

An Investigation into Empirical Equations for Predicting Density and Packing Density Parameters Across Diverse Chemical Compositions: A Theoretical Approach

R. Praveen Kumar

Department of Physics,
Bangalore University, Bengaluru, Karnataka, India.
E-mail: vyasa8273praveen@gmail.com

Susheela K. Lenkenavar

Department of Physics,
Bangalore University, Bengaluru, Karnataka, India.
Corresponding author: sushhh10@gmail.com

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Abstract

This work investigates an empirical equation for predicting the density and packing density parameter for different chemical combinations. The empirical equation suggested by Makishima and Mackenzie (1973) was employed to calculate the values of V_i , which indicates the packing density parameter and the equation proposed by Inaba and Fujino (2010) was utilized to calculate the density values. To determine the density values accurately, V_i is essential. This research focuses on revisiting the density model established by Inaba and Fujino (2010) to increase its accuracy. It is found that the ionic packing ratio is approximately constant and independent of the chemical composition. For different categories of glasses, including silicate, tellurite, and phosphate. The density has been meticulously calculated. These calculations rely on compositional parameters such as molecular weight, molecular fractions, and notably, the ionic radius of various metals. Density values are fundamental to the theoretical examination of radiation properties in the Phy-x/PSD software. Utilizing advanced tools and software allows for the prediction of glass physical parameters, which are indispensable in the fields of optical devices and electronic materials. This research establishes a connection between the composition of oxide glasses and their density. Consequently, it enhances our understanding of the properties and behaviour of these materials.

Keywords- Ionic radius, Phy-x/PSD software, Packing density, Radiation shielding, Makishima and Mackenzie model.

1. Introduction

Glasses have been utilized for several centuries and serve a wide range of aesthetic and technological purposes due to their characteristics such as transparency, refraction, brittleness, and reflection. This amorphous material primarily consists of silica, which is the most prevalent oxide compound in the Earth's crust, with silicon dioxide being the main glass-forming component in nearly all commercial glasses. Additionally, binary oxides like GeO_2 , P_2O_5 , and B_2O_3 are notable glass formers (Feltz, 2001; Kumari et al., 2012) used in the production of chemical glassware and photovoltaic devices. Innovative TeO_2 glasses have been developed for their nuclear radiation shielding properties (Lakshminarayana et al., 2017). Heavy metal oxide glasses have demonstrated excellent performance in gamma ray shielding (Al-Hadeethi and Sayyed, 2019) and the creation of optical materials with unique functionalities. Furthermore, Lithium Alumino-Borate glasses have been engineered to emit bright white light for LED applications, attracting significant interest from researchers worldwide. Glass nano-composites are also gaining attention due to their distinctive electrical and optical properties.

The physical characteristics of glasses play a crucial role in determining their functional attributes. Among these, density is particularly significant, as it can be utilized to derive thermal, optical, and elastic, refractive index, Young's modulus properties, all of which are influenced by the glass composition. Some researchers argue that the density of glass is additive, allowing for calculations based on its composition (Ahmmad et al., 2021a). The ability to calculate and predict density from glass composition is essential and has garnered global interest among researchers. Inaba and Fujino (2010) proposed an empirical relationship that theoretically links glass composition to its density. This model has been widely adopted by researchers to estimate the theoretical density of glasses based on their composition, achieving notable success in minimizing density error to less than $\pm 10\%$. Nevertheless, in scientific contexts, such an error can significantly impact the material's physical properties.

The methodology for determining both the density and the packing density parameter based on chemical compositions has been established. A primary objective of my research is to re-evaluate the theoretical models to enhance their efficiency. We have conducted systematic calculations of the density for a range of oxide glasses, including tellurite, borate, silicate, germanate, and phosphate, among others. In this research have displayed the density values of silicate, phosphate, tellurite glasses, calculated using the equation proposed by Inaba and Fujino (2010) and Makishima and Mackenzie (1973).

The packing density parameter can be determined using the methods developed by Makishima and Mackenzie (1973). By integrating the packing density parameter (V_i) values into the Inaba and Fujino (2010) density model, we can compute the overall density.

