxation times and will be

$$Q^{-1} = \frac{2\pi D^2}{\rho v^2} \int_0^\infty \frac{\omega n E dE}{1 + \omega^2 \tau^2}$$

(3)

The oxygen atoms per unit volume ($n$) or the centers of energy loss can be taken as a summation of the probable activation energies as;

$$n = \int_0^\infty n(E) dE$$

(4)

The parameter $n(E)$ can be described in terms of the ultrasonic velocity ($v$) the angular frequency ($\omega$) and the density ($\rho$) [20] as;

$$n(E) = E^{-1}_h \exp\left(-\frac{E}{E_h}\right)$$

$$= \frac{\rho v^2}{2 zz D^2} \int_0^\infty C(E) dE$$

(5)

Where $zz$ is a constant and the $\int_0^\infty C(E) dE$ is the total number of centers of energy loss. The last parameter can be deduced from $\alpha-T$ relation. The quantitative exploration of the central-force model [17-20] revealed that;

- There is a predictable oscillation of oxygen atoms well with atomic limits,
- Such a well had single minima corresponds to the equilibrium of oscillated oxygen atoms,
- These minima agree with small O oscillations. The minima will flatted at higher anharmonic oscillations,
- The energy of the transmitted ultrasonic wave (longitudinal or shear) disfigured the well,
- The well had a potential energy $U$ and an elongation $e$ based on the longitudinal or shear oscillations of O atoms as shown in the next equation,

$$U_L = -aa_1 (\frac{1}{r} + \frac{1}{2el_0 - r}) + aa_2 (\frac{1}{r_m} + \frac{1}{(2el_0 - r)^m})$$

$$U_T = \frac{-2a}{(e^{2l_0^2} + d^2)^{1/2}} + \frac{2b}{(e^{2l_0^2} + d^2)^{m/2}}$$

$$e = L/2l_0, b = al_0^{m-1}/m$$

(6)
where $aa_1$ and $aa_2$ are constants, $m$ takes values from 6-12, $L$ is the cation-cation distance and $l_0$ expressed bond length in a definite glass structure. The term $U/2$ is a suitable expression for the potential energy $U$ and in this case, characterized the alternate potential energy anion and cation (regarded as a heavier atom) as shown in Fig. (4).

Low-temperature parameters are alternate potential energy, centers of energy loss, elongation, or contraction of the two-well potential. Moreover, the deformation potential is found to be sensitive to the variations of the modifier content. The number of centers of energy loss is related to the elastic moduli as a function of modifier content. Table 6 collected bond energy ($U_0$), constant (a), constant (b), experimental and theoretical deformation potentials ($D_{exp}$) and ($D_{th}$), and percentages of elongations and contractions of binary TeO$_2$-V$_2$O$_5$ glasses as shown in Figs. (5, 6, 7, 8). It is clear that Fig.9. showed an increase of percentage longitudinal elongations with the increase in percentage transverse contractions, which means that the glass network structure increased horizontally in longitudinal chains and decreased vertically in transverse chains, confirming the increase in the dimensions of the 3D network structure and consequently the increase in molar volume.

**2-3 Correlation between bulk modulus and molar volume**

It has been proposed the following equation, which correlates experimental bulk modulus ($K_e$) with molar volume of the glass ($V_M$) [25, 26],

$$K_e V_M^b = C$$  \hspace{1cm} (7)

The constant $C$ and power $b$ have values depend strongly on the type of glass and its composition. The last equation suggests that a decrease in molar volume should lead to an increase in bulk modulus. The molar volume was deduced from the density measurement and the chemical composition. As density decreases, then there is an increase in glass molar volume, with a corresponding decrease in glass compactness or atomic packing density. Unfortunately, this is not true for the present TeO$_2$–V$_2$O$_5$ glasses. The relation between bulk modulus and molar volume reveals a forward proportionality as shown in Fig 10. This suggests that the best fitting of the semi-empirical formula (7) to the data of these glasses was achieved at a negative value of $b$. It is a well-known fact that in V$_2$O$_5$-contained tellurite glasses vanadium, ions can be found in either four-fold coordinated (VO$_4$ tetrahedron), or five-fold coordinated (VO$_5$ trigonal bipyramid) structural units [15, 16, 21, 27]. Thus, the observed changes in molar volume and bulk modulus of TeO$_2$–V$_2$O$_5$ glasses may be associated with either, the network modification, or, the difference between the molar volume of each component oxide. Previous studies on pure tellurite and binary vanadium tellurite glasses [15, 16, 21, 27]. by using ultrasonic and IR techniques concluded that:
i- The network of pure TeO$_2$ glass is composed of TeO$_4$ tetragonal bipyramids and Te–O–Te linkages.

