ORIGINAL RESEARCH PAPER

Volume - 10 | Issue - 08 | August - 2021 | PRINT ISSN No. 2277 - 8179 | DOI : 10.36106/ijsr

INTERNATIONAL JOURNAL OF SCIENTIFIC RESEARCH

CALCULATION AND ANALYSIS OF EFFECTIVE ATOMIC NUMBER USING AUTO Z-EFFECTIVE METHOD FOR BORO-SILICATE GLASS SERIES GLASS [$Li_2O – B_2O_3 – SiO_2$ – XO] WITH THIRD (5D) D-BLOCK (HF–HG) TRANSITION METALS ELEMENTS (X)

Physics

Dr Sangeet Markanda

Department of Physics, University College, Chunni Kalan, F.G.S., Punjab, India.

ABSTRACT

The impact of the doping of the transition metals with Lithium Oxide provides significant data in Boro-silicate materials. Hence their comprehensive study with Lithium in Boro-silicate glass studied in the present paper. Z-effective shows non consistence in study respective to energy and even more anomalous with respective to the atomic number at lowest energy levels (0.01 MeV). Variations in Z-effective are high with increase in energy among all 5d metals used in given series of glass. For 1 to 100 MeV a small variation observed in data as it ranges 9 to 21 (Z-effective). Even variation is symmetrical within the 5d transition metals except for Hf (72) and Ta (73)

KEYWORDS

Z-effective, Boro-Silicate Glasses, Transition metals

INTRODUCTION:

Z-Effective is studying the exposure of radiation on different materials. It is the influence of the electron cloud of the radiation from the material. In glasses it provides the field of use of specific glass composition. For example, a Boro-silicate glass having one of the important applications is a simulation of the human skin and tissues by borosilicate glasses having same Z-Effective as that of human skin and tissues. Also, their relative low costs make them even more significant[1][2][3].

The interest for bulk metallic glasses (MGs) has been steadily increasing during recent years, triggered in part by their unique mechanical properties, in many cases superior to their crystalline counterparts. Named MGs can be twice as strong as steels, exhibit more elasticity and fracture toughness as compared ceramics and be less brittle than conventional oxide glasses[4].

In Glasses structure we analyse the interaction of the X-rays and γ- rays with given series[5][6]. The amount of radiation absorbed by the given glass is influenced by the Z - effect of the glass[7][8]. Z-Effective is the electron cloud interaction with radiation. It is the effective atomic number per unit mass and provide the packing of the atoms in compound [9] [10]. To calculate Z-effective various methods various methods used widely. These methods basically characterized into three main categories.

Transition metals are defined as the elements which have incompletely filled *d* orbitals in its ground state at any one of its oxidation states. For example, in this paper, we chose (I) oxidation state.

Calculation Methods

The compound has been used for evaluation of Z-effective

Compound $Li_2O – B_2O_3 – SiO_2 – XO$

Mole fraction (0.1) (0.5) (0.3) (0.1)

Initially we must find out the following basic parameters **A, Z, W, Ni, f_i & M** are *Atomic Weight, Atomic Number, Weight Percentage, Formula Units, Fraction, Molecular Weight* of individual atoms respectively. *Fraction* calculated by dividing the formula unit of the individual atom by the sum of formula units of all atoms[11].

At last *Molecular Weight* evaluated by multiple formula unit off with respective atomic weight e.g. Mn (Z = 25) = n× A [12]. Similarly, for other atoms the above parameters calculated and drawn the table1.

Table No. 1: Calculation Of Formula Units And Fraction

Elements	A	W	Z	$\sum n_i$	f_i	M
B	10.81	0.16	5	1	0.256	10.8
O	15.99	0.58	8	2.3	0.6	36.8
Li	6.941	0.046	3	0.2	0.051	1.4
Si	28.1	0.14	14	0.3	0.077	8.43
Mn	54.94	0.077	25	0.1	0.026	5.5
Total		1		3.9		62.92

Next step is to evaluate the given values for individual atoms for different energy levels. **µm** Total attenuation with coherent scattering, to evaluate **µm** NIST XCOM database had been used on given **NIST**[13] [14]. Then **f (A) m** & **∑f (A/Z) m** is the total weighing factor & weighing factor per atoms in compound respectively calculated using following formulae[15][16][17].

$$\mathbf{f(A)m = W \times f_i \times \mu m} \qquad (1)$$

$$\mathbf{f(A/Z)m} = \frac{\text{f(A)m}}{\text{Atomic No.(Z)}} \qquad (2)$$

Table No. 2: Calculations Of f (A) m & ∑f (A/Z) m For Boron (Z=5)

	B		
Energy	**µm**	**fAm**	**F (A/Z) m**
1.17	1.26	3.48	0.70

Similarly, above these values calculated for rest of atoms.

