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Calculation of effective atomic numbers and electron densities of different types of material for total photon interaction in the continuous energy region via different methods

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ABSTRACT

Effective atomic number (Z_{eff}) and electron density (N_{eff}) are convenient parameters used to characterise the radiation response of a multi-element material in the technical and industrial applications, radiation shielding design, absorbed dose and build-up factor calculations. Thus, it is very significant to choose accurate method to determine these parameters unambiguously. In the present study, effective atomic numbers and electron densities of different types of materials have been calculated by using a direct method and an interpolation method for total photon interaction in the energy region of 1 keV to 100 GeV. In addition, agreements and disagreements of the used methods have been discussed, and from the results, significant variations have been observed between the methods used to compute for the materials in the different energy regions.

Anahtar Kelimeler: Shielding material, effective atomic number, radiation interaction

Farklı metotlar ile sürekli enerji aralığında toplam foton etkileşimi için farklı tipteki malzemelerin etkin atom numarası ve elektron yoğunluklarının hesaplanması

ÖZ

Etkin atom numarası (Z_{eff}) ve elektron yoğunluğu (N_{eff}) teknik ve endüstriyel uygulamalarda, radyasyon zırhlama tasarımında, soğurma dozu ve foton çoğalma faktörü hesaplamalarında çoklu elementli bir malzemenin radyasyona tepkisini karakterize etmek için kullanılan uygun parametrelerdir. Dolayısıyla, bu parametreleri tartışmasız bir şekilde belirlemek için doğru metodu seçmek çok önemlidir. Bu çalışmada, farklı tipteki malzemelerin etkin atom numarası ve elektron yoğunlukları 1 keV - 100 GeV enerji aralığında toplam foton etkileşimi için doğrudan ve interpolasyon metotları kullanılarak hesaplanmıştır. Ayrıca, metotların uyumluluğu ve uyumsuzlukları tartışılmış ve sonuçlardan, farklı enerji bölgelerinde malzemeler için hesaplamak için kullanılan metotlar arasında önemli farklılıklar gözlenmiştir.
Keywords: Zırhlayıcı malzeme, etkin atom numarası, radyasyon etkileşimi

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1. INTRODUCTION

Radiation interaction with matter has become an important subject with the extensive use of X and/or gamma rays in various fields such as reactors, nuclear power plants, nuclear engineering and space technology, nuclear diagnostics, nuclear medicine, radiation dosimetry and radiation biophysics, technological and engineering applications. Because of the increasing usage of the radiations, it should be noted the risks on human health. Therefore, the use of shielding is very important in the fields. To choose an appropriate type of material, it should be determined radiation matter interaction parameters such as mass attenuation coefficient, effective atomic number and electron density.

Effective atomic number (Z_{eff}) is introduced firstly by Hine [1]. Then, it has been developed by different researchers. There are different available methods used to compute Z_{eff} for different type of materials such as direct method [2-4], interpolation method [5, 6], ratio cross-section method [7-16] and empirical method [1]. As a result, literature is rich of experimental as well as theoretical studies regarding effective atomic number and electron density, but there are a few studies dealing with the comparison of the methods used to compute Z_{eff} and N_{eff} in different materials [4,17]. Especially recently, Elmahroug et al. determined radiation matter interaction parameters of some shielding materials for total photon interaction [15]. Mann et al. studied shielding behaviors of some polymer and plastic materials for gamma-rays [21]. Tapan et al. investigated pumice materials in physical and chemical properties for shielding [22]. This prompted us to focus on this study.

Our aim is to compare the direct method and interpolation method commonly used to compute Z_{eff} and N_{eff} in shielding, polymer, plastic and pumice materials used in cement, concrete, brick, and ceramic industries as an additive and aggregate material. The processes were used both new materials (Sample 5-12) and well known materials such as mylar film, PVS for total photon interaction in the wide energy range from 1 keV to 100 GeV. The chemical compositions of the selected materials have been given in Table 1 [15,21] and Table 2 [22].

Table 1. Chemical composition (%) of the shielding materials, Sample 1-4 [21] and Sample 5-12 [15].

