ARTICLE IN PRESS

Journal of Non-Crystalline Solids xxx (xxxx) xxx–xxx

Contents lists available at ScienceDirect

Journal of Non-Crystalline Solids

journal homepage: www.elsevier.com/locate/jnoncrysol

Effect of PbO on the shielding behavior of ZnO–P2O5 glass system using Monte Carlo simulation

Ashok Kumar[a], M.I. Sayyed[b], Mengge Dong[c,*], Xiangxin Xue[c,*]

[a] Department of Physics, University College, Benra-Dhuri, Punjab, India
[b] Physics Department, University of Tabuk, Tabuk, Saudi Arabia
[c] Department of Resource and Environment, School of Metallurgy, Northeastern University, Shenyang 110819, China

ARTICLE INFO

Keywords:
Shielding
MCNP5
glass
radiation

ABSTRACT

In this work, MCNP5 as a Monte Carlo code is used to calculate gamma ray attenuation coefficient of x PbO-(50 − x) ZnO- 50 P_2O_5 glasses where x = 10, 20, 30, 40 and 50 mol% at 0.122, 0.356, 0.511, 0.662, 0.84, 1.17, 1.275 and 1.33 MeV photon energies. The simulated results of mass attenuation coefficients were compared with the output of XCOM program. Good agreement was observed between simulated and XCOM results. The obtained mass attenuation coefficients were further used to calculate the effective atomic number, electron density, half value layer and mean free path. The maximum values of mass attenuation coefficients and effective atomic number were found for PZPb50 glass sample. The results from this study indicate that the MCNP5 code used in this work may be utilized as a better alternative to experimental work to make supplementary calculations on the photon attenuation characteristics of other materials and glass systems. The lower values of the mean free path of the selected samples as compared to the standard shielding concretes; establishes them as suitable gamma shields. PZPB50 is the best among the selected shielding glasses.

1. Introduction

In the field of radiation physics, the knowledge of shielding parameters such as mass attenuation coefficient (μ_m), electron density(N_e), effective atomic number (Z_{eff}), half value layer(HVL), mean free path (MFP) etc. is very important [1–3]. Radiation exposure is controlled by using shielding materials for gamma rays and neutron [4]. Due to low cost and ability to mould to any construction design, concrete and building material is widely used as radiation shielding material [5,6]. But concrete suffer from many limitations such as addition of moisture content, opaque to visible light, loss of water and crack formation [7]. Due to these limitations, there is need of better shielding material. The best alternative is to use glasses for radiation shielding than concrete [5,8]. Several workers have been studied the borate, borosilicate and phosphate glasses doped with oxides of heavy metals used for shielding applications [9–17].

Lead glasses have many extraordinary properties like excellent infrared transmission, large density, high non linear optical susceptibility and high refractive index [5]. These glasses are extensively used for various applications such as optical or electronic applications, radiation protection, sealing applications and in immobilization of radioactive wastes [18]. PbO is not a network forming oxide by itself but it can be replaced by other network forming oxides such as SiO_2, P_2O_5 and B_2O_3 [19]. Phosphate glasses have various interesting properties like higher absorption coefficient, low glass transition temperature, high thermal expansion coefficient and low optical dispersion [10].

MCNP5 is a Monte Carlo code used for the simulation of different physical interactions [20,21]. In general, before utilizing in practical onsite radiation protection applications, materials are first tested for their radiation shielding effectiveness using Monte Carlo simulations. Therefore in the present study, the effect of PbO on the shielding behavior of ZnO–P_2O_5 glass systems has been studied by calculating the mass attenuation coefficients using MCNP5 simulation code for the xPbO-(50 − x) ZnO-50 P_2O_5 glasses where x = 10, 20, 30, 40 and 50 mol% [22]. The obtained results are compared with the values obtained using XCOM [23]. XCOM is software that can generate mass attenuation coefficients for the different materials in the energy range 1 keV–100 GeV for various interaction processes like coherent and incoherent scattering, photoelectric absorption and pair production. The other shielding properties like Z_{eff}, N_e, MFP, HVL are also obtained. The effect of addition of PbO and the photon energy has also been studied on these parameters. The gamma ray shielding effectiveness of the selected glasses has also been compared among themselves and with the shielding properties of the standard concretes [24] in terms of HVL and

* Corresponding authors.
E-mail addresses: mg_dong@163.com, 1610514@stu.neu.edu.cn (M. Dong), xuexx@mail.neu.edu.cn (X. Xue).

https://doi.org/10.1016/j.jnoncrysol.2017.12.001
Received 29 October 2017; Received in revised form 1 December 2017; Accepted 2 December 2017

Table 1
The chemical composition and the densities of the x PbO-(50 − x) ZnO-50 P_2O_5 glasses.

Glass sample	PbO	ZnO	P2O5	Density
PZPb0	0	50	50	3.177
PZPb10	10	40	50	3.493
PZPb20	20	30	50	4.121
PZPb30	30	20	50	4.419
PZPb40	40	10	50	4.802
PZPb50	50	0	50	4.845

MFP to establish that the selected glasses have better gamma ray shielding efficiency.