Furthermore, we can work towards estimating the elastic moduli and Poisson's ratio of glass using the parameters of packing density and dissociation energy. A model that incorporates the dissociation energy of bonds and the ionic radii of elements can be utilized to calculate the elastic moduli of glasses. This methodology was proposed by Makishima and Mackenzie (1973). Density is essential for determining molar volume, Young's modulus, Poisson's ratio, elastic moduli, and various other properties (Nagendra and Narsimhulu, 2018; Shi et al., 2020; Wu et al., 2020), also the determination of density value is of great importance in the calculation of radiation shielding properties, including the tenth value layer (TVL), electronic cross section (ECS), equivalent atomic number (Z_{eq}), fast neutron removal cross section (FNRCs), and effective conductivity (C_{eff}) as well as effective electron density (Agar et al., 2019; Al-Buriahi and Rammah, 2019; Ersundu et al., 2018; Issa et al., 2020; Stalin et al., 2020). These values are critical for advancing the development of radiation shielding materials. Accordingly, we are actively working on models that pertain to theoretical density.

2. Theoretical Procedure

It is well established that glasses can be classified into network formers, network modifiers, and other categories. This research focuses on several glass systems, including silicate, phosphate, and tellurite. Network formers such as SiO_2 , P_2O_5 , and TeO_2 are notable examples. The oxide variants of these compounds have been used in glass manufacturing. The density values for the different glass compositions analyzed in this study are shown in **Table 1**, **Table 2** and **Table 3**. By employing the density model and referencing the contributions of Inaba and Fujino (2010) we effectively calculated the packing density parameters and their related density values.

In this paper, we have revisited the model for the theoretical calculation of the density of glasses from their chemical compositions. The research incorporates the models of Makishima and Mackenzie (1973) alongside the empirical equation put forth by Inaba and Fujino (2010).

The packing density V_t is defined by

$$V_t = \frac{\rho}{M} \sum_i V_i X_i \quad (1)$$

M is the effective molecular weight, ρ is the density, X_i is the mole fraction of component i and V_i is the packing density parameter.

$$V_i = \frac{4}{3} \pi \cdot N_A \cdot (X \cdot r_M^3 + Y \cdot r_O^3) \quad (2)$$

This is the most important formula to determine packing density parameter, here we have used ionic radius of metals and oxygen atoms proposed by Shannon and Prewitt (1970) to calculate V_i .

The Equations numbered (1) and (2) have been referenced from the research conducted by Makishima and Mackenzie (1973). Many researchers have referred these equations (Adamu et al., 2022; Ahmmad et al., 2021a; Ahmmad et al., 2021b; Ahmed et al., 2022; Bishnoi et al., 2019; Effendy et al., 2020; Plucinski and Zwanziger, 2015; Wilkinson et al., 2019).

Table 1. Composition and density, ρ (10^3 kg/m^3) of various various glass compositions.

Compositions (Silicate)	This work (ρ)	Inaba and Fujino (2010) work (ρ)	Interglad (ρ)	Coordination number
20Li ₂ O–80SiO ₂	2.32	2.27	2.28	4
20Li ₂ O–80SiO ₂	2.14	-	2.28	6
30Li ₂ O–70SiO ₂	2.29	2.36	2.33	4
30Li ₂ O–70SiO ₂	2.08	-	-	6
30Na ₂ O–70SiO ₂	2.52	2.47	-	6
30BaO–70SiO ₂	2.81	3.58	-	6
40BaO–60SiO ₂	3.04	4.01	4.02	6
40CaO–60SiO ₂	2.56	2.77	-	6
20Li ₂ O–24Al ₂ O ₃ –56SiO ₂	2.19	2.44	-	6
20Li ₂ O–24Al ₂ O ₃ –56SiO ₂	2.38	2.44	-	4
30Li ₂ O–10Al ₂ O ₃ –60SiO ₂	2.10	2.40	-	6
30Na ₂ O–10Al ₂ O ₃ –60SiO ₂	2.54	2.47	-	4
30Na ₂ O–10Al ₂ O ₃ –60SiO ₂	2.40	2.47	-	6
30MgO–10Al ₂ O ₃ –60SiO ₂	2.58	2.61	-	4
30MgO–10Al ₂ O ₃ –60SiO ₂	2.41	2.61	-	6
20Li ₂ O–20MgO–60SiO ₂	2.21	2.52	-	4
20Li ₂ O–20MgO–60SiO ₂	2.41	2.61	-	6
20Li ₂ O–20CaO–60SiO ₂	2.25	2.60	-	6
20K ₂ O–20SrO–60SiO ₂	2.60	2.93	-	6
20Na ₂ O–20BaO–60SiO ₂	2.70	3.39	-	6
20Na ₂ O–20CaO–60SiO ₂	2.49	2.65	-	6
20K ₂ O–20CaO–60SiO ₂	2.45	2.60	-	6

