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# Construction of mathematical equation to predict the densities of $B_aO$ - $B_2O_3$ - $Bi_2O_3$ glass system using the percentage weights of its constituents

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## Abstract

Glass systems are now a trending topic of research for radiation shielding. It takes time to fabricate the glass and then to measure its density, following which other properties are determined. Some chemicals' manufacturers write on the chemical containers the health effect of such chemicals if they get contact with eyes or skin and when inhaled. It's therefore of great importance to devise non experimental technique to study the physical and shielding properties of glass systems. The aim of this work is to construct a mathematical equation capable of reproducing and predicting densities of glasses in the system given by "yBaO - xBi2O3 - (100 – x -y) B2O3", where (10 ≤ y ≤ 24 wt% and 0 ≤ x ≤ 100 – y) wt%) so, as to avoid the repetitive fabrication of each member of this system and to cut the cost of fabrication and to assure safety from the chemical exposure. We made used of the existing samples to study the nature of the densities in such system and came up with an equation, using which the densities could be reproduced and some others could be predicted by deciding the weight percentages of the constituent chemicals. The formula has a minimum percentage accuracy of 97.4 %. The use of this formula for studying radiation shielding properties of glasses in this system is therefore of great importance.

**Keywords:** Prediction of Density; Density of Glass System; Density Computation; Calculation of Glass Density; Density from Weight Percentage; Glass Shielding

## 1. Introduction

The use of radiation becomes a daily practice in various aspects of life, particularly for workers in radiological departments, nuclear power and research centers, and in agricultural, geological and other scientific researches. However, the various degrees of the hazardous effects of radiation (1–3) makes it necessary for scientist to develop some means of protection, among which is the use of shielding materials (4) used to reduce the radiation energy to a safety level. (1,5).

The popular materials used for radiation shielding are concrete, used more commonly in hospitals and nuclear energy and research centers (6,7). Clay blocks, rocks and lead-based materials were also in used for radiation shielding (8). However, these materials have thermal instability and have limitation to use only in some particular situations.

Glasses are now a days doped with minerals, nano particles or heavy metal oxides (7), etc. to form glass systems. These glass systems are becoming the alternative shielding materials with better optical and chemical properties and environmental friendly; they are non-toxic, non-corrosive and have high coefficient of radiation attenuation (7,9).

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There are various properties associated with glass systems as shielding materials, these properties include high linear and mass coefficients of attenuation (LAC) and (MAC) respectively, low values of mean free path (MFP), halve value layer (HVL) and tenth value layer (TVL) (7,10). All these properties are related to high value of density and therefore determination of density becomes one of the major aspects of research in studying the shielding properties of glass systems. Among the most promising dopants in glass systems is bismuth oxide ($Bi_2O_3$) which is highly dense and therefore contributes to the overall high density of the end product (11,12).

To determine the density, the glass system has to be manufactured and then the density is calculated using its measured mass and volume, or by the use of other liquid with known densities as in Archimedes' Principle. This process consumes time and has cost implication. We therefore, in this work aimed at developing a mathematical formula to predict the density of glass system containing Boron Oxide ($B_2O_3$) and Barium Oxide (BaO) doped with Bismuth Oxide ($Bi_2O_3$) according to the system $yBaO - xBi_2O_3 - (100 - x - y)B_2O_3$, where ($10 \leq y \leq 24$ wt% and $0 \leq x \leq 100 - y$) wt%). The formula is used by inputting the percentage weights (wt %) of its constituent components BaO, $Bi_2O_3$ and $B_2O_3$ and then solved mathematically to predict the density of the glasses of this system with high degree of accuracy.

Previously, (13) developed a mathematical polynomial equation (Equation 1) as a non-experimental way to determine the density of silicate glasses at room temperature.

$$\rho = b_o + \sum_{i=1}^{n}\left[ b_i C_i + \sum_{k=i}^{n}\left( b_{ik} C_i C_k + \sum_{m=k}^{n} b_{ikm} C_i C_k C_m \right)\right] \quad \ldots\ldots\ldots\ldots (1)$$

Where $\rho$ is the density of the silicate glass, $b_o$ is a constant equals to 2.121560704, $b_i$, $b_{ik}$, $b_{ikm}$, are coefficients of the model. $C_i$, $C_k$ and $C_m$ are the concentrations in mol% of the glass components excluding silica, and n is the total number of the glass components, also excluding silica (13).

