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Developing a Mathematical Formula that can Calculate the Density of MoO_3-B_2O_3-Bi_2O_3 Glass System from Weight Percentages of its Components.

[1*]ALHASSAN, M; [2]USMAN M; [3]MUAZU, SI

[1]Department of Physics, Federal University Dutsin-Ma, Katsina State, Nigeria*
[2]Multimedia University, Malaysia
[3]Department of Physics, Kano State College of Education and Preliminary Studies, Kano State, Nigeria

**Corresponding Author Email: alhasanmuhammad@ymail.com*
Co-Authors Email: muhusman55@gmail.com, simm.phy@gmail.com

ABSTRACT: Research on glass systems for radiation shielding involves the fabrication of different samples in a sequential manner. In order to determine their shielding properties their densities have to be found experimentally. This procedure causes time and capital consumption and is associated with health risk due to the biological harms of some chemicals involved in it. Therefore, the objective of this work is to reduce the cost, time and health risks by developing a mathematical model to calculate the density of MoO_3 - B_2O_3 - Bi_2O_3 glass system from weight percentages of its components using Phy-X/PSD software and Python Programming. The input needed are the densities and percentage weights of the constituent components. The coding made in Python programming language to test the formula shows its ability to reproduce or predict densities of the required samples of this glass system with accuracy within 99.59 – 99.88%. Therefore, making use of this formula will simplify the difficulty of refabricating glasses defined by the expression $yMoO_3$ - xB_2O_3 - $(100 – y – x)$ Bi_2O_3 for research purposes, which will reduce the financial cost and health risks.

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Exposure to radiation results in two categories of harmful effects, stochastic effects, and deterministic effects. Both can be avoided or minimized by using radiation shielding (Alhassan et al., 2020). Glass systems are glasses doped with some additives for radiation shielding purpose. The additives can be minerals, nano particles, heavy metal oxides (HMO) such as tellurite oxide (TeO2), bismuth oxide (Bi_2O_3), tungsten oxide, lead oxide (PbO) (Abouhaswa et al., 2020) or molybdenum oxide (MoO_3) (Perişanoğlu et al., 2020) etc. A glass system usually comprises of multiple members in a sequential order and has a general expression that represents all the members of that system. The members may differ in the molar percentage, mol%, or weight percentage, wt%, of one or more component(s) in the glass formation. The popularity of glass systems in the field of radiation shielding increases due to their advantages over conventional lead shields, concretes, stones, etc. The advantages of glass over the other materials include their improved photon attenuation (Perişanoğlu et al., 2020), their special mechanical, optical, chemical, physical, thermal, electrical and semiconducting properties. Also, the radiation attenuation ability of glass system is not limited to gamma or x-rays photons, but also to charged particles and neutrons. Moreover, the glass systems are environmentally friendly (Kaur et al., 2019), and their unique properties can be improved. Some of the common methods used for glass fabrication are the conventional solid-state

**Corresponding Author Email: alhasanmuhammad@ymail.com*

process or melt quenching (Abouhaswa et al., 2020), sol gel and fast cooling methods (Gomaa et al., 2021). Glass formers are of two categories; some such as Silicon oxide (SiO_2) and Boron oxide (B_2O_3) can form glass alone, the two can also be combined to form borosilicate glass. The other category is of glass formers that cannot form glass alone, unless if combined with other glass former(s) in relatively larger compositions, or with some metal oxide(s). Examples of this category are Tellurium oxide (TeO_2) (Kavaz et al., 2020) and Bismuth Oxide (Bi_2O_3). Fabrication of glass usually involves the measurement of masses of the compositions, mixing them, heating the mixture until melted, molding, annealing (Abouhaswa et al., 2020) and cooling (Kaur et al., 2019; Kavaz et al., 2020). This has to be done for each sample in the glass system. This process may involve higher and higher temperature as some components are added to the new samples (Abouhaswa et al., 2020).

Glass Density is an important feature used in industries for quality control and weight reduction for easier transportation and application (Fluegel, 2007). However, in the field of radiation protection high density is a prerequisite quality and a property that determines many other aspects and features of shielding materials. If a sample in the series got spoiled or damaged prior to the experimental tests, glass of such composition must be refabricated. This is a time-consuming approach and costly. Furthermore, some of the chemicals involved in glass fabrication are biologically harmful to skin, eye or lungs when inhaled. Therefore, the objective of this work is to reduce cost, time and health risks, by developing a mathematical model for the calculation of the density of $yMoO_3$ - xB_2O_3 - $(100 – y – x)$ Bi_2O_3 glass system.

