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Simulation of Acoustic Properties of Borate and Tellurite Glasses

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***Abstract*—**Makishima and Mackenzie model was used to simulation of acoustic properties (longitudinal and shear ultrasonic wave velocities, elastic moduli theoretically for many tellurite and borate glasses. The model was proposed mainly depending on the values of the experimentally measured density, which are obtained before. In this search work, we are trying to obtain the values of densities of amorphous glasses (as the density depends on the geometry of the network structure of these glasses). In addition, the problem of simulating the slope of linear regression between the experimentally determined bulk modulus and the product of packing density and experimental Young's modulus, were solved in this search work. The results showed good agreement between the experimentally measured values of densities and both ultrasonic wave velocities, and those theoretically determined.

***Keywords*---**Glasses, ultrasonic wave velocities, elastic moduli, Makishima and Mackenzie model.

I. Introduction

TeO_2–BASED glasses have recently become of great interest for use in optical communication systems [1]. Tellurite glasses are well known to have the highest refractive indices among oxide glasses in the visible and near IR region [2]. The systems $TeO_2 – WO_3 – K_2O$, $TeO_2 – WO_3 – Bi_2O_3$ and $TeO_2 – WO_3 – PbO$ are the most promising in this respect because they contain oxides of the heaviest metals, such as tungsten, lead and bismuth [1], [3], [4]. Previous studies [5], [6] on vanadium tellurite glasses showed that they are semiconducting glasses and they switch when a high electrical field is applied. Also, Pure B_2O_3 glass has a random three-dimensional network of BO_3 triangles with a large fraction of almost planar B_3O_6 boroxol rings. It is known that borate glasses show the anomalous composition dependences of physical properties, such as density [7], sound velocity [8], [9] and thermal expansion [10], by the addition of alkali oxide to pure B_2O_3 glass.

Longitudinal and shear ultrasonic wave velocities were measured by [11] in binary Li_2O-$2B_2O_3$ glasses doped with different transition metal oxides (TMOs) (where TMO = V_2O_5, Fe_2O_3, Cr_2O_3, NiO, TiO_2, MnO_2 and CuO) using pulse echo technique. Measurements were carried out at 4 MHz frequency and at room temperature. Elastic moduli and some other physical parameters such as acoustic impedance, Debye temperature, thermal expansion coefficient, and latent heat of melting were calculated. Results indicated that these parameters depend upon the TMO modifier i.e., the ionic radius of the transition metal cation. Quantitative analysis has been carried out, in order to obtain more information about the structure of these glasses, based on bond compression model, and the Makishima and Mackenzie model, i.e., the cation-anion bond of each TMO.

The ternary xV_2O_5–$(40-x)Li_2O$–$60B_2O_3$ glass system, where x = 1, 2, 3, 4 and 6 mol%, was prepared by [12] using normal quenching. The composition dependence of these parameters, in addition to the glass-transition temperature, suggested that vanadium ions were incorporated into these glasses as a network modifier, resulting in the reconversion of BO_4 tetrahedra to BO_3 triangles by the breaking of B–O–B linkages and the formation of non-bridging oxygens (NBOs). The results were explained quantitatively in terms of fractal bond connectivity, average atomic volume, network dimensionality, packing density, number of network bonds per unit volume, cross-link density and atomic ring size. The Makishima and Mackenzie model appeared to be valid for the studied glasses when the fate of BO_4 tetrahedra and creation of NBOs are taken into account.

M. S. Gaafar et al. [13] have introduced the Artificial Neural Network (ANN) technique to simulate and predict important parameters such as density, longitudinal and shear ultrasonic velocities and elastic moduli (Longitudinal and shear moduli) for more than 30 glass compositions. The authors showed that the ANN results were found to be in successful good agreement with those experimentally measured parameters. Then the authors have used the ANN model to predict the acoustic properties of some new tellurite glasses. For this purpose, four glass systems x Nb_2O_5 - (1-x) TeO_2, 0.1 PbO - x Nb_2O_5 - (0.9-x) TeO_2, 0.2 PbO - x Nb_2O_5 - (0.8-x) TeO_2 and 0.05 Bi_2O_3 - x Nb_2O_5 - (0.95-x) were prepared by the authors using melt quenching technique. The results of ultrasonic velocities and elastic moduli showed that the addition of Nb_2O_5 as a network modifier provides oxygen ions to change [TeO_4] tbps into [TeO_3] bps.

In the present search work, many different tellurite and borate glass compositions were used to solve the problems of Makishima and Mackenzie model (as it depends on the experimentally measured density values) to make theoretical determination of the densities of these glasses and

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consequently both the ultrasonic (Longitudinal and Shear) wave velocities theoretically.

II. Theoretical Considerations

Makishima and Mackenzie [14], [15] proposed a theoretical model for the direct calculation of Young's modulus of oxide glasses in terms of their chemical compositions taking into consideration the two parameters; dissociation energy of the oxide constituents per unit volume (G_i) and packing density of glasses (V_t). In a simple one component glass such as fused silica, Young's modulus was given as,

$$E_{(M-M)} = 2V_t G \tag{1}$$

For poly-component glasses, Young's modulus was given as,

$$E_{(M-M)} = 2V_t \sum_i G_i x_i \tag{2}$$

where $E_{(M-M)}$ is Young's modulus, x_i is the molecular fraction of component i in the glass system.