ii- For TeO$_2$–V$_2$O$_5$ glasses, the addition of V$_2$O$_5$, beyond 20 mol% V$_2$O$_5$, changed the continuous tellurite network to continuous vanadate network. This results in the formation of VO$_4$ and VO$_5$ structural units in addition to TeO$_4$ tetragonal bipyramids and TeO$_3$ trigonal pyramids, which are connected to each other through Te–O–Te, Te–O–V and V–O–V linkages. Each VO$_4$ or VO$_5$ structural units has one V=O double bonds.

iii- The Te–O bond length (r = 1.98 Å) in TeO$_2$ is larger than the bond length of V–O (r = 1.83 Å) in V$_2$O$_5$ [15].

In the present case, the molar volume was found to be 31 cm$^3$/mole for the base TeO$_2$ glass and increases from 33.48 cm$^3$/mole in 80TeO$_2$–20V$_2$O$_5$ glass sample to 39.88 cm$^3$/mole in 60TeO$_2$–40V$_2$O$_5$ glass sample. This increase in molar volume is in agreement with the coordination of 4 expected for vanadium ions and its network former role that opens the atomic structure of the glass [28]. The volume occupied by a V$_2$O$_5$ (54.18 cm$^3$/mol) is larger than that of the TeO$_2$ (28.15 cm$^3$/mol). As a result, the substitution of TeO$_2$ by V$_2$O$_5$ and formation of VO$_4$ or VO$_5$ structural units is expected to expand the glass network and increases the molar volume. Also, the increase of V$_2$O$_5$ and expense of TeO$_2$ increases the density of oxygen ions in the glass by a factor of 5/2, which increases the oxygen density from 4.679 x 10$^{28}$ m$^{-3}$ in 80TeO$_2$–20V$_2$O$_5$ glass sample to 4.838 x 10$^{28}$ m$^{-3}$ in 60TeO$_2$–40V$_2$O$_5$ glass sample (Table 5). As a result, the excess molar volume ($\Delta V = V_M - V_C$, where $V_C$ is the crystalline molar volume) increases, which supports this discussion. According to our earlier discussion, Te–O bonds are longer and weaker than V–O bonds [15, 27]. The increase of bulk modulus with increasing V$_2$O$_5$ content confirms the former role of vanadium ions, which increases the cross-linking of glass network due to formation of VO$_4$ and VO$_5$ structural units and stronger Te–O–V linkages. This discussion is supported by the increase of the total packing density and dissociation energy with increasing V$_2$O$_5$ content. The least-square linear regressions performed on ln $K_e$ and ln $V_M$ yields the following semi-empirical relationship,

$$K_e V^{-1.75} = 0.057$$  \hspace{1cm} (8)

with $R^2 = 0.946$, $b = -1.75$ and $C = 0.057$. These $b$ and $C$ values are completely different from those reported previously for V$_2$O$_5$–P$_2$O$_5$ glasses [29] or BaF$_2$–TeO$_2$ glasses [30]. This clarifies that a molar volume is an effective tool in exploring changes in elastic properties of glasses and supports the two points of view [25, 26].
2.4 Correlation between room temperature ultrasonic attenuation and compositional parameters

Recently, a model to predict the composition dependence of ultrasonic attenuation coefficient in inorganic oxide glasses at room temperature has been reported [25, 26]. Based on this model, the ultrasonic attenuation coefficient ($\alpha$) is expressed in terms of oxygen density ([O]), average first-order stretching force constant ($F$), mean atomic ring size ($\ell$), dissociation energy per unit volume ($G_i$), packing density ($V_i$), and experimental bulk modulus ($K$) of the glass according to the following semi-empirical formulas:

$$\alpha = \chi_1 \left(\frac{F}{K_e}\right)^{m/4}$$  \hspace{1cm} (9)

$$\alpha = \chi_2 \left(\frac{[O]}{F}\right)^{m}$$  \hspace{1cm} (10)

$$\alpha = \chi_1 \left(\frac{F}{10G_iV_i^2}\right)^{m/4}$$  \hspace{1cm} (11)

where $\chi_1$ and $\chi_2$ are two frequency-dependent constants, whereas $m$ is a power, its value depends upon the type of the glass. Meanwhile, the average first-order stretching force constant of the glass [20] was estimated from the next equation in the form:

$$F = \frac{\sum x_i n_i f_i}{\sum x_i n_i}$$  \hspace{1cm} (12)