MATERIALS AND METHOD

We made use of a mathematical approach in a similar way that machine learning (ML) works. A python program was written using PyCharm notebook that will ask for the weight percent (wt %) of three glass components Bi_2O_3, B_2O_3 and MoO_3 and calculate the density of a glass with such composition based on (Equation 1).

$$\rho_{theor.} = \frac{100}{\left(\frac{wt\,\%}{\rho}\right)_A + \left(\frac{wt\,\%}{\rho}\right)_B + \left(\frac{wt\,\%}{\rho}\right)_C} \quad (1)$$

Where $\rho_{theor.}$ is the theoretical density of the mixed components, A, B and C, which represent Bi_2O_3, B_2O_3 and MoO_3, wt% is their weight percentages and ρ is the density of each one. Making use of (Equation 1) for this purpose is reported in (Alhassan et al., 2023). The program will then compare the calculated result with experimental one published in (Sayyed et al., 2019). The difference, referred here as the deviation of the theoretical density from the experimental one (dev), resulted in the need of a corrective term represented by (± C) which will correct (Equation 1). This gave rise to (Equation 2).

$$\rho_{comp.} = \rho_{theor.} \pm C \quad (2)$$

Where, $\rho_{comp.}$ is the computed density, ± C is the corrective term.

The deviation which resulted in the need of the addition of the corrective term may be attributed to the chemical interactions between the glass components (Fluegel, 2007).

The analysis of the result obtained from the Python program shows that corrective term for each sample, i, represented by Ci, depends on the product of dev% and $\rho_{theor\_i.}$ for that sample and is given by (Equation 3).

$$C_i = dev\,\% \times \rho_{theor\_i.} \quad (3)$$

The graph showing the relationship between the dev% term and the mol% of the dopant Bi_2O_3 for various samples is plotted. In order to make the density in the constructed formula a function of wt%, conversion of mol% into wt% was performed using Phy-X/PSD software (Şakar et al., 2020). This is because determining the wt% of a component involves less steps and is easier for users than determining its mol%.

The final formula based on (Equation 3) is rewritten in terms of wt% and then tested in the Python program. Statistical assessment of the constructed formula is made for its effectiveness.

How to use the formula: In the constructed formula, only the weight percentage, wt% will be decided by the researcher, while the densities of the constituent components are constants and are shown in Table 1.

Table 1: Densities of glass components.

Component	Density (gcm^{-3})
MoO_3	4.69
B_2O_3	2.46
Bi_2O_3	8.9

Normal mathematical procedure for simplifying equations must be adhered to, in order to get the

computed or predicted density. The wt% shall then be varied and the new inputs will give density of another member glass in the system under study. This enables researchers to predict densities of other glasses with higher or lower mol% or wt% in this glass system.

RESULT AND DISCUSSIONS

The relationship between Ci and dev is shown in (Equation 3). The graph of $dev\,\%$ against the concentration of Bi_2O_3 (mol %) is shown in Figure 1.

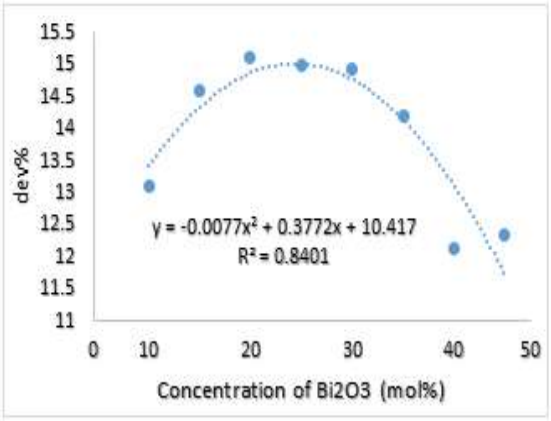

Fig 1: Percentage deviation of density from the experimental density against the concentration (mol %) of Bi_2O_3

The fitting curve equation that defines the general corrective term C for all C_i (s) is shown in Equation 4.

$$dev\,\% = 0.077(mol\,\%)^2_{Bi_2O_3} + 0.3772(mol\,\%)_{Bi_2O_3} + 10.417 \quad (4)$$

Where**,** dev% is the percentage of $\rho_{theor.}$ for each sample that deviates from the experimental densities for the corresponding mol% of Bi_2O_3 present in the sample. Ci is the corrective term for each sample.