The packing density V_t, is defined as;

$$V_t = \left(\frac{\rho_m}{M}\right)\sum_i V_i x_i \tag{3}$$

where M is the effective molecular weight, ρ_m is the density of the poly-components glass system and V_i is the packing factor of the oxide and can be determined from the equation for an oxide A_xO_y having ions A and O with Pauling ionic radii given as;

$$V_i = 6.023\times10^{23}\left(\frac{4\pi}{3}\right)\left[xR_A^3 + yR_O^3\right] \tag{4}$$

where R_A and R_O are the respective ionic radii of the cation and anion.

Makishima and Mackenzie [14], [15] studied the agreement between the experimental values of Young's modulus (E_{M-M}), of many oxide glasses and those calculated from their theoretical model. The agreement was good for the majority of glasses, especially for silica glass, proving that (1) is satisfactory for estimating elastic modulus of a simple one component glass system. A problem appeared for poly-component glasses with Young's modulus values greater than 90 GPa where the theoretically calculated values were found to be less than the measured values. Furthermore, Makishima - Mackenzie model also requires the measured density of glass for which the glass-melting needs to be done before estimating their elastic moduli. Therefore, Makishima and Mackenzie refined their model in order to estimate Young's modulus values directly from the designed compositions without melting.

Makishima and Mackenzie [15] extended their theoretical study and combined Gruneisen's equation with Young's modulus equation of glass to derive new formula for the theoretical calculation of bulk modulus, shear modulus, and Poisson's ratio of glass. According to Gruneisen first rule, the bulk modulus, K, is given as;

$$KV_o = \frac{1}{9}mn|U_o| \tag{5}$$

where V_o is the equilibrium volume found where the net force vanishes, m and n are constants, and U_o is the equilibrium energy for volume V_o. Then, they obtained the;

$$K_{(M-M)} = \left[\frac{m|m-n|}{24\pi}\right]\beta V_t E_{(M-M)} \tag{6}$$

Makishima and Mackenzie pointed out that it was very difficult to calculate m and n which are important factors. They therefore, examined the correlation between bulk modulus and the product of packing density and Young's modulus and found good linearity between the experimentally obtained bulk modulus (using ultrasonic technique) and the product of the packing density multiplied by the experimentally obtained Young's modulus of many glasses. Therefore, the slope (β) of the linear regression was determined, and the bulk modulus of the glass was expressed as;

$$K_{(M-M)} = \beta V_t E_{(M-M)} \tag{7}$$

Still, the problem remains for E values which are greater than 100 GPa. In that case, calculated values are much less than experimental values. Thus, [16] had modified the expression of the packing factor as;

$$C_i = 6.023x10^{23}\frac{\rho}{M}\frac{4}{3}\pi\left(xR_A^3 + yR_B^3\right) \tag{8}$$

and for the polycomponent glass, the C_t factor will therefore be expressed as;

$$C_t = \sum_i C_i x_i \tag{9}$$

Therefore, Young's modulus E_{M-M}, shear modulus $S_{(M-M)}$, and Poisson's ratio $\sigma_{(M-M)}$, are given as;

$$E_{(M-M)} = 2V_t G \tag{10}$$

$$S_{M-M} = \frac{3E_{(M-M)}K_{(M-M)}}{9K_{(M-M)} - E_{(M-M)}} \tag{11}$$

$$\sigma_{M-M} = \frac{E_{(M-M)}}{2S_{(M-M)}} - 1 \tag{12}$$

Now there are two problems; (ρ_m) which is the experimentally obtained density of the poly-components glass system and the slope of the linear regression (β).

Concerning the (ρ_m), [17] derived modified equations on the basis of Makishima - Mackenzie model for direct determination of the elastic modulus of glasses from their compositions. According to the traditional crystalline model of glass structure, the authors assumed that a polycomponent glass is a mixture of microcrystals with the same local structure of corresponding oxide (A_xO_y) component i, so the Young's modulus coefficient E_i, of the component i can be given as,

$$E_i = 2V_iG_i \tag{13}$$

where V_i is the packing density factor of component i which is equivalent to (V_t) only when the glass is simple one component system. If the A – O bond energy of oxide A_xO_y is similar, in the crystal or in the glass, the packing factor (V_i) can be evaluated from the basic properties of oxide A_xO_y as,

$$V_i = \left(\frac{\rho_i}{M_i}\right)6.023\times10^{23}\left(\frac{4\pi}{3}\right)\left[xR_A^3 + yR_O^3\right] \tag{14}$$

Based on the foundational definition of specific modulus [18], the specific modulus coefficient (S_i), of component i in a glass can be expressed as;

$$S_i = \frac{E_i}{\rho_i} = 2G_i\frac{V_i}{\rho_i} \tag{15}$$

Substituting (14) for (15), the modulus coefficient, S_i, can be rewritten as;

$$S_i = 2\left(\frac{G_i}{M_i}\right)6.023\times10^{23}\left(\frac{4\pi}{3}\right)\left[xR_A^3 + yR_O^3\right] \tag{16}$$