The calculation of the packing density parameter is performed using Equation (2), which is fundamental for determining the density of glass systems. We utilized the density model to calculate the density of the glass system (Inaba and Fujino, 2010).

$$\text{i.e. } \rho = 0.53 \cdot \frac{\sum M_i X_i}{\sum V_i X_i} \quad (3)$$

Upon determining the density using Equation (3), we have recognized that a modification is essential for enhancing its accuracy. We have introduced a revised equation, designated as Equation (7), aimed at minimizing errors.

Table 2. Density values of phosphate glass compositions for coordination number 4 and 6.

Compositions (Phosphate)	This work (ρ)	Inaba and Fujino (2010) work (ρ)	Interglad (ρ)	Coordination number
50Li ₂ O–50P ₂ O ₅	2.16	2.46	-	4
50Li ₂ O–50P ₂ O ₅	1.92		-	6
50MgO–50P ₂ O ₅	2.59	2.47	2.46	4
50MgO–50P ₂ O ₅	2.40		-	6
50CaO–50P ₂ O ₅	2.55	2.70	2.68	6
50SrO–50P ₂ O ₅	3.00	3.22	3.20	6
50BaO–50P ₂ O ₅	3.19	3.64	-	6
30Li ₂ O–10Al ₂ O ₃ –60P ₂ O ₅	2.24	2.51	-	4

Table 3. Density values of tellurite glass compositions for coordination number 4 and 6.

Compositions (Tellurite)	This work (ρ)	Inaba and Fujino (2010) work (ρ)	Interglad (ρ)	Coordination number
20Li ₂ O–80TeO ₂	4.46	4.80	-	4
20Li ₂ O–80TeO ₂	3.99		-	6
20Na ₂ O–80TeO ₂	5.07	4.86	4.86	4
20Na ₂ O–80TeO ₂	4.77		4.86	6
20ZnO–80TeO ₂	6.23	5.76	5.53	4
20ZnO–80TeO ₂	5.82		5.53	6
10Al ₂ O ₃ –90TeO ₂	5.54	5.32	-	4
10Al ₂ O ₃ –90TeO ₂	5.21		-	6
20WO ₃ –80TeO ₂	6.25	6.17	-	4
20WO ₃ –80TeO ₂	5.89		-	6
10TiO ₂ –90TeO ₂	5.72	5.05	-	4
10TiO ₂ –90TeO ₂	5.38		-	6
10Nb ₂ O ₅ –90TeO ₂	5.98	5.50	-	4
10Nb ₂ O ₅ –90TeO ₂	5.63		-	6
20Fe ₂ O ₃ –80TeO ₂	5.69	5.22	-	4
20Fe ₂ O ₃ –80TeO ₂	5.34		-	6
10Sb ₂ O ₃ –90TeO ₂	6.35	5.90	-	4
10Sb ₂ O ₃ –90TeO ₂	5.99		-	6
20MoO ₃ –80TeO ₂	5.56	5.62	-	4
20MoO ₃ –80TeO ₂	5.24		-	6

3. Result and Discussion

We have used the ionic packing ratio V_p expression to compute the density (Inaba and Fujino, 2010).

$$V_p = \rho \cdot \frac{\sum(V_i \cdot X_i)}{\sum(M_i \cdot X_i)} \quad (4)$$

Here, M_i stands for molar weight (kg/mol), X_i signifies molar fraction (mol%), ρ represents density (kg/m³), V_i is the packing density parameter (m³/mol),

$$V_i = \frac{4}{3} \pi \cdot N_A \cdot (X \cdot r_M^3 + Y \cdot r_O^3).$$

Equation (2) represents the formula used to calculate the packing density parameter (V_i). In this context, X denotes the number of metal atoms, while Y indicates the number of oxygen atoms in the compound M_XO_Y . For instance, in the case of SiO₂, X is equal to 1 and Y is equal to 2 (M_XO_Y -- SiO₂ -- $X=1$, $Y=2$, similarly in Al₂O₃ $X=2$, $Y=3$). Here, N_A stands for Avogadro's number (mol⁻¹), with r_M and r_O indicating the ionic radii of the metal and oxygen, respectively. This investigation employed ionic radii (Shannon and Prewitt, 1970). We have included the ionic radii in **Table 5**.