Where $n_i$ is the number of network bonds per cation (coordination number of cation) in oxide component $i$ with cation-anion bond length $r_i$ and first-order stretching force constant $f_i = 17/r_i^3$. It is worth predicting the composition dependence of the ultrasonic attenuation coefficient in the present TeO$_2$–V$_2$O$_5$ glasses by using the above and first-order stretching force constant semi-empirical formulas [25, 26]. Table 7 collected the calculated values for average stretching force constant, besides those of ($F/K_e$), ($F/10G_iV_i^2$) and ($\alpha F$) for the investigated TeO$_2$–V$_2$O$_5$ glass samples. The frequency dependence of room temperature ultrasonic attenuation is shown in Fig. 11 for 80TeO$_2$–20V$_2$O$_5$ and 60TeO$_2$–40V$_2$O$_5$ glass samples. The increase in ultrasonic attenuation with increasing the frequency was fitted by a linear relation $\alpha = \mu \omega^{\gamma}$ where $\mu$ is a new constant, its value depends strongly the glass composition. This behavior is reasonable and agrees well with Abd El-Moneim’s approaches [25-27].

Fig.12 illustrates how the quantity ($F\alpha$) varies with ($F/K_e$) ratio at 2, 4, 5 and 6 MHz frequencies. It was found that, for a fixed frequency, there is an inverse proportionality
between \((F\alpha)\) and \((F / K_e)\). This suggests that the best fitting of the semi-empirical formula (9) to the ultrasonic attenuation data of the same present TeO\(_2\)-V\(_2\)O\(_5\) glasses was achieved at a negative value of \(m\). The equations of the fitted curves in Fig. 12 can be represented by the following semi-empirical relationships;

\[
\alpha_{2\text{MHz}} = \frac{15391}{F} (F / K_e)^{-1.55}
\]

with \(R^2 = 0.351\), \((m/4) = 0.155\) and \(\chi_1 = 15391\);

\[
\alpha_{4\text{MHz}} = \frac{21379}{F} (F / K_e)^{-1.52}
\]

with \(R^2 = 0.532\), \((m/4) = 1.52\) and \(\chi_1 = 21379\);

\[
\alpha_{5\text{MHz}} = \frac{40628}{F} (F / K_e)^{-1.76}
\]

with \(R^2 = 0.527\), \((m/4) = 1.76\) and \(\chi_1 = 40628\);

\[
\alpha_{6\text{MHz}} = \frac{40126}{F} (F / K_e)^{-1.71}
\]

with \(R^2 = 0.500\), \((m/4) = 1.71\) and \(\chi_1 = 40126\);

As expected, \(\chi_1\) is a frequency dependent constant, whereas the power \((m/4)\) has a very close values (ranged between -1.52 and -1.76). The corresponding \(m\) values are ranged between -6.08 and –7.04. In a previous work [26, 27], the applicability of the same schematic relationship (9) has been verified for other types of glass systems [25-28]. It has been found that, the best fitting of this schematic relationship to the ultrasonic attenuation data was achieved for V\(_2\)O\(_5\)-P\(_2\)O\(_5\) glasses when \((m/4) = 7.398\) [26], and for BaF\(_2\)-TeO\(_2\) glasses when \((m/4) = 8.077\) [27].

The relationship between \((F\alpha /[O])\) ratio and the estimated average atomic ring size \((\ell)\) is illustrated in **Fig.13** for 2, 4, 5 and 6 MHz frequencies. Performing the least-square linear regressions on \((F\alpha /[O])\) and \((\ell)\) yields the following relationships for the ultrasonic attenuation coefficient;

\[
\alpha_{2\text{MHz}} = 4.656 \frac{[O]}{F} \ell^{-5.16}
\]

with \(R^2 = 0.314\), \(\chi_2 = 4.656\) and \(m = -5.16\).

\[
\alpha_{4\text{MHz}} = 7.459 \frac{[O]}{F} \ell^{-5.05}
\]

with \(R^2 = 0.497\), \(\chi_2 = 7.459\) and \(m = -5.05\).
\[ \alpha_{5MHz} = 4.711 \frac{[O]}{F} \ell^{-5.97} \quad (19) \]

with \( R^2 = 0.499, \chi_2 = 4.711 \) and \( m = -5.97 \).