The conversion of various values of mol% to wt% for Bi_2O_3 is achieved using Phy-X/PSD and the general equation for such conversion for the glass system under study is given by (Equation 5).

$$(wt\,\%)_{Bi_2O_3} = 27.56\ln(mol\,\%)_{Bi_2O_3} - 25.559 \quad (5)$$

Using (Equation 1) and (Equation 4) into (Equation 3), and then (Equation 3) into (Equation 2), we arrived at the constructed formula, (Equation 6).

$$\rho_{comp.} = \frac{89.583 + 0.049e^{0.0720(wt\%)_{Bi_2O_3}} - 0.956e^{0.0366(wt\%)_{Bi_2O_3}}}{\left(\frac{wt\%}{\rho}\right)_{MoO_3} + \left(\frac{wt\%}{\rho}\right)_{Bi_2O_3} + \left(\frac{wt\%}{\rho}\right)_{B_2O_3}} \quad ...6$$

Where $(wt\,\%)_{Bi_2O_3}$ is the weight percentage of Bi_2O_3, and $\left(\frac{wt\%}{\rho}\right)_{MoO_3}$, $\left(\frac{wt\%}{\rho}\right)_{Bi_2O_3}$, $\left(\frac{wt\%}{\rho}\right)_{B_2O_3}$ are the ratios of the weight percentages and densities of the components MoO_3, Bi_2O_3 and B_2O_3 respectively.

The Python program which requests the weight percentage of each of the three components of this glass system and return the predicted density was executed to test the accuracy of the formula (Equation 6), in comparison with the experimental densities MoBiB1, MoBiB2, MoBiB3 and MoBiB4 with Bi_2O_3 equals 30, 35, 40 and 45 mol% respectively. These glasses were fabricated by (Sayyed et al., 2019). The glasses labelled here as G1, G2, G3 and G4 are the glasses with wt% which are equivalent to 30, 35, 40 and 45 mol% of Bi_2O_3 respectively. We extrapolated four other densities in this series G5, G6, G7 and G8 for glasses with Bi_2O_3 equals 10, 15, 20 and 25 mol% respectively using Microsoft Excel. The four experimental densities and the four extrapolated densities are shown in Figure 2. The equivalence of mol% and wt% for the experimental and the extrapolated glasses are shown in Table 2. The result in Figure 3 shows the densities of glass system found experimentally and using the built mathematical formula in this work.

The percentage accuracy for the computed densities with respect to the experimental densities for G1 – G4 is within 99.59 – 99.97 and the mean percentage accuracy is 99.53957 gcm^{-3}. The comparison between the reproduced/predicted densities and the experimental/extrapolated densities is shown in Figure 3 and Figure 4 respectively.

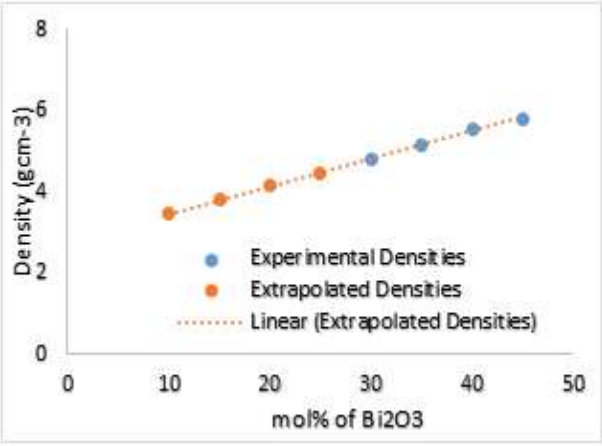

Fig 2: The experimental and extrapolated densities for various mol% of Bi_2O_3.