Sample	Symbol	Elemental composition (% by weight)
Polyvinyl chloride (PVC)	S1	H(4.84),C(38.44),Cl(56.73)
Air-equivalent plastic (C-552)	S2	H(2.47),C(50.17),O(0.46),F(46.53),Si(0.40)
Radio chromic dye film (nylon base)	S3	H(10.20),C(65.44),N(9.89),O(14.47)
Polyethylene terephthalate (mylar)	S4	H(4.20),C(62.51),O(33.31)
Flexi- Boron	S5	H(2.76),B(25.3),C(20.1),O(24.2),Si(26.9), Fe(0.41),Zn(0.26)
7.5% Lithium Polyethylene	S6	H(7.84),Li(7.5),C(57.76),O(26.13)
8.97% Borated Polyethylene	S7	H(6.68),B(8.97),C(27.2),N(5.28),O(51.9)
Self Extinguishing Borated Polythylene	S8	H(5.84),B(1),C(18.02),O(47.83),Na(0.19), Mg(0.14),Al(24.94),Si(0.26),S(0.02),Ca(1.53), Fe(0.02),Sr(0.1)
5.45% Borated Polyethylene	S9	H(5.72),B(5.45),C(25.96),O(39.69),Na(0.23),Mg(0.76), Al(11.92),Si(1.37),S(0.13),Ca(8.37),Fe(0.09),Sr(0.53)
High Temperature Boron Silicone	S10	H(4.74),B(1.08),C(11.01),O(46.56),Na(0.12),Al(18.75), Si(17.54),Fe(0.02),Zn(0.19)
Polykast Dry Mix	S11	H(10.3),B(0.9),C(46),O(32.5),Mg(0.04),Al(0.03),Si(0.43), S(3.99),Ca(5.72),Fe(0.05)
Field castable Heat Resistant shielding	S12	H(3.37),B(1.56),O(58.7),Na(0.59),Mg(0.5),Al(23.9),Si(2.13), S(0.19),Ca(8.83),Fe(0.27)

Table 2. Concentration of compounds in Pumice group, P1-P6, Tapan et al. [22].

Compound	P1	P2	P3	P4	P5	P6
SiO_2	71.813	77.653	76.781	75.812	76.7659	72.245
Al_2O_3	12.737	14.019	13.979	14.074	13.926	15.682
Fe_2O_3	5.525	1.663	1.964	1.955	2.485	3.921
CaO	2.019	0.521	0.491	0.521	1.032	1.654
MgO	0.643	0.000	0.000	0.000	0.010	0.000
TiO_2	0.502	0.100	0.120	0.110	0.170	0.341
Na_2O	2.612	1.243	1.142	2.195	1.423	1.574
K_2O	4.038	4.720	5.451	5.263	4.158	4.442
P_2O_5	0.030	0.040	0.030	0.030	0.020	0.120
Cl	0.080	0.040	0.040	0.040	0.010	0.020

2. CALCULATION

2.1. Direct method

The effective atomic numbers of the materials can be calculated by the following practical formula [2]:

$$Z_{eff} = \frac{\sum_i f_i A_i (\mu/\rho)_i}{\sum_j f_j \frac{A_j}{Z_j} (\mu/\rho)_j} \quad (1)$$

, where f_i is the molar fraction, A_i is the atomic weight (IUPAC, 2007) [18], Z_j is the atomic number, $(\mu/\rho)_i$ is the mass attenuation coefficient. The total mass attenuation coefficients of elements present in the materials have been obtained from the WinXCom [19, 20], computer program. In this method, the quantities are directly used in the relation without employing any additional interpolation or fitting procedure. The detailed explanation on this method can be found elsewhere [2].