Another approach to none experimentally determine the density of glass is the use of machine learning ML. Where computer is trained using large number of training data, which is the mole percentages (mol %) or weight percentages (wt %) and their corresponding resulted densities in literature, in order to be able to predict the densities of other glasses with different concentrations of similar components. This work is also based on densities of $SiO_2$ in combination with some oxides (14).

A glass system $(80 - x)B_2O_3 - xBi_2O_3 - 20BaO$, where (x = 10, 20, 30, 40, 50 and 60 mol%) was fabricated and the densities of the individual members were determined experimentally by (15) and in the present work, the mathematical formula was constructed in order to reproduce those experimental densities and to predict other densities which follow the same sequence by the use of wt% of the components.

The importance of the present work is in the simplification of the way to reproduce the densities in (15), and to predict the densities of the glass system $yBaO - xBi_2O_3 - (100 - x - y)B_2O_3$, where ($10 \leq y \leq 24$ wt% and $0 \leq x \leq 100 - y$ wt%), within less time and capital consumption and to assure safety from the health effect of some glass constituents. Furthermore, the steps involved in calculating wt% are less compared to calculation of mol%, therefore the construction and the use of this formula will be more time-saving than other techniques which involves the use of mol%.

### 1.1. Hypothesis

The following hypotheses were made:

- Density of mixture made from various components say $X_1$, $X_2$ and $X_3$ which are not chemically interacting with each other can be calculated theoretically using (Equation 2).

$$\rho_{theor.} = \frac{100}{(\frac{wt\,\%}{\rho})_A + (\frac{wt\,\%}{\rho})_B + (\frac{wt\,\%}{\rho})_C} \quad \ldots\ldots\ldots\ldots\ldots\ldots (2)$$

Where $\rho_{theor.}$ is the theoretical density of the mixture and $\rho$ is the densities of the components, $X_1$, $X_2$ and $X_3$.

- There is Physical and Chemical interactions between the components $X_1$, $X_2$ and $X_3$ (13). This interaction may cause the real density of the mixture to deviate from the theoretical densities.

- Let the deviation be represented by a term say (± d) which should be added to $\rho_{theor.}$ so that the computed density $\rho_{comp.}$ will be equal to the experimental densities, as shown in (Equation 3).

$$\rho_{comp} = \rho_{theor.} \pm d \quad \text{..... (3)}$$

Where, $\rho_{comp.}$ is the computed density, ± d is the term added to $\rho_{theor.}$ in order to correct its deviation from the experimental densities due to physical and chemical interactions between the molecules of the constituent components.

## 2. Methodology

We made used of Phy-X/PSD to determine the equivalent wt% for various mol% in the glasses reported by (15). The graph of wt% against the mol% was plotted (Figure 1) to get (Equation 4) which describes the mathematical relationship between the two units in this particular glass system. To determine the term, d, we developed a Python Programming code to request for the wt% of the three components of the members of this glass system and calculate the theoretical density, it then compares the theoretical density and the experimental one and return their difference. The difference is the parameter, d, and the values of "d" are plotted against various wt% of the dopant to get a general equation for all d(s) in this system (Equation 5).

Densities of the glasses reported in (15) can then be reproduced, and that of other glasses with various wt% can also be predicted.

Let's define d in ($gcm^{-3}$) as the deviation of the $\rho_{theor.}$ from the experimental densities for various concentrations, c in (mol %), of the dopant, $Bi_2O_3$. The graph of d against $Bi_2O_3$ represents an equation which defines how $\rho_{theor.}$ deviates from the experimental densities for various c. The equation of the curve represents ± d and is added to the $\rho_{theor.}$ to form a general equation for all the samples in the system.

## 3. Results and discussion

The relationship between mol% converted into wt% for the glass system under study is shown in figure 1.