Then the specific modulus of a poly-component glass can be expressed, based on the modified additive rule, as;

$$S = \gamma\sum_i S_i x_i \tag{17}$$

where (γ) is the modified coefficient introduced by the authors. Equation (14) was established under assumption that oxide A_xO_y has the same co-ordination number regardless of the oxide being in the crystal or in the glass. However, (16) was established under assumption that oxide A_xO_y has the same co-ordination number regardless of the oxide being in the crystal or in the glass. However, the local structure of each oxide component in glass is, in general, somewhat different to that in its crystal state. Experiments carried out by the authors showed that the difference in results is mainly due to variation of the packing density of oxide component in glass. If the local structure of oxides does not change when added them into glass, the density of the glass based on the additive rule (ρ_i) can be simply evaluated by integrating the densities of the oxide components weighted by their molecular fractions. However, the measured densities are, in fact, different to the calculated values due to the variation of their co-ordination structures. Such a difference between the measured and calculated densities of glass just reflects the variation of local structures of oxide components in the glass. The modified coefficient (γ) is therefore defined as;

$$\gamma = \frac{\sum_i \rho_i x_i}{\rho_m} \tag{18}$$

where ρ_m is the measured density of the glass. Therefore, the problem of (ρ_m) is the density of the poly-components glass system can be solved by linear regression between (ρ_m) is the density of the poly-components glass system and the density of the glass composition based on the additive rule (ρ_i) of different glass compositions and the slope of regression will be equals to the coefficient (γ). Therefore, the density can be obtained theoretically using (18) which take the form;

$$\rho_{cal} = \gamma\sum_i \rho_i x_i \tag{19}$$

where (ρ_{cal}) is the calculated density of amorphous glass composition. Moreover, the problem of the slope (β) of the linear regression between the experimental bulk modulus K_e and the product of V_t and experimental Young's modulus (E_e) was solved. Then, the ultrasonic velocities (U_l, the longitudinal velocity and U_s, the shear velocity) can be computed using equations;

$$L = \rho U_l^2$$
$$S = \rho U_s^2$$
$$E = 2(1+\sigma)S \tag{20}$$
$$K = L - \left(\left(\tfrac{4}{3}\right)S\right)$$

III. Analysis and Discussions

A. Density Calculation

The density of the glass network depends upon many factors such as structural changes, coordination number, cross-link density, and dimensionality of interstitial spaces.

According to [19] the primary structural units of tellurium glasses having high TeO_2 content are composed mostly of TeO_4 trigonal bi-pyramids, and most of the tellurium atoms are connected at vertices by Te-O-Te linkage.

TABLE I

MEASURED DENSITY (**ρ (M)**), THEORETICAL DENSITY (**ρ (CAL)**), MEASURED LONGITUDINAL VELOCITY (**U_L (M)**), THEORETICAL LONGITUDINAL VELOCITY (**U_L (CAL)**), MEASURED SHEAR VELOCITY (**U_S (M)**), THEORETICAL SHEAR VELOCITY (**U_S (CAL)**), EXPERIMENTAL BULK MODULUS (**K_E (M)**), THEORETICAL BULK MODULUS (**K (CAL)**) AND V_T.E, THE PRODUCT OF PACKING DENSITY AND THEORETICAL YOUNG'S MODULUS FOR TELLURITE GLASSES