\[ \alpha_{6MHz} = 5.931 \frac{[O]}{F} \ell^{-5.77} \quad (20) \]

with \( R^2 = 0.464, \chi_2 = 5.931 \) and \( m = -5.77 \). As expected, the schematic relationships (17)- (20) have approximately the same value of \( m \) (ranged between – 5.05 and – 5.97). This supports the fact that the power \( m \) is a frequency independent parameter. At the same time, the constant \( \chi_2 \) has values depend strongly upon the ultrasonic frequency. These results agree very well with semi-empirical formulas [25, 26] and support all the above discussion.

Besides the above, one of the authors [27] has eliminated the experimental bulk modulus \( (K_v) \) in equations (7) and (9) and finally reported the following semi-empirical relationship, which relates the ultrasonic attenuation coefficient with both the average first-order starching force constant and molar volume of the glass,

\[ \alpha = \frac{\chi_3}{F} \left[ F V_M^b \right]^{m/4} \quad (21) \]

where \( \chi_3 = \chi_1 / C^{m/4} \) is a new constant, its value depends upon the applied ultrasonic frequency and type of the glass. It is worth predicting changes in the ultrasonic attenuation coefficient by using the last semi-empirical formula. Substituting the value \( b = -1.75 \) in equation (21) yields the following schematic relationship for the present TeO\(_2\)–V\(_2\)O\(_5\) glasses;

\[ \alpha = \frac{\chi_3}{F} \left[ F / V_M^{1.75} \right]^{m/4} \quad (22) \]

Fig. 14 shows the relation between \( (F\chi) \) and \( (F/V_M^{1.75}) \) at 2, 4, 5 and 6 MHz frequencies. There is an inverse proportionality between \( (F\chi) \) and \( (FV_M^{-1.75}) \), which again suggests a negative value for the power \( m \). The equations of the fitted curves can be represented by the following semi-empirical relationships;

\[ \alpha_{2MHz} = \frac{157.3}{F} [F/V_M^{1.75}]^{-1.72} \quad (23) \]

with \( R^2 = 0.392, (m/4) = -1.72 \) and \( \chi_3 = 157.3 \).

\[ \alpha_{5MHz} = \frac{252.8}{F} [F/V_M^{1.75}]^{-1.63} \quad (24) \]

with \( R^2 = 0.554, (m/4) = -1.63 \) and \( \chi_3 = 252.8 \).
\[
\alpha_{5\text{MHz}} = \frac{220.7}{F} \left[ F/V_M^{1.75} \right]^{-1.97}
\] (25)

with \( R^2 = 0.597, (m/4) = -1.97 \) and \( \chi_3 = 220.7 \).

\[
\alpha_{6\text{MHz}} = \frac{257.5}{F} \left[ F/V_M^{1.75} \right]^{-1.90}
\] (26)

with \( R^2 = 0.56, (m/4) = -1.9 \) and \( \chi_3 = 257.5 \). One interning observation is that, the semi-empirical relationships (23) – (26) have \( (m/4) \) values very close to each other and to those observed in the semi-empirical relationships (13) – (16), which supports our discussion. This confirms the validity of Abd El-Moneim's approaches [25-27] for the investigated The present findings will complete the previous works in the physical properties, technological advances, smart glasses, and structure-applications of tellurite glasses [31-36].

The least-square linear regression performed on \( \log(F\alpha) \) and \( \log(F/10G_iV_r^2) \) at the same 2, 4, 5 and 6 MHz frequencies (Fig. 15) yields the following schematic relationships;

\[
\alpha_{2\text{MHz}} = \frac{3189}{F} (F/10G_iV_r^2)^{-0.95}
\] (27)

with \( R^2 = 0.026, (m/4) = -0.95 \) and \( \chi_1 = 3189 \).

\[
\alpha_{4\text{MHz}} = \frac{619}{F} (F/10G_iV_r^2)^{0.277}
\] (28)

with \( R^2 = 0.003, (m/4) = 0.277 \) and \( \chi_1 = 619 \).

\[
\alpha_{5\text{MHz}} = \frac{2276}{F} (F/10G_iV_r^2)^{-0.42}
\] (29)

with \( R^2 = 0.006, (m/4) = -0.42 \) and \( \chi_1 = 2276 \).

\[
\alpha_{6\text{MHz}} = \frac{1180}{F} (F/10G_iV_r^2)^{0.034}
\] (30)

with \( R^2 = 0.00004, (m/4) = 0.034 \) and \( \chi_1 = 1180 \).