Table 4. Compositional parameter and V_i for various glass compositions.

Parameter unit	Packing density parameter V_i 10^{-6} m/mol	Packing density parameter V_i 10^{-6} m/mol
Co-ordination number	4	6
NWF		
SiO ₂	13.3	14.0
B ₂ O ₃	19.9	20.9
GeO ₂	13.4	14.2
P ₂ O ₅	33.2	35.0
V ₂ O ₃	20.1	21.6
TeO ₂	13.2	14.3
V ₂ O ₅	33.4	35.4
As ₂ O ₅	33.3	35.1
Sb ₂ O ₃	22.1	23.0
Sb ₂ O ₅	35.4	36.8
IMO		
BeO	7.15	-
TiO ₂	13.4	14.4
ZnO	7.17	7.94
Al ₂ O ₃	20.2	21.5
ZrO ₂	13.8	14.8
CdO	7.8	9.08
Fe ₂ O ₃	20.5	22.1
Ga ₂ O ₃	20.4	22.0
PbO	9.01	11.2
ThO ₂	-	15.9
NWM		
Li ₂ O	7.67	9.14
MgO	7.10	7.87
CaO	-	9.45
Na ₂ O	11.5	12.3
CoO	7.12	7.96
CuO	7.17	8.07
MnO ₂	14.0	15.3
Sc ₂ O ₃	-	22.8
K ₂ O	19.6	20.2
SrO	-	11.1
SnO	7.05	7.75
Cu ₂ O	7.72	9.22
MoO ₃	20.1	21.3
SnO ₂	13.7	14.7
Cr ₂ O ₃	20.2	21.6
BaO	-	13.1
Rb ₂ O	-	24.6
Y ₂ O ₃	-	24.4
Ag ₂ O	12.0	14.6
WO ₃	20.1	21.3
PbO ₂	15.6	18.1
Nb ₂ O ₅	33.7	35.9
In ₂ O ₃	21.1	23.3
La ₂ O ₃	-	26.3
Pr ₂ O ₃	-	25.7
Nd ₂ O ₃	-	25.6
Sm ₂ O ₃	-	25.2
Eu ₂ O ₃	-	28.8
Gd ₂ O ₃	-	24.9
Dy ₂ O ₃	-	26.9
Er ₂ O ₃	-	24.3
Tm ₂ O ₃	-	26.3
Yb ₂ O ₃	-	26.1
Bi ₂ O ₃	24.6	26.3

Table 5. Radii values of various ions. Adopted from “revised effective ionic radii and systematic studies of interatomic distances in halides and Chalconides” By Shannon and Prewitt (1970).

Ion	Charge	Coordination number	Crystal radius (Å)	Ionic radius (Å)
Al	3	4	0.53	0.39
		6	0.675	0.535
B	3	4	0.25	0.11
		6	0.41	0.27
Ba	2	4	-	-
		6	1.49	1.35
Li	1	4	0.73	0.59
		6	0.9	0.76
Na	1	4	1.13	0.99
		6	1.16	1.02
Si	4	4	0.4	0.26
		6	0.54	0.4
O	-2	4	1.24	1.38
		6	1.26	1.4

The ionic radii database provides a variety of values that correspond to different coordination numbers of oxygen. Additionally, metals exhibit varying coordination numbers, such as 4 and 6. Consequently, the packing density parameter V_i has been computed for both 4 and 6 coordination numbers of oxygen, and similar calculations have been performed for metals with coordination numbers of 4 and 6, as presented in **Table 4**. To make the comparison of the density contributions from each oxide more straightforward, they are divided into three categories: network former oxides (NWF), intermediate oxides (IMO), and network modifier oxides (NWM).