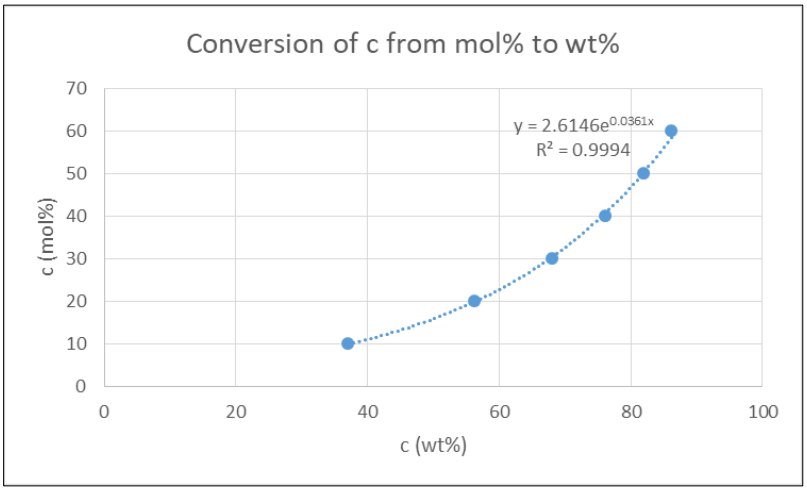


**Figure 1** A graph showing the relationship between c in mol% and in wt%.

The equation that defines the curve is shown in (Equation 4).

$$mol\% = 2.6146^{0.0361(wt\%)_{Bi_2O_3}} \quad \text{.....(4)}$$

The graph of deviation of densities found theoretically from the experimental ones, d in ($gcm^{-3}$), for various concentrations of $Bi_2O_3$ in (mol%), c, is shown in figure 2.

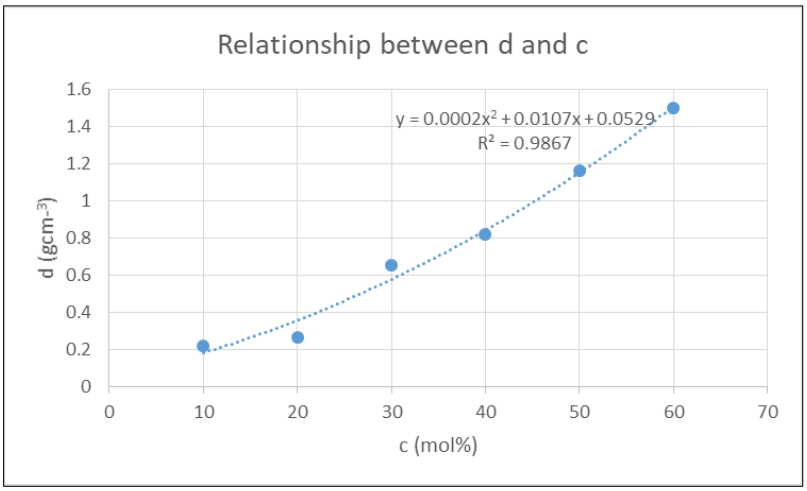


**Figure 2** Relationship between the deviation of the theoretical and experimental densities with respect to the concentration of the dopant $Bi_2O_3$ in mol %.

The curve showing the relationship between d ($gcm^{-3}$) and c (mol %) of $Bi_2O_3$ is defined by (Equation 5).

$$d = 0.0002c^2 + 0.0107c + 0.0529 \qquad \text{……..(5)}$$

Where c is in mol %.

With the help of (Equation 4) into (Equation 5), the representation of d in wt % is achieved. and therefore, (Equation 3) is rewrite as (Equation 6).

$$\rho_{comp.} = \frac{100}{(\frac{wt\%}{\rho})_{BaO} + (\frac{wt\%}{\rho})_{B_2O_3} + (\frac{wt\%}{\rho})_{Bi_2O_3}} - \left[0.0014e^{0.072(wt\%)_{Bi_2O_3}} + 0.028e^{0.036(wt\%)_{Bi_2O_3}} - 0.1\right] \text{……(6)}$$

The densities of glasses B1 - B6 in (15) could be reproduced using (Equation 6). Let the reproduced densities represent glasses B'1 – B'6 as shown in table 1. The sets of data for each glass Bi (where i = 1, 2, ...6) are transformed into set of data for B'i (where i = 1, 2, ...6) respectively before being inputted into (Equation 6) to determine the computed densities.