These results suggest that ultrasonic attenuation data of TeO$_2$–V$_2$O$_5$ glasses are not predictable from the semi-empirical relationships (11). Equations (27) – (30) have values of \( \chi_1 \) and \( (m/4) \) completely different from those obtained from fitting of the semi-empirical relationships (9) to the data of the same studied TeO$_2$–V$_2$O$_5$ glasses. This means that the calculated values of packing
density and dissociation energy per unit volume in the present study are not the correct values for predicting bulk modulus and ultrasonic attenuation coefficient of TeO$_2$–V$_2$O$_5$ glasses. This explains also why all investigated glass samples have a theoretical bulk modulus ($K_m = 10G_iV_i^2$) [22, 23] greater than the experimental bulk modulus ($K_e$).

3-Conclusions:

The impact of adding V$_2$O$_5$ into TeO$_2$ glass was as follows:

• Firstly, the average bond stretching force constants ($F$), the number of network bonds per unit volume $n_b$, the ring diameter $\ell$ decreased, while the average crosslink density $\bar{n}_i$, the packing density $V_i$ increased, the dissociation energy $G_i$ increased, increased, and the values of ($K_{bc}/K$) ratio are less than 3, which is attributed to the open 3D structure,

• Secondly; the increment of V$_2$O$_5$ structural units in the tellurite network is congruent with the increment of the number of centers of energy loss increases, the acoustic activation energy increases, and a dual-well potential will be formed as a direct result of the oscillations of oxygen atoms. The oscillations are created from the effect of the ultrasonic energy; the created potential well suffers from some changes as the supposed ultrasonic energy increases. The potential well will change from an equilibrium state to a flat-bottom state to a dual-well potential, the last well corresponds well to the ultrasonic activation energy within the elastic limits, and besides that and more ultrasonic energy effect on the oxygen atoms will change the elasticity of the well and it will be no longer matching the proper activation energies. So, the well will be wracked. Therefore, the increment of the bulk modulus of TeO$_2$–V$_2$O$_5$ glasses as a function of V$_2$O$_5$ will increase the deformation potential of the presented dual-well state.

• Thirdly; the correlations between ultrasonic attenuation coefficient ($\alpha$) can be expressed in terms of oxygen density ([O]), average first-order stretching force constant ($F$), mean atomic ring size ($\ell$), dissociation energy per unit volume ($G_i$), packing density ($V_i$), and experimental bulk modulus ($K$) of the glass according to the following semi-empirical formulas have achieved.

The impact of the present findings indicates that V$_2$O$_5$ didn’t act to fill the interstices and was added to the longitudinal chains, confirming the increase in molar volume with the increase in V$_2$O$_5$ content, and consequently the structure becomes more open with V$_2$O$_5$ content.
Credit authorship contribution statement:
R. El-Mallawany: Idea, data curation, methodology, validation, investigation, writing original draft.
Amin Abdel Moniem, and M S. Gafaar: data curation, methodology, calculations and shared in the analysis. All authors provided critical feedback and helped shape the research, analysis, and manuscript.

Prime novel statement:
All authors agree with this final version of the MS and also declare it was not submitted or published in other journals nor any other kind of publication. The authors declare that there is no financial interest in this work.

Declaration of Competing Interest:
The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data and materials:
All the data included in the study is available in the supplementary materials.

4-References:
4. Aşkın, MI Sayyed, A Sharma, M Dal, R El-Mallawany, MR Kaçal, Investigation of the gamma ray shielding parameters of (100-x)[0.5 Li₂O–0.1 B₂O₃–0.4 P₂O₅]-xTeO₂ glasses using Geant4 and FLUKA codes, Journal of Non-Crystalline Solids 521, 119489 (2019)
4. R El-Mallawany, AH El-Sayed, MMHA El-Gawad, ESR and electrical conductivity studies of (TeO₂) 0.95 (CeO₂) 0.05 semiconducting glasses, Materials chemistry and physics 41 (2), 87-91 (1995).
5. R El-Mallawany, A Abd El-Moneim, Comparison between the elastic moduli of tellurite and phosphate glasses, physica status solidi (a) 166 (2), 829-834 (1998)


Table 1: Glass compositions, density, molar volume, experimental bulk modulus and Poisson’s ratio of binary TeO$_2$-V$_2$O$_5$ glasses [15].