Glass compositions (mol. %)														ρ (M)	ρ (cal)	U_l (M)	U_l (cal)	U_s (M)	U_s (cal)	K_e (M)	K_{th} (cal)	$V_t.E_{(M-M)}$
TeO_2	WO_3	K_2O	CeO_2	CuO	B_2O_3	Li_2O	Bi_2O_3	V_2O_5	La_2O_3	Nb_2O_5	PbO	Sm_2O_3	BaO									
0.8	0.2	0												5.766	5.664	3366	3381	1951	1932	36.1	36.6	29.0
0.8	0.15	0.05												5.453	5.432	3288	3310	1888	1897	33.0	33.4	25.3
0.8	0.1	0.1												5.091	5.199	3190	3229	1805	1857	29.7	30.3	21.0
0.8	0.05	0.15												4.766	4.967	3130	3139	1734	1811	27.6	27.2	17.8
0.8	0	0.2												4.500	4.735	3058	3035	1681	1757	25.1	24.1	15.6
0.9			0.1											5.706	5.561	3429	3351	2102	1939	33.5	34.6	26.2
0.84				0.16										5.622	5.471	3390	3375	1981	1949	35.2	34.6	26.2
0.821				0.179										5.707	5.482	3476	3383	1887	1952	41.9	34.9	26.5
0.81				0.19										5.785	5.489	3477	3388	2034	1954	38.0	35.1	26.6
0.797				0.203										5.608	5.497	3684	3394	2232	1957	38.9	35.3	26.7
0.1					0.6	0.3								2.580	2.509	5869	6242	3381	3369	49.5	59.8	45.3
0.2					0.5	0.3								2.919	2.813	5556	5580	3089	3065	53.0	52.3	39.7
0.3					0.4	0.3								3.177	3.117	5090	5021	2875	2806	47.3	45.9	34.8
0.35					0.35	0.3								3.404	3.269	4714	4772	2752	2689	41.3	42.9	32.6
0.5							0	0.5						3.996	4.274	3655	3617	2096	1936	30.0	34.6	26.2
0.5							0.05	0.45						4.376	4.537	3591	3569	2056	1937	31.8	35.1	26.6
0.5							0.1	0.4						4.797	4.800	3507	3520	1995	1935	33.5	35.5	26.9
0.5							0.15	0.35						5.188	5.063	3416	3470	1937	1932	34.6	35.8	27.1
0.5							0.2	0.3						5.624	5.326	3330	3421	1882	1926	35.8	36.0	27.3
0.5							0.25	0.25						6.031	5.589	3250	3371	1833	1920	36.7	36.1	27.3
0.65				0				0.35						3.996	4.604	3992	3763	2362	2042	34.0	39.6	30.0
0.65				0.075				0.275						4.376	4.815	3694	3587	2159	1953	32.5	37.5	28.4
0.65				0.1				0.25						4.797	4.885	3364	3524	1950	1922	30.0	36.6	27.8
0.65				0.125				0.225						5.188	4.955	3210	3459	1859	1891	29.6	35.7	27.0
0.65				0.15				0.2						5.624	5.025	3066	3392	1769	1859	29.4	34.6	26.3
0.65				0.175				0.175						6.031	5.095	2939	3322	1682	1827	29.4	33.5	25.4
0.9									0.1					5.685	5.452	3415	3351	2093	1945	33.1	33.7	25.6
0.669										0.124	0.207			5.888	5.705	3294	3287	1906	1884	35.3	34.6	26.3
0.75									0.04		0.21			6.145	6.138	3038	2994	1711	1730	32.7	30.5	23.2
0.9												0.1		5.782	5.557	3447	3386	2149	1975	33.1	34.8	26.4
1														5.101	5.374	3404	3438	2010	1999	33.1	34.9	26.5
0.85	0.15													5.250	5.591	3532	3398	2031	1950	36.6	36.2	27.5
0.8	0.2													5.766	5.664	3366	3429	1951	1959	36.1	37.6	28.5
0.79	0.21													5.390	5.678	3561	3435	2080	1961	37.0	37.9	28.7
0.67	0.33													5.700	5.852	3555	3509	2098	1983	38.6	41.4	31.4
0.77	0.14												0.09	5.669	5.580	3378	3360	1952	1930	35.9	35.3	26.8
0.74	0.21		0.05											5.781	5.772	3408	3416	2011	1939	36.0	38.4	29.1
0.77	0.2								0.03					6.027	5.687	3480	3445	2035	1967	39.7	38.2	28.9
0.5	0.3										0.2			6.680	6.506	3169	3182	1786	1793	38.7	38.0	28.8
0.75	0.2											0.05		6.110	5.755	3515	3470	2067	1986	40.7	39.0	29.6
0.95										0.05				5.475	5.323	3352	3439	1876	1981	35.8	35.1	26.6
0.9										0.1				5.414	5.272	3464	3568	1911	2039	38.6	37.9	28.7
0.85										0.15				5.302	5.222	3677	3692	1949	2096	44.8	40.6	30.8
0.8										0.2				5.242	5.171	3922	3812	2087	2150	50.2	43.3	32.8
0.9											0.1			5.845	5.722	3091	3259	1746	1890	32.1	33.5	25.4
0.7										0.2	0.1			5.529	5.520	3767	3789	2079	2124	46.6	46.0	34.9
0.7										0.1	0.2			6.025	5.970	3151	3249	1784	1842	34.3	36.0	27.3
0.6										0.2	0.2			5.904	5.868	3692	3503	2177	1954	43.2	42.1	32.0
0.75							0.05			0.2				5.33	5.324	3633	3680	1879	2092	45.3	41.0	31.1
0.7							0.05			0.25				5.13	5.273	3990	3803	2175	2149	49.3	43.8	33.2

TABLE II

MEASURED DENSITY (**ρ (M)**), THEORETICAL DENSITY (**ρ (CAL)**), MEASURED LONGITUDINAL VELOCITY (**U_L (M)**), THEORETICAL LONGITUDINAL VELOCITY (**U_L (CAL)**), MEASURED SHEAR VELOCITY (**U_S (M)**), THEORETICAL SHEAR VELOCITY (**U_S (CAL)**), EXPERIMENTAL BULK MODULUS (**K_E (M)**), THEORETICAL BULK MODULUS (**K (CAL)**) AND V_T.E, THE PRODUCT OF PACKING DENSITY AND THEORETICAL YOUNG'S MODULUS FOR BORATE GLASSES