**Table 1** Transformation of mol % into wt % for various glasses.

| Sample | $B_2O_3$ (mol %) | $Bi_2O_3$ (mol %) | BaO (mol %) | | Sample | $B_2O_3$ (wt %) | $Bi_2O_3$ (wt %) | BaO (wt %) |
|---|---|---|---|---|---|---|---|---|
| B1 | 70 | 10 | 20 | | B'1 | 38.7 | 37.0 | 24.3 |
| B2 | 60 | 20 | 20 | | B'2 | 25.2 | 56.3 | 18.5 |
| B3 | 50 | 30 | 20 | | B'3 | 17.0 | 68.1 | 14.9 |
| B4 | 40 | 40 | 20 | | B'4 | 11.4 | 76.1 | 12.5 |
| B5 | 30 | 50 | 20 | | B'5 | 07.3 | 81.9 | 10.8 |
| B6 | 20 | 60 | 20 | | B'6 | 04.3 | 86.2 | 09.5 |

The computed densities are compared with the experimental ones in figure 3.

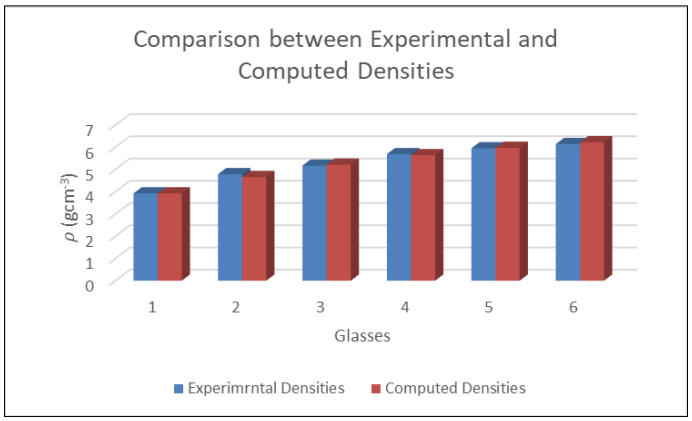


**Figure 3** The histogram showing the closeness of the computed densities to the experimental ones

The histogram (Figure 3) shows the computed densities and the experimental ones and also shows the accuracy of the constructed formula, which was evaluated statistically to have percentage accuracy within 97.388 – 99.924 % ($gcm^{-3}$), with average percentage accuracy of 98.982 % ($gcm^{-3}$).

Some predicted densities for various concentrations of BaO, $B_2O_3$ and $Bi_2O_3$, based on the developed formula in this work are shown in (Table 2). For other shielding properties, after predicting the densities, Phy-X/PSD software (16) can be used.

**Table 2** Some Predicted Densities for various concentrations of $B_2O_3$, $Bi_2O_3$ and BaO

| **BaO (wt %)** | **$B_2O_3$ (wt %)** | **$Bi_2O_3$ (wt %)** | **$\rho$ ($gcm^{-3}$)** |
|---|---|---|---|
| 10 | 50 | 40 | 3.5252 |
| | 51 | 39 | 3.4905 |
| | 52 | 38 | 3.4559 |
| | 53 | 37 | 3.4218 |
| 11 | 53 | 36 | 3.4187 |
| | 54 | 35 | 3.3852 |
| | 55 | 34 | 3.3522 |
| | 56 | 33 | 3.3198 |
| 12 | 56 | 32 | 3.3164 |
| | | 31 | 3.3488 |
| | | 30 | 3.3164 |
| | | 29 | 3.2846 |
| 13 | 39 | 48 | 3.9548 |
| | 40 | 47 | 3.9109 |
| | 41 | 46 | 3.868 |
| | 42 | 45 | 3.8258 |
| 14 | 42 | 44 | 3.8228 |
| | 43 | 43 | 3.7814 |
| | 44 | 42 | 3.7408 |
| | 45 | 41 | 3.7009 |

## 4. Conclusion

An equation capable of reproducing and predicting densities of glasses in the system $yBaO - xBi_2O_3 - (100 - x - y)B_2O_3$, where ($10 \leq y \leq 24$ wt% and $0 \leq x \leq 100 - y$) wt%) is developed by studying the deviation of the theoretically calculated densities from the experimentally found densities in literature. This work simplifies the tedious experimental production of all samples in this system, and also simplifies the relatively longer time approach of calculating mol % for each component in the glass formation, and the use of this equation makes research on the glass system under study cheaper and safer.

The percentage accuracy of the formula is within 97.388 – 99.924%, with average of 98.982%. This indicates the suitability of this formula for calculating density of glass in the system under study and for sample prediction for research purpose.

## Compliance with ethical standards

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### *Disclosure of conflict of interest*

The authors declare that there is no conflict of interest in publishing this article in this journal.

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