Last step we must calculate values of **µg, σt, σa, Zeff**. Where **µg** is Glass mass Attenuation Coefficient, **σt** is Total cross section and **σa** is a cross section per atom[1][2][3].

$$\mathbf{\mu g} = \sum_{\text{allatoms}}[W \times \mu m] \qquad (3)$$

$$\mathbf{\sigma t} = \sum_{\text{allatoms}}[M \times \mu g] \qquad (4)$$

$$\mathbf{\sigma a} = \frac{\sigma t}{\sum ni} \qquad (5)$$

$$\text{Z-effective} = \frac{\sigma a}{\sum f(A/Z)m} \qquad (6)$$

Table No. 3: Table Of Calculation Of Z-effective

Energy (MeV)	∑f (A/Z) m	µg	σt	σa	Z-Eff
0.01	21.5	20.1	1267.4	325	15.1
0.1	0.323	0.17	10.66	2.73	8.47
1	0.127	0.0619	3.89	0.999	7.85
10	0.0412	0.0207	1.31	0.34	8.13
100	0.0353	0.0197	1.24	0.327	8.99

Data Analysis

The graph plotted Z-effective verses energy in MeV (fig 1.1). Where trends show 5d transition metals show higher values of Z-effective at exceptionally low energy 0.01 to 0.1 MeV. Variation of Z-effective with energy on exponential scale of energy show same pattern for all the 5d transition metals in given glass composition except Hf (72) and Ta (73). Anomalies in Hf are observed at extremely low energy values in comparison to the rest of 5d transition metals. However, Ta indicates anomalous variation then the rest family metals except around 1 MeV energy values. Its Z-Effective value varies around These values suddenly dropped to 9 values for 0.1 MeV. Among all the metals used in series Ta (z=73) shows larger variation with minimum dip in Z-effective at 1 MeV.

Whole series undergoes the sharp dip in Z-effective with Ta(z=73) having the minimum value of Z-effective 9.411974 at 1 MeV. For energy varies from 1 MeV to 100 MeV slightly increase observed for giving glass series with all 5d transition metals. The study within the group of 5d transition metals Z-effective absolute consistent observed except the Hf (72) and Ta (73). Values of Z-effective began with small increase and then sudden dip at 1 MeV rest going on increasing with small change with respective energy values. Except first two elements in series rest elements show no significant changes with respective atomic numbers. Since z-effective for Ta (73) floating around 10, shows more significance in applications for shielding glass over a wide range of Energy values. With Increase in energy (0.01MeV- 100MeV) Z-effective remains inconsistently for all the First (5*d*) d-block Series (Hf–Hg) transition metals in given series of Boro-Silicate Glass.

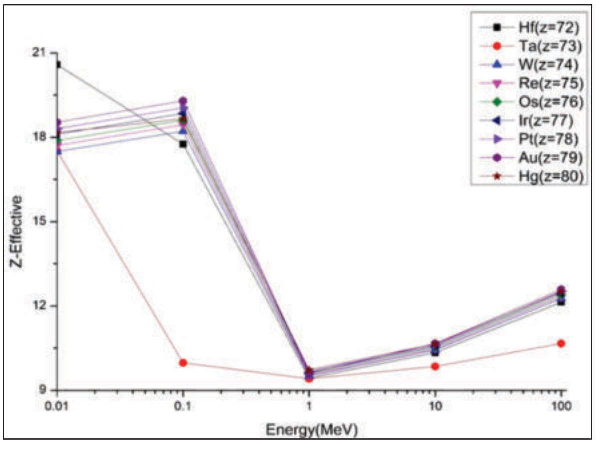

Fig1.1. Graph plotted Z-effective verses energy in MeV

CONCLUSIONS

Variations in Z-effective are high with increase in energy among all 5d metals used in given series of glass. From 1 to 100 MeV a small variation observed in data as it ranges 9 to 21 (Z-effective). All over variation is symmetrical within the 5d transition metals except for Hf(72) and Ta (73) given boro-silicate glass series. Analysis indicates possible shielding properties of Ta(73) over wide range of incident energy with boro-silicate glasses. Calculated Data applications are for experimental references and for preparation of protecting glass from radiation. These values reflect the influence of the 5d transition metals in boro-silicate glass series with alkaline earth metals but with their individual minor variations in it.