Glass compositions (mol. %)											ρ (M)	ρ (cal)	U_l (M)	U_l (cal)	U_s (M)	U_s (cal)	K_e (M)	K_{th} (cal)	$V_t.E_{(M-M)}$
B_2O_3	WO_3	Li_2O	Na_2O	Fe_2O_3	P_2O_5	Al_2O_3	ZnO	V_2O_5	PbO	PbF_2									
0.8	0	0.2									2.124	2.198	5890	5531	3250	2765	43.8	43.3	36.1
0.795	0.005	0.2									2.159	2.219	5723	5527	3207	2842	41.1	42.7	35.6
0.79	0.01	0.2									2.191	2.240	5662	5480	3204	2786	40.3	43.1	35.9
0.785	0.015	0.2									2.212	2.261	5626	5457	3187	2790	40.1	42.9	35.8
0.78	0.02	0.2									2.236	2.282	5557	5446	3183	2800	38.9	42.9	35.8
0.775	0.025	0.2									2.249	2.303	5510	5420	3168	2808	38.2	42.4	35.3
0.75	0.05	0.2									2.404	2.408	5406	5290	3108	2695	39.3	44.0	36.7
0.725	0.075	0.2									2.543	2.512	5353	5208	3042	2663	41.5	44.9	37.4
0.7	0.1	0.2									2.707	2.617	5237	5117	2960	2631	42.6	45.9	38.2
0.675	0.125	0.2									2.760	2.721	5222	5039	2938	2618	43.5	44.9	37.4
0.7125			0.2375	0.05	0						2.302	2.357	5631	5566	3228	3156	41.0	38.4	32.0
0.69375			0.23125	0.05	0.025						2.324	2.353	5350	5318	3057	3157	37.6	34.9	29.1
0.675			0.225	0.05	0.05						2.331	2.349	5278	5258	3030	3123	36.4	34.5	28.8
0.65625			0.21875	0.05	0.075						2.333	2.345	5177	5164	2965	3103	35.2	33.2	27.7
0.6375			0.2125	0.05	0.1						2.357	2.340	5128	5146	2934	3066	34.9	33.0	27.5
0.6			0.2	0.05	0.15						2.397	2.332	5036	5105	2895	3012	34.0	32.7	27.2
0.67			0.29			0.04	0				2.280	2.274	5412	5415	3056	3031	38.4	38.9	32.4
0.6365			0.2755			0.038	0.05				2.335	2.412	5362	5383	3022	3029	38.7	39.1	32.6
0.603			0.261			0.036	0.1				2.435	2.551	5328	5369	2992	3019	40.1	40.6	33.8
0.5695			0.2465			0.034	0.15				2.563	2.689	5331	5360	2992	3004	42.2	42.8	35.7
0.536			0.232			0.032	0.2				2.632	2.827	5324	5313	2986	2993	43.3	42.8	35.7
0.5025			0.2175			0.03	0.25				2.728	2.966	5315	5271	2970	2976	45.0	43.6	36.3
0.469			0.203			0.028	0.3				2.846	3.104	5310	5231	2953	2956	47.2	44.7	37.3
0.4355			0.1885			0.026	0.35				2.938	3.242	5292	5171	2940	2935	48.4	44.8	37.3
0.6		0.39						0.01			2.281	2.114	6355	6148	3905	3410	45.7	47.1	39.3
0.6		0.38						0.02			2.299	2.126	6290	6095	3853	3387	45.4	46.5	38.7
0.6		0.37						0.03			2.316	2.138	6135	6045	3676	3365	45.5	45.9	38.2
0.6		0.36						0.04			2.331	2.150	5831	5997	3421	3343	42.9	45.3	37.7
0.6		0.34						0.06			2.363	2.174	5639	5908	3264	3303	41.6	44.3	36.9
0.7		0	0.3								2.344	2.466	5710	5879	3199	3304	44.4	44.4	37.0
0.7		0.05	0.25								2.360	2.453	5952	5976	3362	3347	48.0	45.9	38.2
0.7		0.1	0.2								2.350	2.440	6122	6076	3483	3392	50.1	47.4	39.5
0.7		0.15	0.15								2.340	2.427	6265	6181	3555	3437	52.4	49.0	40.9
0.7		0.2	0.1								2.330	2.415	6370	6289	3595	3484	54.4	50.8	42.3
0.7		0.25	0.05								2.320	2.402	6527	6402	3709	3532	56.3	52.7	43.9
0.6									0.4	0	5.239	5.270	6766	6520	3923	3581	35.7	43.7	36.4
0.6									0.35	0.05	5.383	5.215	3700	3969	2176	2214	39.5	44.3	36.9
0.6									0.3	0.1	5.261	5.159	3690	4018	2170	2243	42.0	44.8	37.4
0.6									0.25	0.15	5.279	5.104	3850	4067	2265	2272	38.9	45.4	37.8
0.6									0.2	0.2	5.223	5.048	3700	4115	2176	2301	45.1	45.8	38.2
0.6									0.15	0.25	5.282	4.993	4000	4163	2350	2330	52.6	46.3	38.6
0.667			0.333						0		2.377	2.457	4300	4209	2530	2359	45.9	48.1	40.1
0.6			0.3						0.1		2.850	3.146	5771	6153	3240	3477	44.0	44.6	37.2
0.533			0.267						0.2		3.252	3.835	5200	5238	2950	2959	40.9	40.0	33.3