<table>
<thead>
<tr>
<th>V$_2$O$_5$ (mol%)</th>
<th>Density (g/cm$^3$)</th>
<th>$V_M$ (cm$^3$/mol)</th>
<th>$K_x$ (GPa)</th>
<th>$\sigma_x$</th>
<th>$V_C$ (cm$^3$/mol)</th>
<th>$\Delta V$ (cm$^3$/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0 [21]</td>
<td>5.105</td>
<td>31.00</td>
<td>31.70</td>
<td>0.233</td>
<td>28.15</td>
<td>2.85</td>
</tr>
<tr>
<td>20</td>
<td>4.900</td>
<td>33.48</td>
<td>27.20</td>
<td>0.360</td>
<td>33.36</td>
<td>0.124</td>
</tr>
<tr>
<td>25</td>
<td>4.620</td>
<td>35.48</td>
<td>30.50</td>
<td>0.350</td>
<td>34.66</td>
<td>0.823</td>
</tr>
<tr>
<td>30</td>
<td>4.500</td>
<td>35.70</td>
<td>28.80</td>
<td>0.323</td>
<td>35.96</td>
<td>0.259</td>
</tr>
<tr>
<td>35</td>
<td>4.300</td>
<td>38.66</td>
<td>33.90</td>
<td>0.337</td>
<td>37.26</td>
<td>1.400</td>
</tr>
<tr>
<td>40</td>
<td>4.230</td>
<td>39.88</td>
<td>37.30</td>
<td>0.338</td>
<td>38.56</td>
<td>1.320</td>
</tr>
</tbody>
</table>

Table 2: Theoretical elastic moduli according to bond compression model for TeO$_2$-V$_2$O$_5$ glasses.

<table>
<thead>
<tr>
<th>V$_2$O$_5$ (mol%)</th>
<th>$n_b$ ($10^{28}$ m$^{-3}$)</th>
<th>$F$ (N/m)</th>
<th>$\ell$ (nm)</th>
<th>$\bar{\sigma}_e$</th>
<th>$\sigma_{bc}$</th>
<th>$K_{bc}$ (GPa)</th>
<th>$K_{bc} / K_x$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0 [21]</td>
<td>7.74 [21]</td>
<td>216.0</td>
<td>0.500</td>
<td>2.00</td>
<td>0.235</td>
<td>73.3</td>
<td>2.31</td>
</tr>
<tr>
<td>20</td>
<td>7.56</td>
<td>230.5</td>
<td>0.535</td>
<td>2.33</td>
<td>0.227</td>
<td>73.3</td>
<td>2.70</td>
</tr>
<tr>
<td>25</td>
<td>7.16</td>
<td>233.9</td>
<td>0.521</td>
<td>2.40</td>
<td>0.225</td>
<td>69.7</td>
<td>2.30</td>
</tr>
<tr>
<td>30</td>
<td>7.11</td>
<td>237.3</td>
<td>0.531</td>
<td>2.46</td>
<td>0.224</td>
<td>69.6</td>
<td>2.40</td>
</tr>
<tr>
<td>35</td>
<td>6.78</td>
<td>240.5</td>
<td>0.510</td>
<td>2.52</td>
<td>0.222</td>
<td>66.6</td>
<td>2.00</td>
</tr>
<tr>
<td>40</td>
<td>6.65</td>
<td>243.7</td>
<td>0.499</td>
<td>2.57</td>
<td>0.221</td>
<td>65.6</td>
<td>1.80</td>
</tr>
</tbody>
</table>
Table 3: Theoretically calculated total dissociation energy per unit volume, total packing density, bulk modulus and Poisson's ratio of binary TeO₂-V₂O₅ glasses on the basis of MM model [22, 23].