The formula $V_i = \frac{4}{3} \pi \cdot N_A \cdot (X \cdot r_M^3 + Y \cdot r_O^3)$ yields highly accurate measurements for different coordination numbers, reflecting the variation in ionic radii of metals and oxygen based on the coordination number. For example, in SiO_2 with a coordination number of 4, the ionic radii for silicon and oxygen are 0.26 Å and 1.38 Å, while for a coordination number 6, the ionic radii are 0.4 Å and 1.4 Å, respectively. Therefore, Equation (2) is the most reliable empirical equation for determining V_i (Makishima and Mackenzie, 1973).

$$\rho = \frac{M \cdot V_t}{\sum V_i X_i} \quad (5)$$

Here, V_i is the packing density which is 0.53, It is assumed that the ionic packing density or ratio remains relatively constant, regardless of the chemical composition. this is the formula proposed by Makishima and McKenzie (1973). In a similar manner, we can express another formula from the Rocherulle et al. (1989) model as follows:

$$C_t = \sum \frac{\rho_i}{M_i} V_i X_i \quad (6)$$

The density calculations can be performed using the density models outlined in Equations (5) and (6), in this paper we have used Equation (3) to calculate density values. When calculating density values using this formula, one must consider potential errors in the measurement of glass composition. The primary source of this deviation is the assumption that the ionic packing ratio is a constant value of 0.53, which does not vary with changes in chemical composition.

The calculated densities of oxide glasses for coordination numbers 4 and 6 are presented in **Table 1**, **Table 2** and **Table 3**, while the packing density parameter (V_i) values are summarized in **Table 4**. The V_i values are free from error, however, there are discrepancies in the density values. Upon reviewing Equation (3),

we determined that modifications are necessary to reduce the errors, specifically by adding the values 0.35 and 0.75 to the equation we can reduce the errors.

Modified equation is

$$\rho = 0.53 \cdot \frac{\sum M_i X_i}{\sum V_i X_i} + 0.35 \text{ and } \rho = 0.53 \cdot \frac{\sum M_i X_i}{\sum V_i X_i} + 0.75 \quad (7)$$

$$V_m = \frac{\sum M_i X_i}{\rho_{glass}} \quad (8)$$

We have calculated density values using Equation (7) and the density values have been presented in the **Table 6**, One significant aspect to consider is that density values vary with changes in ionic radius as the coordination number changes. In **Table 6**, we have outlined the density values for coordination numbers 4 and 6, The experimental density values have been sourced from existing literature (Al-Hadeethi and Sayyed, 2019; Al-Hadeethi et al., 2020; El-Mallawany et al., 2018; Massera et al., 2010; Yasaka et al., 2019; Koudelka et al., 2017). Some elements do not possess coordination number 4. The density values for coordination number 6 are reported with greater precision than those for coordination number 4. Consequently, we can calculate density values corresponding to a coordination number of 6.

Following Equation (7), it is essential to add 0.35 for binary and tertiary glass systems, while for quaternary systems and beyond, an addition of 0.75 is required.

Equation (8) enables us to calculate the molar volume, thereby establishing density as a vital parameter.

$$\rho = 0.53 \cdot \frac{\sum M_i X_i}{\sum V_i X_i} + 0.35 \dots \dots \dots \text{for Binary and Tertiary.}$$

$$\rho = 0.53 \cdot \frac{\sum M_i X_i}{\sum V_i X_i} + 0.75 \dots \dots \dots \text{for Quaternary, Senary, e.t.c.}$$

Tellurite glass serves as a valuable material in various fields, including lasers, nonlinear applications, photonics, and communication systems. It is frequently chosen for its stability at ambient temperatures and its advantageous thermal, optical, and electrical characteristics (Shannon and Prewitt, 1970).

The histogram graphs illustrate the distribution of density in relation to frequency expressed as a percentage. **Figures 1** and **2** depict the frequency of specific density values within a dataset, facilitating the identification of density distribution patterns. The histogram in **Figure 1** displays the density of silicate glass compositions. Density values range from 2.3 to 2.45, varying with the chemical composition, and the average density shows an increase consistent with the information in **Table 1**, **Table 2** and **Table 3**. The results indicate that the density is largely influenced by the molecular weight of the oxide that forms the network (Kumari et al., 2012).

Table 6. Density (g/cm³) Values of various glasses estimated using modified equation.