Table 2: The mol% and wt% of the compositions of the glasses G1 - G8

Glass type	MoO_3		B_2O_3		Bi_2O_3	
	mol%	wt%	mol%	wt%	mol%	wt%
G1	20	14.2	50	17.1	30	68.7
G2	20	12.9	45	14.0	35	73.1
G3	20	11.8	40	11.5	40	76.7
G4	20	11.0	35	09.3	45	79.8
G5	20	23.2	70	39.3	10	37.5
G6	20	20.0	65	31.4	15	48.6
G7	20	17.6	60	25.5	20	56.9
G8	20	15.7	55	20.9	25	63.5

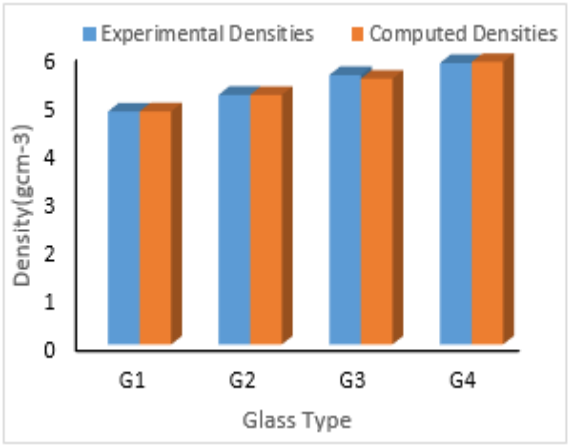

Fig 3: The comparison between the computed densities and the experimental densities.

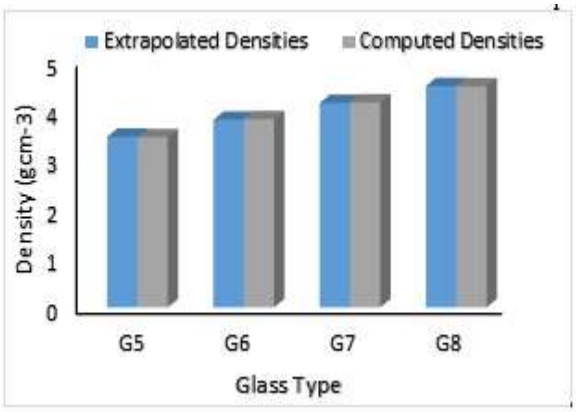

Fig 4*:* The comparison between the computed densities and the extrapolated densities.

The calculated densities and the extrapolated densities are shown in Figure 4, The percentage accuracy for the computed densities with respect to the extrapolated densities is within 99.66 – 99.88% and the mean percentage accuracy is 99.74%. This high percentage accuracy means an excellent agreement between the computed densities and both the experimental and the extrapolated densities, and further implies that, the constructed formula can be used to reproduced the densities of the glasses by inserting the appropriate wt% of the three components which forms the glass system and their respective densities and also other members of this series can be predicted by varying the wt% of the components in (Equation 6). Some predicted densities using this formula for various wt% of $yMoO_3$, where $10 \leq y \leq 13$ wt% and various wt% of B_2O_3 and Bi_2O_3 are show in Table 3**.**

Table 3: Predicted densities of some glasses of various wt% of MoO_3, B_2O_3 and Bi_2O_3.

Compositions (wt %)			Predicted Density (gcm^{-3})
MoO_3	B_2O_3	Bi_2O_3	
10	50	40	3.2065
	51	39	3.1749
	52	38	3.1439
	53	37	3.1136
11	53	36	3.1052
	54	35	3.0756
	55	34	3.0466
	56	33	3.0181
12	56	32	3.0101
	57	31	2.9823
	58	30	2.9550
	59	29	2.9282
13	39	48	3.5702
	40	47	3.5305
	41	46	3.4917
	42	45	3.4538

Table 3 shows predicted densities of glasses with wt% of MoO_3 fixed at 10, 11, 12 and 13 wt% while for each case varying wt% of Bi_2O_3 and B_2O_3. More densities can also be predicted using (Equation 6); however, the accuracy is higher at wt% of MoO_3 within $10 \leq y \leq 15$ wt% while x can be within $0 \leq x \leq 100 - y$ wt%. The limitation of this formula is due to the fact that no universal model in ML can predict all entities of a particular system efficiently (Stergiou et al., 2023). Thus, variation of some features results either in adopting new model or to end up with poor result. Therefore, this formula is used effectively within the specified ranges of x and y.

Conclusion: We constructed a mathematical formula in a similar way that machine learning works. The formula can be used to reproduce/predict densities of the glass system $yMoO_3 - xB_2O_3 - (100 - x - y)\ Bi_2O_3$, where ($10 \leq y \leq 15$ wt% and $0 \leq x \leq 100 - y$ wt %) with excellent percentage accuracy of at least 99.59% gcm^{-3}. The use of this formula can reduce the financial cost and time of reproducing members of this glass system.

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