<table>
<thead>
<tr>
<th>V₂O₅ (mol%)</th>
<th>$G_i$ (kcal/cm³)</th>
<th>$V_i$ (cm³/mole)</th>
<th>$\bar{V}$ (cm³/mole)</th>
<th>$K_w$ (GPa)</th>
<th>$\sigma_w$</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>13.66</td>
<td>0.5639</td>
<td>8.81</td>
<td>43.44</td>
<td>0.2537</td>
</tr>
<tr>
<td>25</td>
<td>13.85</td>
<td>0.5573</td>
<td>8.87</td>
<td>43.02</td>
<td>0.2508</td>
</tr>
<tr>
<td>30</td>
<td>14.03</td>
<td>0.5756</td>
<td>8.50</td>
<td>46.49</td>
<td>0.2587</td>
</tr>
<tr>
<td>35</td>
<td>14.22</td>
<td>0.5695</td>
<td>8.79</td>
<td>46.11</td>
<td>0.2561</td>
</tr>
<tr>
<td>40</td>
<td>14.40</td>
<td>0.5782</td>
<td>8.67</td>
<td>48.14</td>
<td>0.2598</td>
</tr>
</tbody>
</table>

Table 4: Room temperature ultrasonic attenuation coefficient of binary TeO₂-V₂O₅ glasses [16].

<table>
<thead>
<tr>
<th>V₂O₅ (mo%)</th>
<th>$\alpha$ (dB/cm)</th>
<th>2 MHz</th>
<th>4MHz</th>
<th>5MHz</th>
<th>6MHz</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td></td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>20</td>
<td></td>
<td>1.77</td>
<td>2.95</td>
<td>3.14</td>
<td>3.50</td>
</tr>
<tr>
<td>25</td>
<td></td>
<td>3.51</td>
<td>4.71</td>
<td>5.52</td>
<td>6.01</td>
</tr>
<tr>
<td>30</td>
<td></td>
<td>3.00</td>
<td>4.25</td>
<td>5.00</td>
<td>5.63</td>
</tr>
<tr>
<td>35</td>
<td></td>
<td>2.75</td>
<td>4.03</td>
<td>5.00</td>
<td>5.25</td>
</tr>
<tr>
<td>40</td>
<td></td>
<td>3.25</td>
<td>5.06</td>
<td>5.81</td>
<td>6.56</td>
</tr>
</tbody>
</table>
Table 5: Experimental data of peak temperature $T_p$, attenuation coefficient at peak, acoustic activation energy and number of loss centers of binary TeO$_2$-V$_2$O$_5$ glasses [16].

<table>
<thead>
<tr>
<th>V$_2$O$_5$ (mol%)</th>
<th>$T_p$ (K)</th>
<th>Peak loss at 6 MHz (dB/cm)</th>
<th>$V$ (eV)</th>
<th>[O] ($10^{28}$ m$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>238</td>
<td>5.40</td>
<td>0.068</td>
<td>4.679</td>
</tr>
<tr>
<td>25</td>
<td>255</td>
<td>6.75</td>
<td>0.166</td>
<td>4.633</td>
</tr>
<tr>
<td>30</td>
<td>238</td>
<td>9.10</td>
<td>0.174</td>
<td>4.794</td>
</tr>
<tr>
<td>35</td>
<td>228</td>
<td>7.15</td>
<td>0.207</td>
<td>4.752</td>
</tr>
<tr>
<td>40</td>
<td>238</td>
<td>7.00</td>
<td>0.223</td>
<td>4.838</td>
</tr>
</tbody>
</table>

Table 6: Bond energy ($U_0$), constant (a), constant (b), experimental and theoretical deformation potentials ($D_{exp}$) and ($D_{th}$) and percentages of elongations and contractions for binary TeO$_2$-V$_2$O$_5$ glasses.

<table>
<thead>
<tr>
<th>V$_2$O$_5$ content</th>
<th>$U_0$ (eV)</th>
<th>a (eV)</th>
<th>b x 10$^{-7}$ (eV)</th>
<th>$D_{exp}$ (eV)</th>
<th>$D_{th}$ (eV)</th>
<th>%e (long)</th>
<th>%c (Trans)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>4.396869</td>
<td>0.984349</td>
<td>2.6899</td>
<td>0.250</td>
<td>0.253</td>
<td>35.8</td>
<td>-4.3</td>
</tr>
<tr>
<td>25</td>
<td>4.526174</td>
<td>1.012024</td>
<td>2.7378</td>
<td>0.453</td>
<td>0.453</td>
<td>45.3</td>
<td>-8.7</td>
</tr>
<tr>
<td>30</td>
<td>4.655478</td>
<td>1.039627</td>
<td>2.7843</td>
<td>0.468</td>
<td>0.467</td>
<td>41.2</td>
<td>-6.5</td>
</tr>
<tr>
<td>35</td>
<td>4.784783</td>
<td>1.067156</td>
<td>2.8294</td>
<td>0.525</td>
<td>0.525</td>
<td>38.6</td>
<td>-5.7</td>
</tr>
<tr>
<td>40</td>
<td>4.914088</td>
<td>1.094613</td>
<td>2.8730</td>
<td>0.552</td>
<td>0.555</td>
<td>37.0</td>
<td>-4.8</td>
</tr>
</tbody>
</table>
Table 7: Room temperature ultrasonic attenuation coefficient and bulk modulus, and calculated average stretching force constant, total dissociation energy per unit volume of binary TeO$_2$-V$_2$O$_5$ glasses.