It was suggested [20], [21] that, an addition of alkali oxide modifier to TeO_2 glass, the strengths of the Te-O_{ax} and Te-O_{eq} bonds become weak and the TeO_4 trigonal bi-pyramid network breaks up, and are accompanied by creation of non-bridging oxygen atoms in both Te-O_{eq} and Te-O_{ax} bonds. Yoko et al. [21] proposed a mechanism for the change of coordination number of Te^{4+} from 4 through (3+1) polyhedron to 3, as the alkali oxide modifier content is varied. Uchino and Yoko [22] reported that the Te-O_{ax} bonds in TeO_4 trigonal bi-pyramid are much weaker than the Te-O_{eq} bonds. Thus in tellurium glasses with alkali oxide as modifier, there is a structural change in coordination polyhedron induced by the change in modifier concentration.

For borate glasses, [23]–[27] used ultrasonic techniques to study the binary system xM_2O – $(1-x)B_2O_3$; (M: Li, Na, K, Rb, or Cs) where x is the mole fraction of M_2O. They proposed a model to explain the effect of adding alkali to B_2O_3: The elastic properties of these glasses were analyzed in terms of

three structural units defined as $B\varnothing_3 \equiv$ a; $M^+B\varnothing_2O^- \equiv$ b and $M^+$is $^-$represents a bridging oxygen and O ∅c; where $\equiv B\phi_4^-$ non-bridging oxygen. They assumed that these structural units have their respective elastic constants defined on the basis of a thermodynamic equation of deformed body. They showed that the rigidity of the glass was increased with the structural unit (c) while it decreased with the structural unit (b). They found that the structural unit (a) was converted only into the structural unit (c) in the composition range (0<x<0.28) of lithium borate glasses. The sound velocity of lithium borate glasses increased monotonously with increasing modifier in mol% content in this range, whereas, the velocity in the other two binary systems (sodium and potassium borate glasses) showed a single maximum around x = 0.34 mol% for sodium borate glass and around x = 0.30 mol% for potassium borate glass. The authors correlated the occurrence of a single maximum to the increase of non-bridging oxygens. On the other hand, the velocity in binary systems rubidium and cesium borate glasses showed a maximum at about 0.10 mol% for rubidium borate glass and at about 0.06 mol% for cesium borate glass.

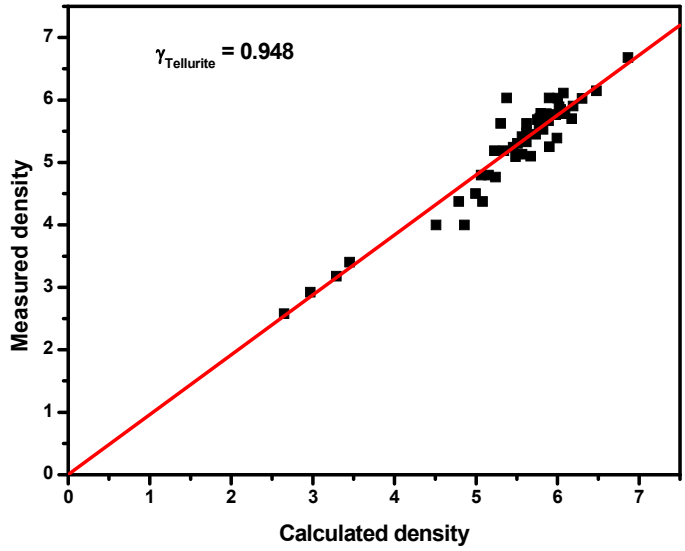

Fig. 1 The relation between the measured densities and the calculated densities of the glass compositions based on the additive rule (ρ_i) for tellurite glasses

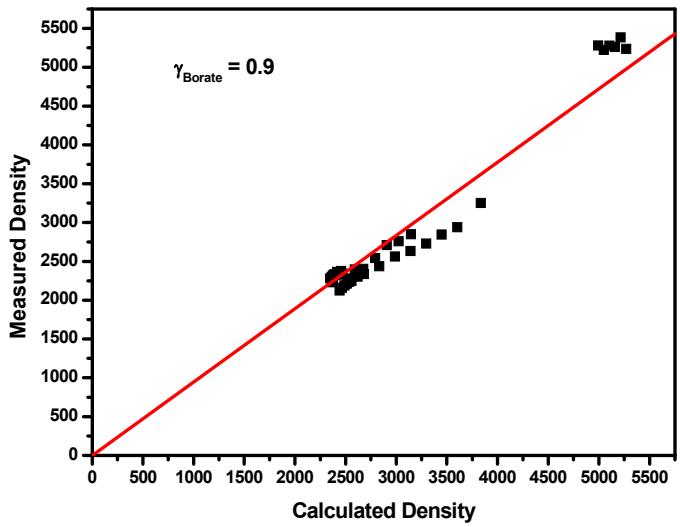

Fig. 2 The relation between the measured densities and the calculated densities of the glass compositions based on the additive rule (ρ_i) for borate glasses