2. Materials and method

The chemical composition and the densities of the x PbO-(50 − x) ZnO-50 P_2O_5glasses has been taken from the sideket. al [22]. and are shown in Table 1. The method of calculation of the different shielding parameters is described in the following sections:

2.1. MCNP5 simulation process

Monte Carlo simulation code, MCNP5 was applied for calculation of μ_m of investigated glass system. MCNP5 is a Monte Carlo code for simulation of different physical interactions in wide energy range. MCNP5 is fully three-dimensional and it uses extended nuclear cross section libraries and uses physics models for particle types [25]. Similar to the methodology in the present investigation, different MCNP5 studies for various radiation applications were found in the literature [25–27]. In this work, each simulation parameters such as cell specifications, surface specifications, material specifications and position determinations of each simulation tools were defined in input file.-Gamma ray sources with different energies were defined as a point isotropic source. The source has been defined in the mode card of MCNP5 input file as a point source at 0.122, 0.356, 0.511, 0.662, 0.84, 1.17, 1.275 and 1.33 MeV photon energies. To examine the μ_m, geometry and material composition of glass sample was defined in input file. Glass sample was located as an attenuator sample between source and detection area. The F4 tally was used to obtain the MCNP simulated data representing average flux in a detector volume for gamma rays emitted from the source. 10^8 particles were tracked as the number of particle [25]. MCNP5 calculations were done by using Intel® Core ™ i7-6700 CPU @3.40 GHzcomputer hardware.

2.2. XCOM software process

XCOM is a software or dataset based on the mixture rule. It can generate attenuation coefficients for different elements in the energy range 1 keV–100 GeV for various interaction processes like coherent and incoherent scattering, photoelectric absorption and pair production.

Generally the mass attenuation coefficients of the glass sample are described by the mixture rule [23]:

$$\mu_m = \sum_{i=1}^{n} w_i \mu_m \tag{1}$$

where w_i and μ_m are the proportion by weight and the mass attenuation coefficient of the ith element respectively present in the glass.

The Z_{eff} (Effective atomic number) of the present glasses were evaluated by the ratio of the effective atomic cross section (σ_a) and electronic cross section (σ_e) of the glasses [28]. For the details knowledge on calculation procedures of σ_a, σ_e and N_e (Electron density) have been found in different literatures [29].

The average distance that a photon moves between collisions is called the MFP. Besides, the thickness of the material where 50% of the intensity of incident photon has been attenuated is called the half value layer (HVL). MFP and HVL can be defined as [30–32]:

$$\mathrm{MFP} = \frac{1}{\mu} \tag{2}$$

$$\mathrm{HVL} = \frac{0.693}{\mu} \tag{3}$$

where μ is the linear attenuation coefficient.

3. Results and discussion

The mass attenuation coefficients of the selected glass samples were calculated using the MCNP 5 computer code (μ_{MCNP5}) and the XCOM software (μ_{XCOM}) at the selected energies of 0.122, 0.356, 0.511, 0.662, 0.84, 1.17, 1.275 and 1.33 MeV respectively along with their % deviations and are presenting in Table 2. The percentage deviations have been calculated using the following relations:

$$\%\mathrm{dev} = \frac{\mu_{XCOM} - \mu_{MCNP5}}{\mu_{XCOM}} \times 100 \tag{4}$$

All the μ_{MCNP5} values are slightly smaller than the μ_{XCOM} values and the smaller values of the % deviations in the values mass attenuation using both the methods establish the validity of present MCNP5 computer code. The variation of the mass attenuation coefficients with photon energies has been shown in Fig. 1 for both kinds of values simultaneously. The μ_{MCNP5} values are represented by dots whereas μ_{XCOM5} values are represented by the line. It is clear from the Fig. 1 that the both the values are in good agreement with each other. It justifies the validity the of present MCNP5 computer code for the calculation of the mass attenuation coefficients for a given sample. The mass attenuation coefficient decreases gradually with photon energy, it is due to the fact that the selected energy region is a Compton scattering dominant region and as the interaction cross section for the Compton

Table 2
Mass attenuation coefficients of the x PbO-(50 − x) ZnO-50 P_2O_5 glasses.

Energy (MeV)	Mass attenuation coefficients (cm^2/g)																	
	PZPb0			PZPb10			PZPb20			PZPb30			PZPb40			PZPb50		
	XCOM	MCNP5	% dev	XCOM	MCNP5	% dev	XCOM	MCNP5	% dev	XCOM	MCNP5	% dev	XCOM	MCNP5	% dev	XCOM	MCNP5	% dev
0.122	0.2045	0.2038	0.36	0.7184	0.7177	0.1	1.128	1.128	0.03	1.463	1.463	0.08	1.741	1.741	0.06	1.976	1.976	0.07
0.356	0.1002	0.0997	0.53	0.1309	0.13	0.68	0.1554	0.1554	0.85	0.1754	0.1754	0.99	0.192	0.192	1.02	0.206	0.206	0.99
0.511	0.085	0.085	0.02	0.0968	0.0965	0.35	0.1062	0.1062	0.6	0.1139	0.1139	0.76	0.1203	0.1203	0.98	0.1257	0.1257	1.07
0.662	0.0755	0.0752	0.43	0.0813	0.0807	0.75	0.086	0.086	0.89	0.0897	0.0897	1.07	0.0929	0.0929	1.18	0.0956	0.0956	1.27
0.84	0.0675	0.0672	0.43	0.0703	0.0698	0.71	0.0727	0.0727	0.91	0.0745	0.0745	1.05	0.0761	0.0761	1.14	0.0774	0.0774	1.26
1.17	0.0572	0.0569	0.62	0.0581	0.0574	1.14	0.0588	0.0588	1.57	0.0594	0.0594	1.9	0.0599	0.0599	2.19	0.0603	0.0603	2.42
1.275	0.0548	0.0545	0.54	0.0554	0.0548	1.01	0.0559	0.0559	1.37	0.0563	0.0563	1.68	0.0567	0.0567	1.93	0.057	0.057	2.14
1.33	0.0536	0.0533	0.56	0.0542	0.0536	1.01	0.0546	0.0546	1.35	0.0549	0.0549	1.62	0.0552	0.0552	1.87	0.0555	0.0555	2.07