Glass matrix	Coordination number	Experimental density value (g/cm ³)	Theoretical density (g/cm ³) Calculated using Equation (7)
70TeO ₂ -10Bi ₂ O ₃ -20ZnO	6	6.16	6.38
10PbO-30WO ₃ -60TeO ₂	4	6.43	6.92
	6		6.49
40BaO-20MoO ₃ -40P ₂ O ₅	6	3.76	3.60
20Bi ₂ O ₃ -25B ₂ O ₃ -45TeO ₂ -10TiO ₂	6	4.67	4.42
30PbO-10ZnO-50TeO ₂ -10B ₂ O ₃	4	6.22	6.92
	6		6.07
46B ₂ O ₃ +20TeO ₂ + 19CaO+10Li ₂ O + 5ZrO ₂	6	3.11	3.11
10ZnO-30BaO-30B ₂ O ₃ -(28.5) TeO ₂ -1.5Sm ₂ O ₃	6	3.95	4.24

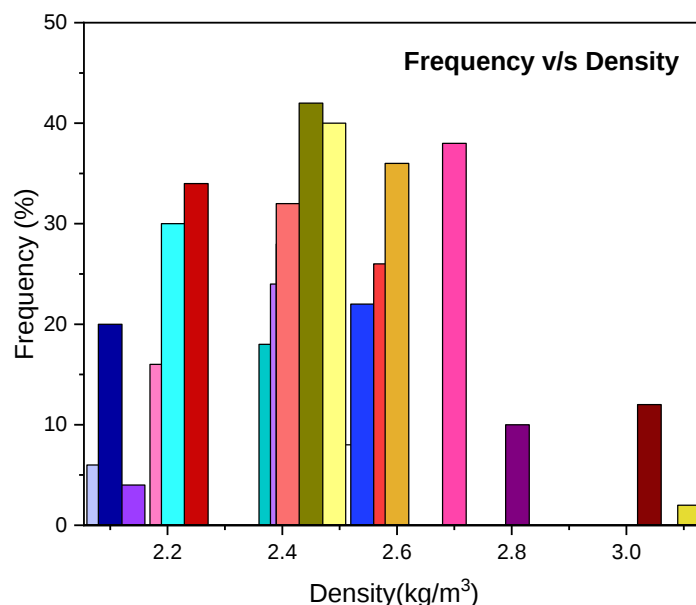


Figure 1. Histogram of silicate glass compositions.

Similarly in **Figure 2** the density of tellurite glass compositions has shown, values range from 4.46 to 5.24, Influenced by the specific chemical compositions. The graphs further showcase the ranges characterized by increased frequencies, potentially reflecting preferred or typical density levels found within the dataset.

In **Figure 3**, the variations of the mean free path (MFP), mass attenuation coefficient (MAC), and half value layer (HVL) are presented, with calculations performed within the energy range of 1.50×10^{-2} to 1.50×10^1 . We have deliberately included **Figure 3** to illustrate that by utilizing density values and the glass matrix, we can calculate various parameters such as Mean Free Path (MFP), Mass Attenuation Coefficient (MAC), and Half Value Layer (HVL), among others. This allows for a comparison between theoretical and experimental studies.

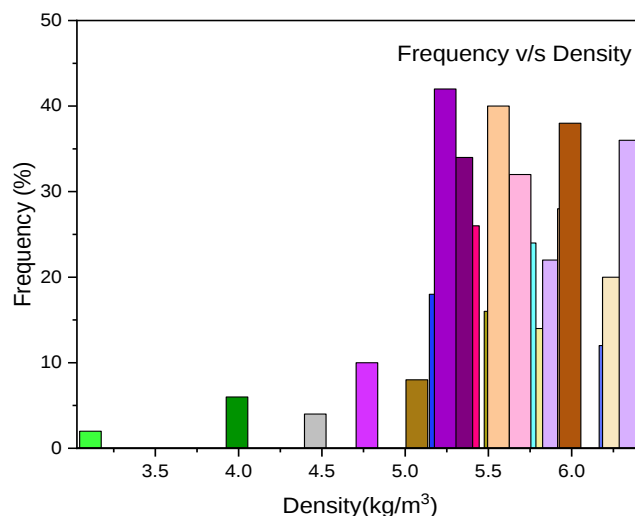


Figure 2. Histogram of tellurite glass compositions.