Figs. 1 and 2 show the relations between the measured densities (ρ_m) for many different tellurite and borate glasses, which were taken from [12], [28]–[43] and the calculated densities of the glass compositions based on the additive rule

(ρ_i). The slopes of the relations which are the modified coefficients ($\gamma_{Tellurite}$& γ_{borate}) for tellurite and borate glasses. The modified coefficients values were found to be as 0.948 and 0.900 for tellurite and borate glasses, respectively. Then (19) will take the following forms;

$$\rho_{cal} = 0.948\sum_i \rho_i x_i \tag{21}$$

for tellurite glasses with correlation factor 99.8 %, and

$$\rho_{cal} = 0.900\sum_i \rho_i x_i \tag{22}$$

for borate glasses with correlation factor 99.4 %. Results of the measured densities and calculated densities are listed in Tables I and II for tellurite glasses and borate glasses, respectively.

As can be seen in Figs. 1 and 2, there are some deviations from linearity due to the structural changes in tellurite and borate glasses which are not considered in the calculations and have been discussed at the beginning of this section. Also, the presence of four low density glass compositions (which are belong to the glass system TeO_2 – B_2O_3 – Li_2O) as shown in Fig. 1 and Table I, are due to the low mol % content of TeO_2 from 0.1 to 0.35.

B. Ultrasonic Velocities Calculations

Figs. 3 and 4 show the relations between the experimentally determined bulk moduli (K_e) and the product of packing density and Young's modulus ($V_t.E_{M-M}$) for tellurite and borate glass compositions. The slopes ($\beta_{Tellurite}$ & β_{Borate}) were found to be as 1.319 and 1.200 for tellurite and borate glasses, respectively. Then (7) will take the following forms;

$$K_{cal} = 1.319.V_t E_{(M-M)} \tag{23}$$

for tellurite glasses with correlation factor 99.1 %, and

$$K_{cal} = 1.2.V_t E_{(M-M)} \tag{24}$$

for borate glasses with correlation factor 99.5%.

The results of the experimentally determined bulk moduli (K_e), theoretically obtained bulk moduli (K_{cal}) and the product of packing density and Young's moduli ($V_t.E_{M-M}$) for the glass compositions under investigation were listed in Tables I and II. Then both the ultrasonic wave velocities (U_l & U_s) were obtained theoretically using (20) and compared with those experimentally determined as shown in Figs. 5-8 and Tables I and II. The results showed good agreement between those obtained experimentally and theoretically obtained, and the deviations were found to be about 3% on average. Finally, those results led one to conclude that this method is good for theoretical prediction or simulation of both ultrasonic wave velocities for any tellurite or borate glasses using the data of packing densities and dissociation energies of the constituent oxides.

IV. Conclusions

The author's solution was found to be applicable for characterizing amorphous glass materials using the complete theoretical model, which now give a good chance to simulate the structures of glass materials before experimental processing.

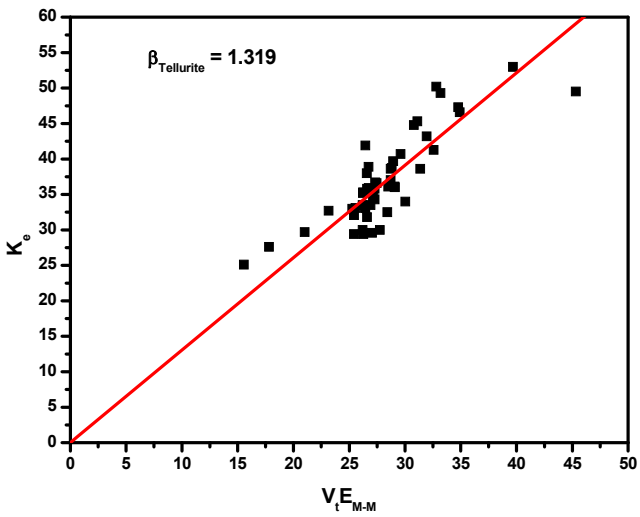

Fig. 3 The relation between the measured bulk moduli and the product of the packing density and calculated Young's modulus for tellurite glasses

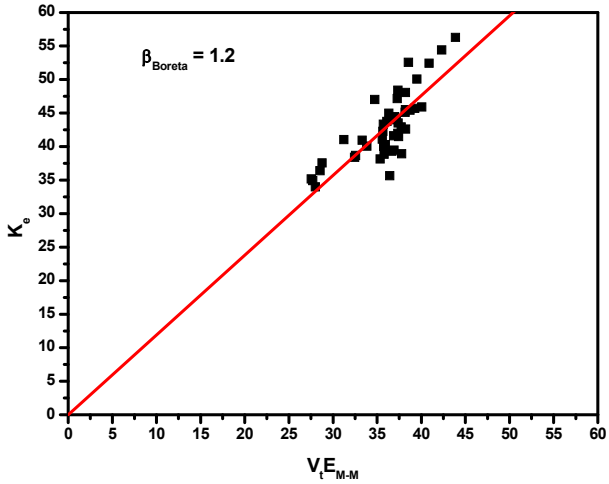

Fig. 4 The relation between the measured bulk moduli and the product of the packing density and calculated Young's modulus for borate glasses