2.2. Interpolation method

The total atomic cross-section can be obtained by dividing the mass attenuation coefficient μ/ρ (cm^2/g) of the compound by the total number of atoms present in one gram of that compound as follows:

$$\sigma_a = \frac{(\mu/\rho)_{comp}}{N_A \sum_i w_i/A_i} (barns/atom) \quad (2)$$

, where $(\mu/\rho)_{comp}$ is the mass attenuation coefficient of the compound, N_A is the Avogadro constant, w_i is the fraction by weight of the element i, and A_i is the atomic weight of the ith element. The total atomic cross-sections of materials have been obtained theoretically by using WinXCom computer program [19, 20]. The values of the total atomic cross-section, σ_a, have been used to determine the effective atomic number, Z_{eff}. The total atomic cross-section values of samples were interpolated in the total atomic cross-section values of elements generated from WinXCom [19, 20] at the selected energy to calculate the effective atomic number (Z_{eff}) using the following logarithmic interpolation formula [5]:

$$Z_{eff} = \frac{Z_1(\log\sigma_2 - \log\sigma) + Z_2(\log\sigma - \log\sigma_1)}{\log\sigma_2 - \log\sigma_1} \quad (3)$$

, where σ_1 and σ_2 are the elemental cross section (barns/atom) in between which the atomic cross section σ of the material lies and Z_1 and Z_2 are atomic numbers of the elements corresponding to the cross sections σ_1 and σ_2, respectively.

2.3. Electron density (N_{eff})

For an element, electron density, n_e which is expressed in number of electrons per unit mass is given through:

$$n_e = \frac{N_A Z}{A} \quad (4)$$

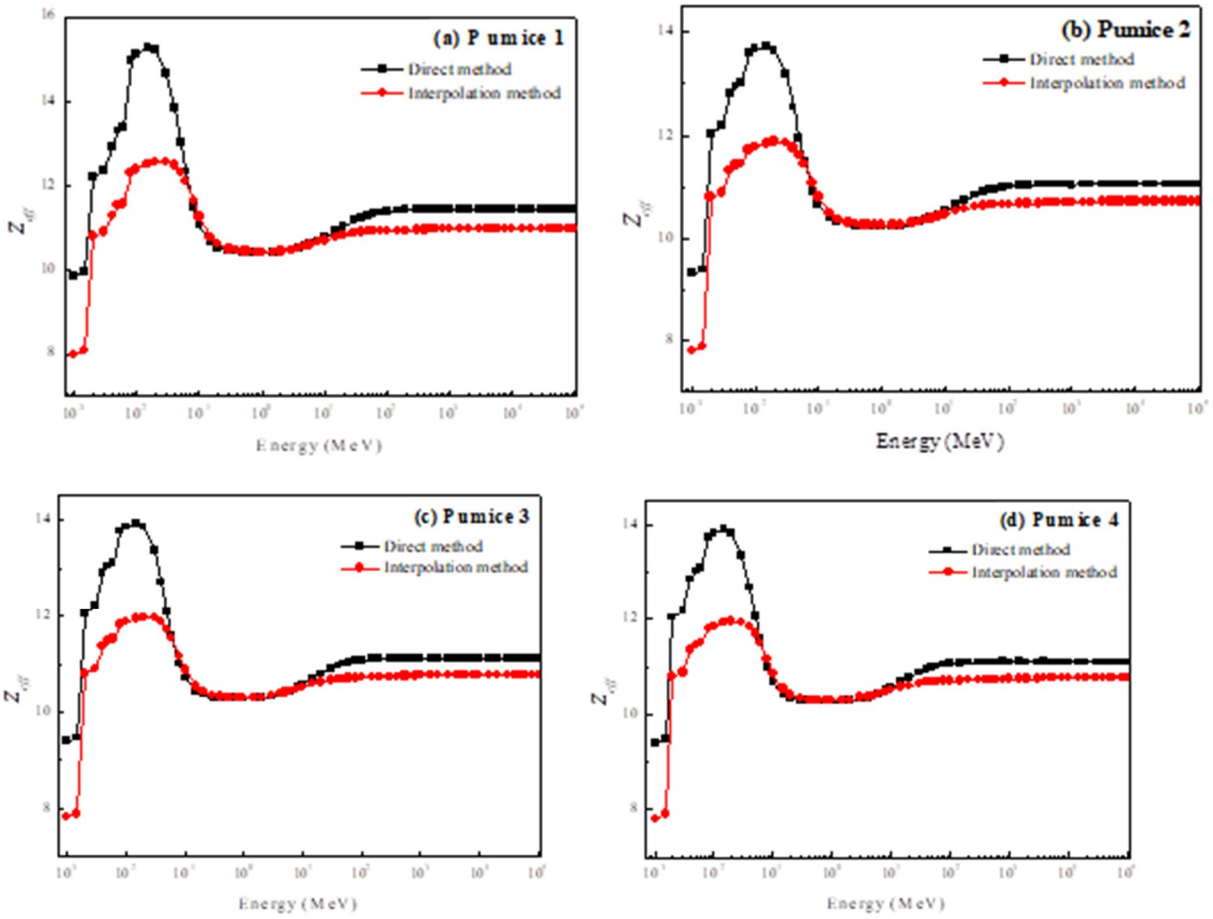
This expression can be generalized to a multi-element material, thus the electron density is expressed by the following relation [2]:

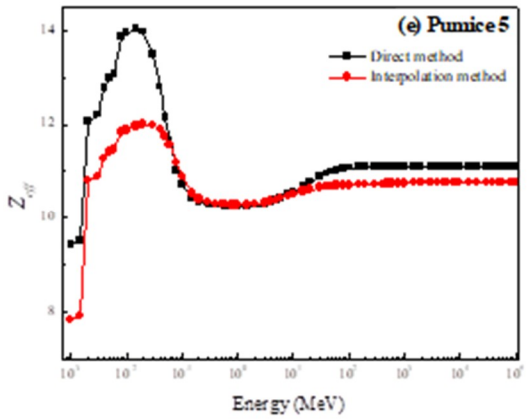
$$N_{eff} = N_A \frac{nZ_{eff}}{\sum_i n_i A_i} = N_A \frac{Z_{eff}}{<A>} \left(\frac{electrons}{g}\right) \quad (5)$$

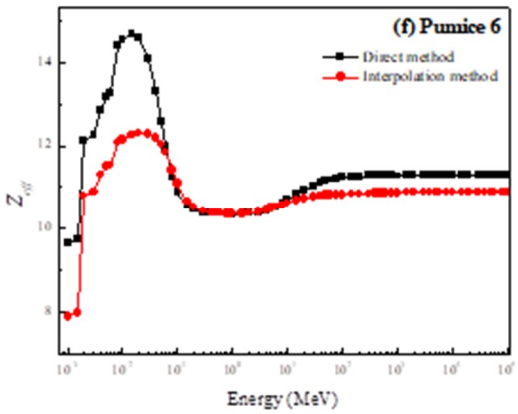
, where $< A >$ is the average atomic mass of materials.

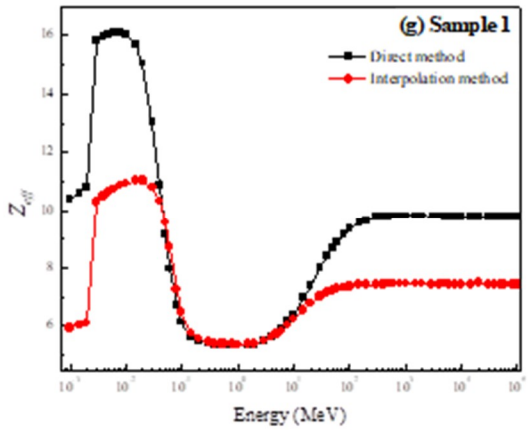
3. RESULTS AND DISCUSSION

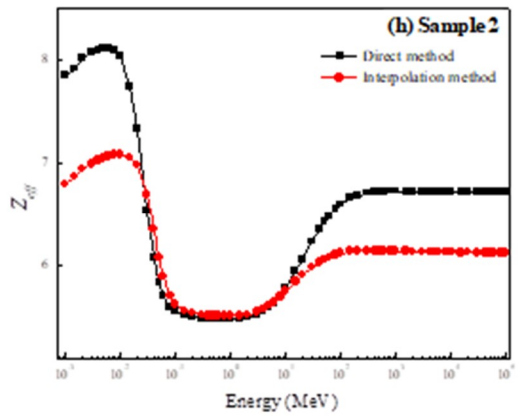
Because Z_{eff} is convenient parameter for understanding the radiation interaction mechanism with material for potential usage, it is very significant to be determined precisely before their some applications such as physical, technological and engineering. In this study, Z_{eff} values were calculated by using the Eq. (1) and Eq. (3) for total photon interaction. For the given materials the variation of Z_{eff} with energy is mainly dominated by different partial photon interaction processes namely photoelectric absorption, Compton scattering and pair production in the continuous energy region 1keV-100 GeV. Differences in Z_{eff} values for all materials, calculated by direct and interpolation methods, are shown in Fig. 1 (a)-(s).

