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Elastic Properties Of Biba(K)O_3ferroelectric Oxide Glass

M. S. Emam
Department of Basic Science, Canadian International Collage, Egypt
Corresponding Author: M. S. Emam

ABSTRACT: *Based on the pair distribution functions of $(Bi_2O_3)_{90-x}(K_2O)_x(BaO)_{10}$,$(Bi_2O_3)_{90-x}(BaO)_x(K_2O)_{10}$ferroelectric oxide glass,we have been obtained the pair potential of all components. By applying Schofield's equations, the elastic constants have been calculated. Velocity of sound, elastic moduli, Debye temperature has been obtained as a function of Bi_2O_3, BaO and K_2O contents. The calculated results are in good well agreement with available experimental data.*

KEYWORDS: *Oxide glasses, elastic constant, and mechanical properties*

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I. INTRODUCTION

Ferroelectric oxide glasses which consist of network formers and modifiers provide a wide range of excellent properties and new applications technologies by selecting suitable chemical composition. . Any change in composition of a former or modifier of glass results in a change in density, local structure of cations (e.g., coordination number) which reflect on the change of the mechanical properties of glass such as Young's moduli *Y* and bulk moduli *B*. Another important parameter is Debye temperature θ_D which represents the temperature at which nearly all the vibrational modes are excited, its increase implies an increase in the rigidly. BiBa(K)O_3 ferroelectric oxide glass is investigated because it characterized as ferroelectric and low temperature superconductor materials. Since the strength of materials increases with their elastic moduli, so it is possible to evaluate strength indirectly from their elastic property [1]. In this study, elastic properties of 2 series of simulated ferroelectric oxide glasses of are computed, series 1 is$(Bi_2O_3)_{90-x}(K_2O)_x(BaO)_{10}$, series 2 is$(Bi_2O_3)_{90-x}(BaO)_x(K_2O)_{10}$($x$=0, 10,20,30, and 40).

II. THEORY

The pair potential *V(r)* is computed form pair distribution function *g(r)* according to the following relation [2, 3]

$$V(r) = -K_B T \ln(g(r)) \quad (1)$$

whereK_B is the Boltzman's constant and *T* is the temperature.
Figure 1 show the empirical pair potential computed from pair distribution *g(r)* which used in computation of elastic constant.
The pair potential is used along with that of Schofield equations [4] to compute the elastic constant, the integrals I_1 and I_2 are given by

$$I_1 = \frac{\rho}{2k_BT}\int_v g(r)rV'(r)dr \quad (2)$$

$$I_2 = \frac{\rho}{2k_BT}\int_v g(r)r^2V''(r)dr \quad (3)$$

Where $V'(r)$ and $V''(r)$ are the first and second derivatives of pair potential*V(r)* andρ is density.
These I_1 and I_2 integrals are in turn related to the elastic constant [5] as

$$C_{11} = \varrho k_BT\left(3+\frac{2I_1}{15}+\frac{I_2}{5}\right) \quad (4)$$

$$C_{12} = \varrho k_BT\left(1+\frac{2I_1}{5}+\frac{I_2}{15}\right) \quad (5)$$

The longitudinal and transverse velocity of sound can be calculated from [4]

$$v_L^2 = \frac{C_{11}}{\rho} \quad (6)$$

$$v_T^2 = \frac{C_{44}}{\rho} \quad (7)$$

Then the mean velocity is

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_T^3} + \frac{1}{v_L^3}\right)\right]^{-\frac{1}{3}} \quad (8)$$

From the longitudinal and transvere sound velosity we can get the mechanical properties such as the Young's modulus Y

$$Y = \rho v_T^2 \frac{3v_L^2 - 4v_T^2}{v_L^2 - v_T^2} \quad (9)$$

Bulk modulus B

$$B = \rho \frac{3v_L^2 - 4v_T^2}{3} \quad (10)$$

Debye temperature [6] of the ferroelectric oxide glasses was calculated from the relation

$$\theta_D = \frac{h}{k_B} \sqrt[3]{\frac{9\rho}{4\pi}} v_m \quad (11)$$

Where *h* is planck's constant.

III. RESULTS AND DISCUSSION

In our previous theoretical work, we compute the pair distribution function g(r) of same ferroelectric oxide glasses which used in the present work to carry out the pair potential. Figure 1 shows the pair potential with is computed from the computed pair distribution functiong(r).