REFERENCES:

1. Markanda. S. An analytic review of the different methods for evaluating the Z-effective of the series of glass [Li2O – B2O3 – SiO2 – MnO]" International Journal of Advance Research in Science and Engineering in Volume 06, Issue 11 and November (2017) : 2019-2023 (P)
2. Markanda. S, Krishan. B. "An analytic analysis of Z-effective for the series of glass [Li2O – B2O3 – SiO2 – XO] with First (3d) d-block (Sc–Zn) transition metals Elements(X)" published in International Journal of Latest Trends in Engineering and Technology in December (2017). Vol.9 ,Issue-3,
3. Markanda. S, Krishan. B . "An analytic analysis of Z-effective for the series of glass [Li2O – B2O3 – SiO2-XO] with Second (4d) d-block (Y–Cd) transition metals Elements(X)" published in International Journal of Latest Trends in Engineering and Technology in December (2017). Vol.9 ,Issue-3,
4. Fornell, J., Et al. "Yielding and intrinsic plasticity of Ti–Zr–Ni–Cu–Be bulk metallic glass." *International Journal of Plasticity*25.8 (2009): 1540-1559(P).
5. A. M. Ali, A. M. El-Khayatt & I. Akkurt (2016): Determination of effective atomic number and electron density of heavy metal oxide glasses, Radiation Effects andDefects in Solids, 1042-0150 (Print)
6. Singh, H., Singh, K., Gerward, L., Singh, K., Sahota, H. S., & Nathuram, R. (2003). ZnO–PbO–B 2 O 3 glasses as gamma-ray shielding materials. *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, *207*(3), 257-262.
7. Manohara, S. R., Hanagodimath, S. M., Thind, K. S., & Gerward, L. (2008). On the effective atomic number and electron density: a comprehensive set of formulas for all types of materials and energies above 1keV. *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, *266*(18), 3906-3912.
8. Singh, K., Singh, H., Sharma, V., Nathuram, R., Khanna, A., Kumar & Sahota, H. S. (2002). Gamma-ray attenuation coefficients in bismuth borate glasses. *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, *194*(1), 1-6.
9. Sheng, H. W., Luo, W. K., Alamgir, F. M., Bai, J. M., & Ma, E. (2006). Atomic packing and short-to-medium-range order in metallic glasses. *Nature*, *439*(7075), 419-425.
10. Kaewkhao, J., & Limsuwan, P. (2010). Mass attenuation coefficients and effective atomic numbers in phosphate glass containing Bi 2 O 3, PbO and BaO at 662keV. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, *619*(1), 295-297.
11. Singh, K., Singh, H., Sharma, G., Gerward, L., Khanna, A., Kumar, R., ... & Sahota, H. S. (2005). Gamma-ray shielding properties of CaO–SrO–B2O3 glasses. *Radiation Physics and Chemistry*, *72*(2), 225-228.
12. Singh, S., Kumar, A., Singh, D., Thind, K. S., & Mudahar, G. S. (2008). Barium–borate–flyash glasses: as radiation shielding materials. *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, *266*(1), 140-146.
13. M. J. Berger and J. H. Hubbell, *XCOM: Photon Cross Sections Database*, NBSIR, 1987
14. Singh, V. P., Badiger, N. M., & Kucuk, N. (2014). Determination of effective atomic numbers using different methods for some low-Z materials. *Journal of Nuclear Chemistry*, *2014*.
15. Hossain I., Shekaili N. K. & Wagiran H. (2013). Dopant Concentration and Effective Atomic Number of Copper-Doped Potassium Borate Glasses. *Hindawi Publishing Corporation Advances in Materials Science and Engineering*, Article ID 278934, 1-4
16. M. L. Taylor (2012), Robust calculation of effective atomic numbers: The Auto-Zeff software, Medical Physics 39, 1769-1778
17. M. L. Taylor (2011), Robust determination of effective atomic numbers for electron interactions with TLD-100 and TLD-100H thermoluminescent detectors, Nuclear Instruments and Methods B, 269 770-773.