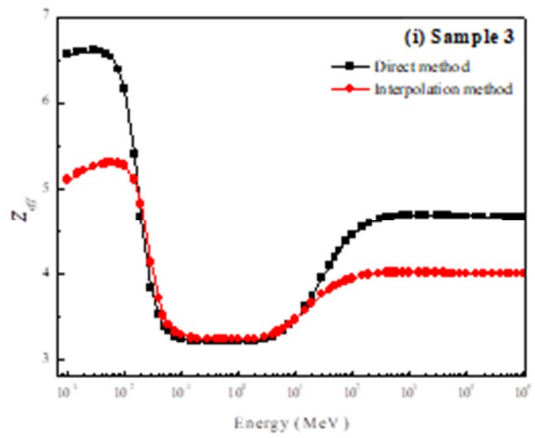


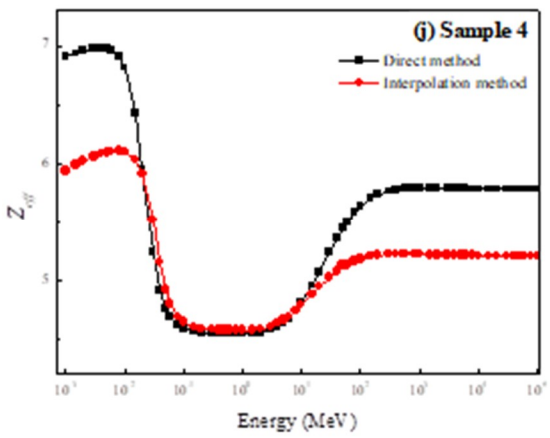

(e) Pumice 5
Direct method
Interpolation method
Z_{eff}
Energy (MeV)

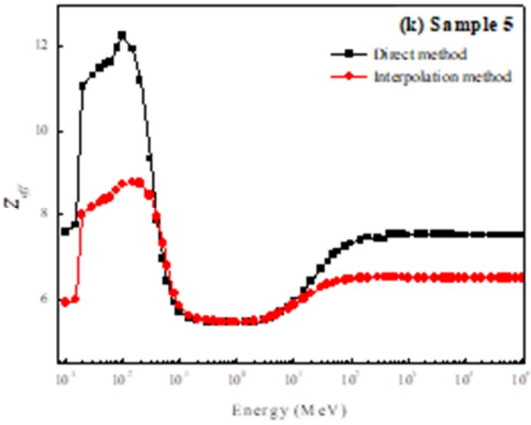

(f) Pumice 6
Direct method
Interpolation method
Z_{eff}
Energy (MeV)

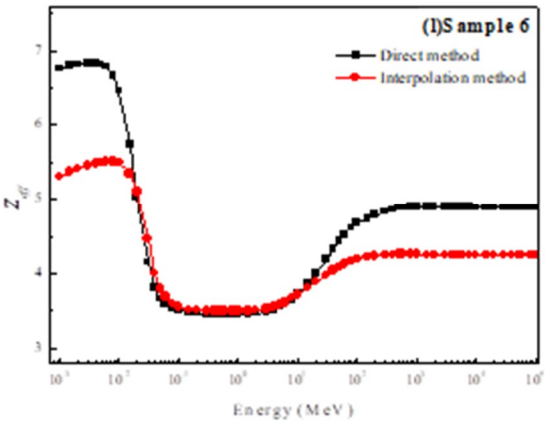

(g) Sample 1
Direct method
Interpolation method
Z_{eff}
Energy (MeV)