Figure 2 shows the variation of the computed Young Y, bulk Bmoduliand Debye temperatureθ_D of $(Bi_2O_3)_{90-x}(K_2O)_x(BaO)_{10}$ ferroelectric oxide glasses with substitution Bi_2O_3 by K_2O.it is clear that the computedelastic moduli increased with subsistution Bi_2O_3 by K_2O. The computed Young Y, bulk Bmoduliand Debye temperature$\theta_D$of $(Bi_2O_3)_{90-x}(BaO)_x(K_2O)_{10}$ ferroelectric oxide glasses with substitution Bi_2O_3 by BaO are shown in Figure 3. Refering to this Figure we can observe that by replacement of Bi_2O_3 by BaO the mentioned computed elastic moduli increased. The increment of the computed elastic moduli of the pervious ferroelectric oxide glasses means increase in rigidity. These manners of increment due to the change of the glass structure accompanied with replacement formers (Bi_2O_3) by modifiers (K_2O and BaO) which appears on the values of the computed pair distribution function *g(r)*.These subsistution caused a increment of computed *g(r)*as shown in Figure 4.It is clear that by using (K_2O) as a modifier the values of the computed elastic moduli are higher than using BaO, thisdue to that the computed g(r)in case of K_2O is higher than BaO.

IV. CONCLUSIONS

The variation in the composition of a former or modifier of glass results in a change in the structure which reflect on the change of the mechanical properties of glass such as the elastic constant such as Young's Y and bulk B moduli, and Debye temperature θ_D. The elastic moduli of $(Bi_2O_3)_{90-x}(K_2O)_x(BaO)_{10}$ and $(Bi_2O_3)_{90-x}(BaO)_x(K_2O)_{10}$ ferroelectric oxide glasses are computed by Schofield equations. The increment of those moduli with substitutions of former (Bi_2O_3) by modifier (BaO and K_2O) is due the change of structure whichreflected on the computed pair distribution function*g(r)*. The (K_2O) as a modifier has a higher effect on improvement the mechanical properties of the ferroelectric oxide glasses rather than (BaO).