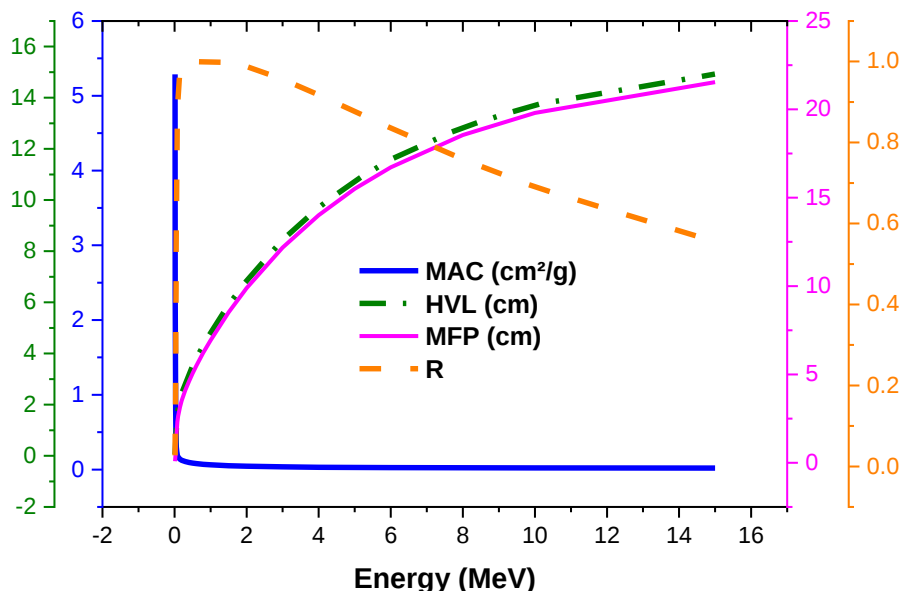


Figure 3. Radiation shielding properties.

Variations in chemical composition lead to notable differences in density, which tends to increase in the order of tellurite > germanate > phosphate > silicate > borate glass systems. The density values associated with silicate, phosphate, and tellurite glass systems are of particular interest. Density and packing density are influenced by several factors, including molecular weight, molar fraction, ionic radii, and the number of metal and oxygen atoms. The theoretical models that stand out include the Bond compression model, the Makishima and Mackenzie model, and the Rocherulle model. The Makishima and Mackenzie model (Makishima and McKenzie, 1973), in addition to the Rocherulle model (Rocherulle et al., 1989), has provided empirical formulas for density calculations. However, we did not employ the Rocherulle model in our computations; instead, we relied on the Makishima and McKenzie (1973) model and the formulas formulated by Inaba and Fujino (2010).

A significant observation from this research indicates that different coordination numbers yield unique density values. The density values, calculated using the newly established formula, reflecting a considerable increase in accuracy. It is important to note that the density values for coordination number 6 are exceptionally precise, and given that all ions have a coordination number of 6, we can determine the density values by employing the ionic radius relevant to this coordination number. The modified formula has a low error rate, effectively lowering the error by approximately $\pm 4\%$. Through an extensive evaluation of the existing formulas and related calculations, we recognized that the formula required adjustments for improved accuracy. The changes we made to the formula demonstrate a consistent linear correlation between the measured density and the calculated values for all oxide glasses examined in this study. With our newly refined formula, we are able to accurately compute the density values for binary, tertiary, quaternary, and other glass systems. Utilizing the density values, we can compute the molar volume based on established relationships. Moreover, these values can be used to evaluate radiation-shielding properties, including mean free path (MFP), mass attenuation coefficient (MAC), and half-value layer (HVL), through the Phy-x/PSD software, enabling us to compare theoretical predictions with experimental data (Agar et al., 2019; Al-Buriahi and Rammah, 2019; Ersundu et al., 2018; Issa et al., 2020; Stalin et al., 2020; Sayyed et al., 2018).

4. Conclusion

Thus, this work is summarised as follows:

- The density values, calculated using the newly established formula, reflecting a considerable increase in accuracy.
- The modified formula is able to lower the error by approximately $\pm 4\%$.
- The changes to the formula demonstrate a consistent linear correlation between the measured density and the calculated values for all oxide glasses examined in this study.

Conflict of Interest

There is no conflict of interest.

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