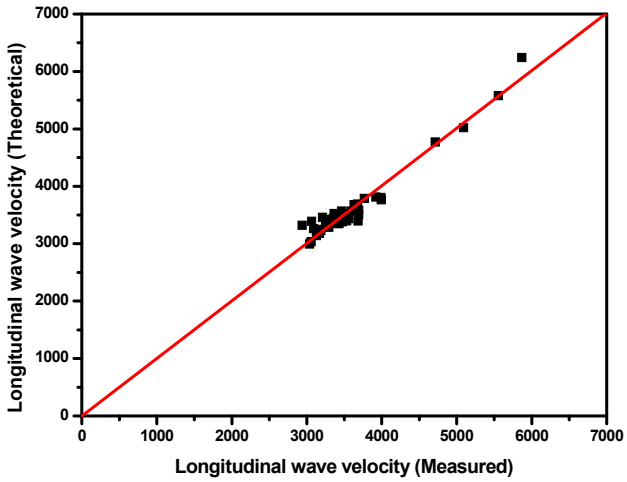

Fig. 5 The relation between the experimentally determined longitudinal ultrasonic wave velocities and the theoretically determined longitudinal ultrasonic wave velocities for Tellurite glasses

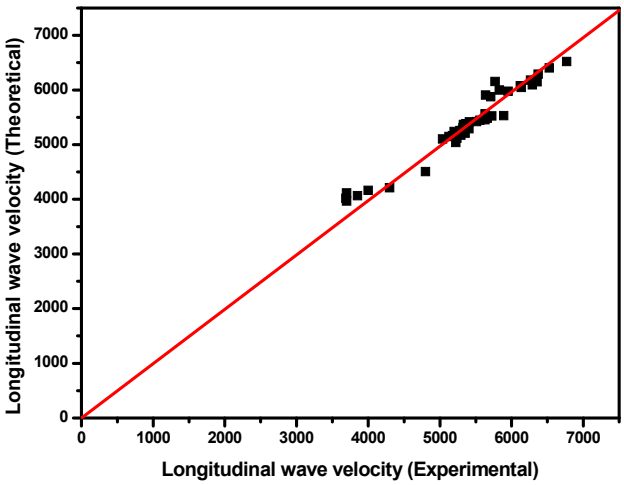

Fig. 6 The relation between the experimentally determined longitudinal ultrasonic wave velocities and the theoretically determined longitudinal ultrasonic wave velocities for borate glasses

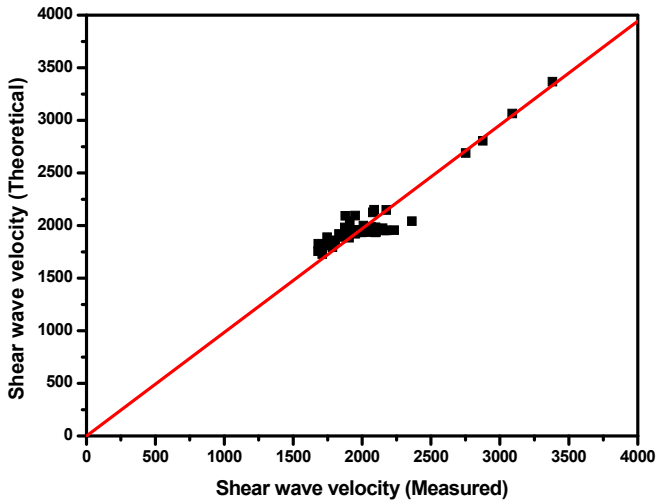

Fig. 7 The relation between the experimentally determined shear ultrasonic wave velocities and the theoretically determined shear ultrasonic wave velocities for tellurite glasses

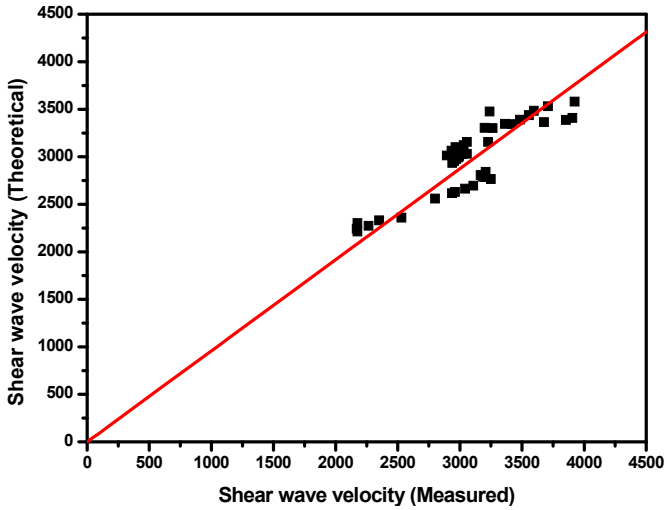

Fig. 8 The relation between the experimentally determined shear ultrasonic wave velocities and the theoretically determined shear ultrasonic wave velocities for borate glasses

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