V. REFERENCES

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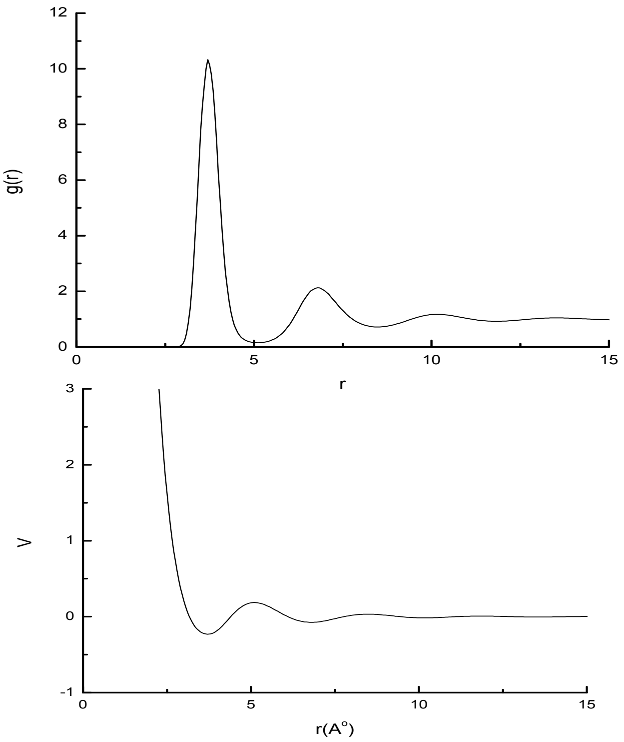
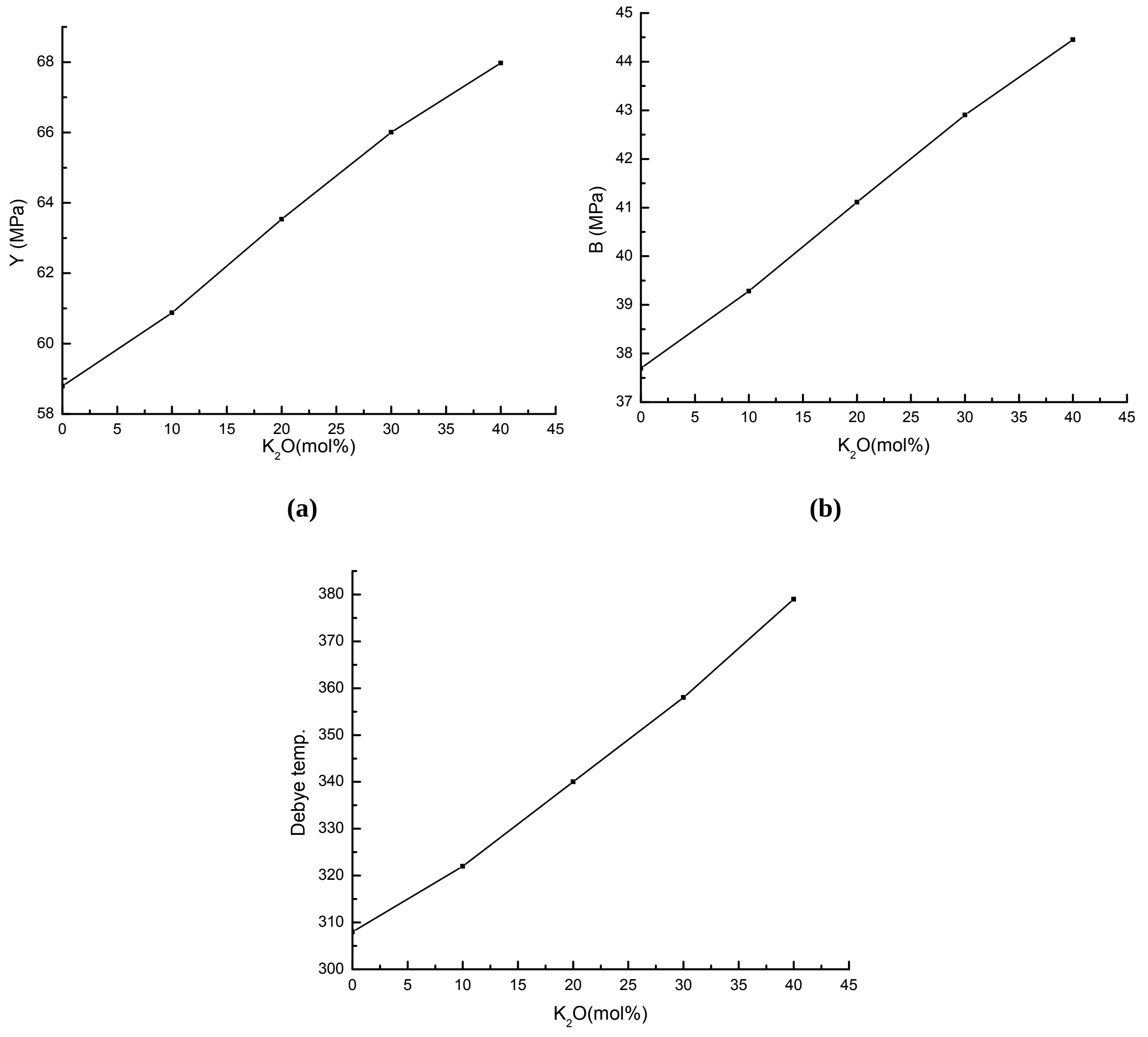


Fig.1: The empirical pair potential *V(r)* computed from the computed pair distribution function *g(r)* of $(Bi_2O_3)_{40}(K_2O)_{50}(BaO)_{10}$ ferroelectric oxide glass.



(a) (b)

(c)

Fig. 2: The computed elastic moduli of $(Bi_2O_3)_{90-x}(K_2O)_x(BaO)_{10}$ ferroelectric oxide glasses with variation of K_2O contents