<table>
<thead>
<tr>
<th>V$_2$O$_5$ (mol%)</th>
<th>$F$ (N/m)</th>
<th>$F/K_c$</th>
<th>$F/10G_iV_i^2$</th>
<th>$F/V_M^{1.75}$</th>
<th>$\alpha F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>216</td>
<td>6.81</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>20</td>
<td>230.5</td>
<td>8.47</td>
<td>5.36</td>
<td>0.495</td>
<td>408</td>
</tr>
<tr>
<td>25</td>
<td>233.9</td>
<td>7.67</td>
<td>5.03</td>
<td>0.453</td>
<td>821</td>
</tr>
<tr>
<td>30</td>
<td>237.3</td>
<td>8.24</td>
<td>5.14</td>
<td>0.455</td>
<td>712</td>
</tr>
<tr>
<td>35</td>
<td>240.5</td>
<td>7.09</td>
<td>5.00</td>
<td>0.401</td>
<td>661</td>
</tr>
<tr>
<td>40</td>
<td>243.7</td>
<td>6.53</td>
<td>5.61</td>
<td>0.385</td>
<td>792</td>
</tr>
</tbody>
</table>
Fig. 1. Two-dimension representation of crosslinks [17].
Fig. 2. Variation of $(K_{bc}/K)$ and ring diameter $l(nm)$ binary TeO₂-V₂O₅ glasses.

Fig. 3. Variation of bulk modulus by using B.C. model ($K_{bc}$), Makishima-Mackenzie models and experimental bulk $K$ for binary TeO₂-V₂O₅ glasses.
Fig. 4. Double well potential and variables considered in a treatment of the deformation potential (CFM).
Fig. 5. Potential wells for longitudinal motion of oxygen atoms at elongations from 0 % to 100 % for binary TeO$_2$-V$_2$O$_5$ glasses.
Fig.6. Effect of addition of V$_2$O$_5$ on the elongation percentages of longitudinal TeO$_2$ network bonds in binary TeO$_2$-V$_2$O$_5$ glasses.
Fig. 7. Potential wells for transverse motion of oxygen atoms at elongations from 0 % to 100 % in binary TeO$_2$-V$_2$O$_5$ glasses.
Fig. 8. Effect of addition of V$_2$O$_5$ on the contraction percentages of transverse TeO$_2$ network bonds in binary TeO$_2$-V$_2$O$_5$ glasses.
Fig. 9. Elongation and contraction effects on structure of binary TeO$_2$–V$_2$O$_5$ glasses.

Fig. 10. Variation of experimental bulk modulus with molar volume in TeO$_2$–V$_2$O$_5$ glasses. The solid line represents the least-square fitting of the data.
Fig. 11: Frequency dependence of ultrasonic attenuation in 80TeO$_2$–20V$_2$O$_5$ and 60TeO$_2$–40V$_2$O$_5$ glass samples. The solid lines represent the least-square fitting of the data.

Fig. 12. Relation between $F\alpha$ and $(F/K)$ in TeO$_2$–V$_2$O$_5$ glasses at different frequencies. The solid lines represent the least-square fitting of the data in binary TeO$_2$–V$_2$O$_5$ glasses.
Fig. 13. Relation between \((F\alpha / |O|)\) and \((\ell)\) in TeO\(_2\)–V\(_2\)O\(_5\) glasses at different frequencies. The solid lines represent the least-square fitting of the data.

Fig. 14. Relation between \(F\alpha\) and \((FV_{M}^{-1.567})\) in TeO\(_2\)–V\(_2\)O\(_5\) glasses at different frequencies. The solid lines represent the least-square fitting of the data.
Fig. 15. Relation between $(F\alpha)$ and $(F/10G_iV_i^2)$ in TeO$_2$–V$_2$O$_5$ glasses at 2 MHz frequency. The solid lines represent the least-square fitting of the data.
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