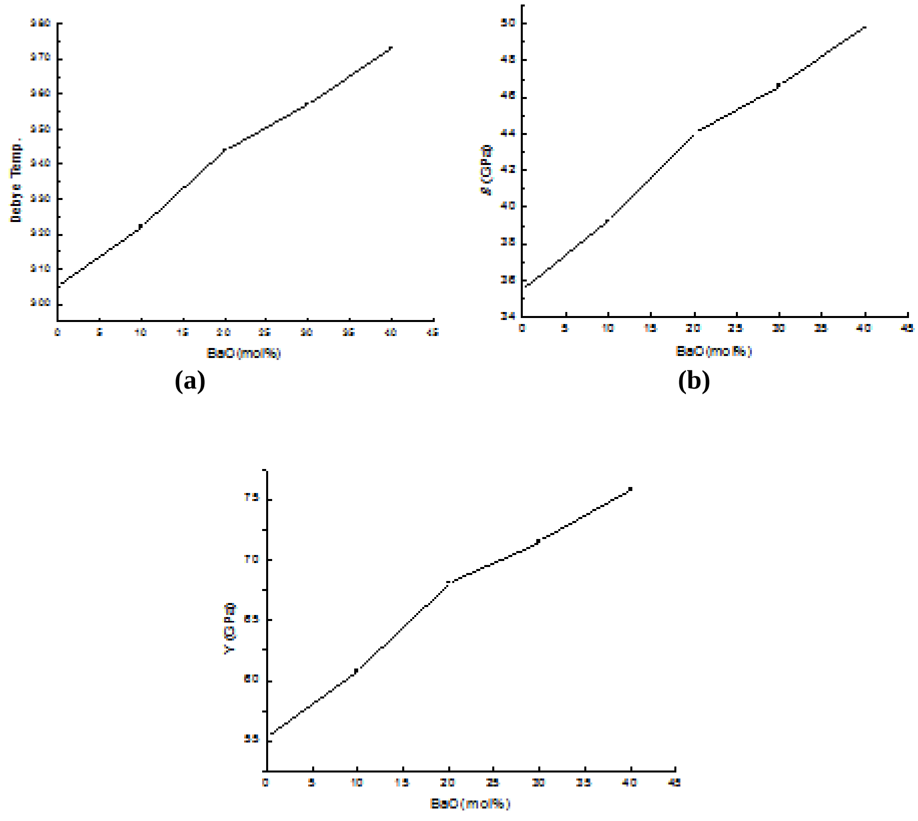


Fig. 3: The computed elastic moduli of $(Bi_2O_3)_{90-x}(BaO)_x(K_2O)_{10}$ ferroelectric oxide glasses with variation of BaO contents

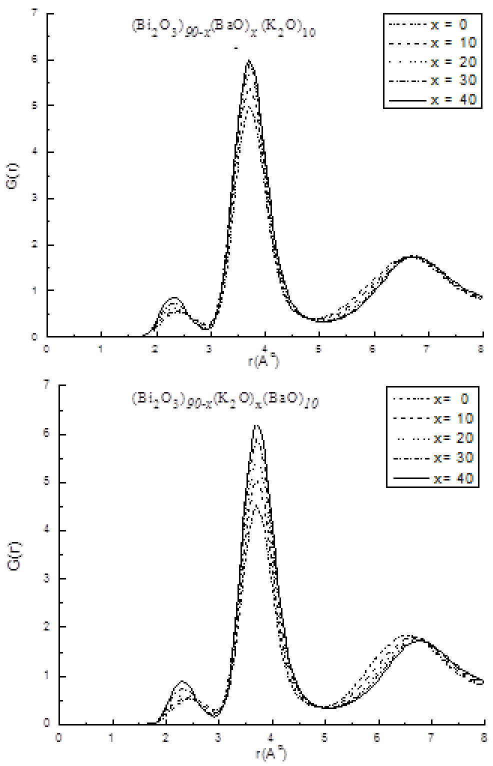


Fig.4: The values of the computed *g(r)*.

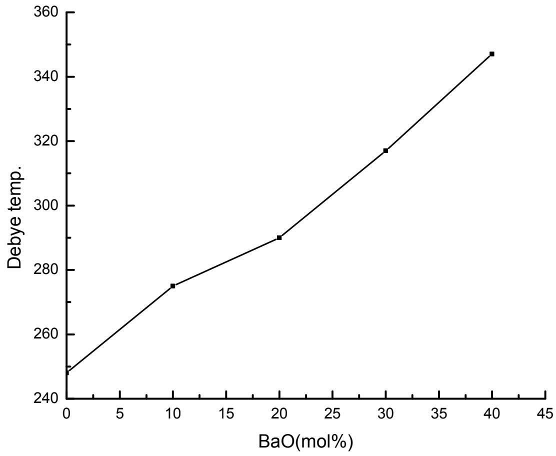


Fig. 5: The computed elastic moduli $(PbO)_{90-x}$ $(BaO)_x(K_2O)_{10}$ ferroelectric oxide glasses with variation of BaO contents.

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