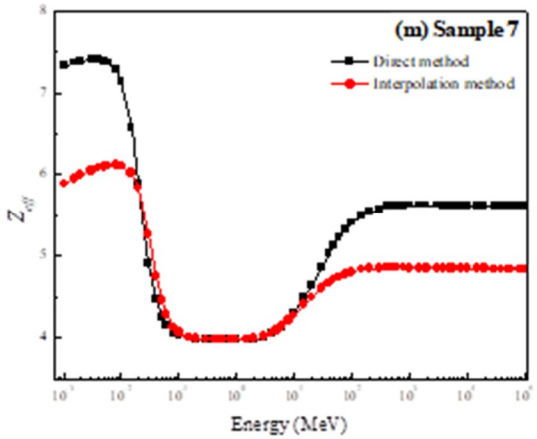

(h) Sample 2
Direct method
Interpolation method
Z_{eff}
Energy (MeV)

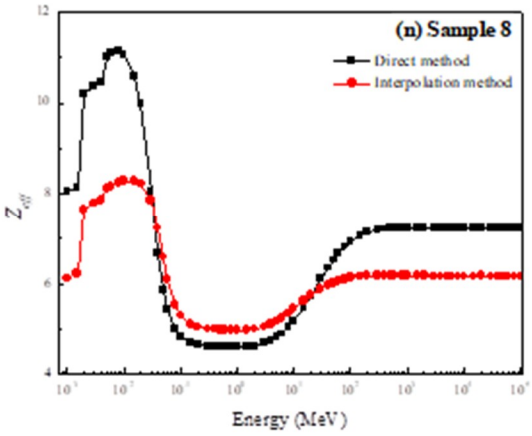

(i) Sample 3
Direct method
Interpolation method
Z_{eff}
Energy (MeV)

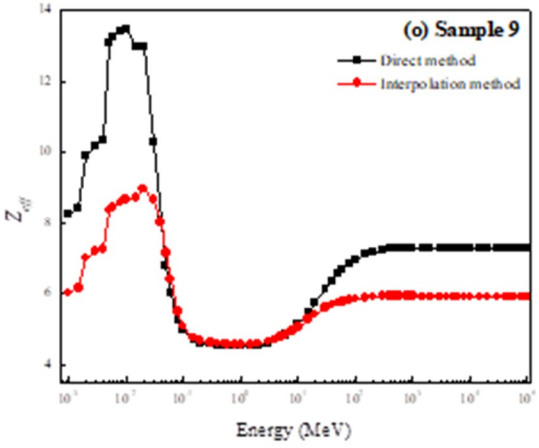

(j) Sample 4
Direct method
Interpolation method
Z_{eff}
Energy (MeV)

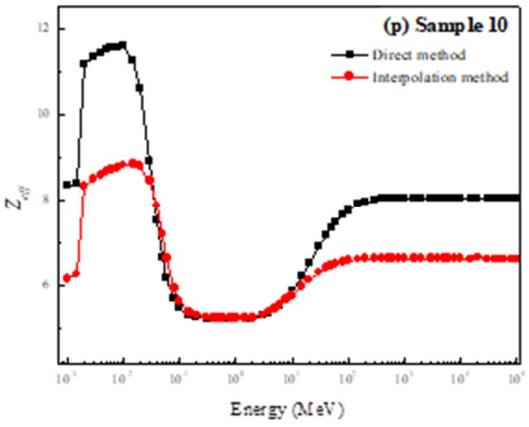

(k) Sample 5
Direct method
Interpolation method
Z_{eff}
Energy (MeV)


(l)Sample 6
Direct method
Interpolation method
Z_{eff}
Energy (MeV)


(m) Sample 7
Direct method
Interpolation method
Z_{eff}
Energy (MeV)


(n) Sample 8
Direct method
Interpolation method
Z_{eff}
Energy (MeV)


(o) Sample 9
Direct method
Interpolation method
Z_{eff}
Energy (MeV)


(p) Sample 10
Direct method
Interpolation method
Z_{eff}
Energy (MeV)

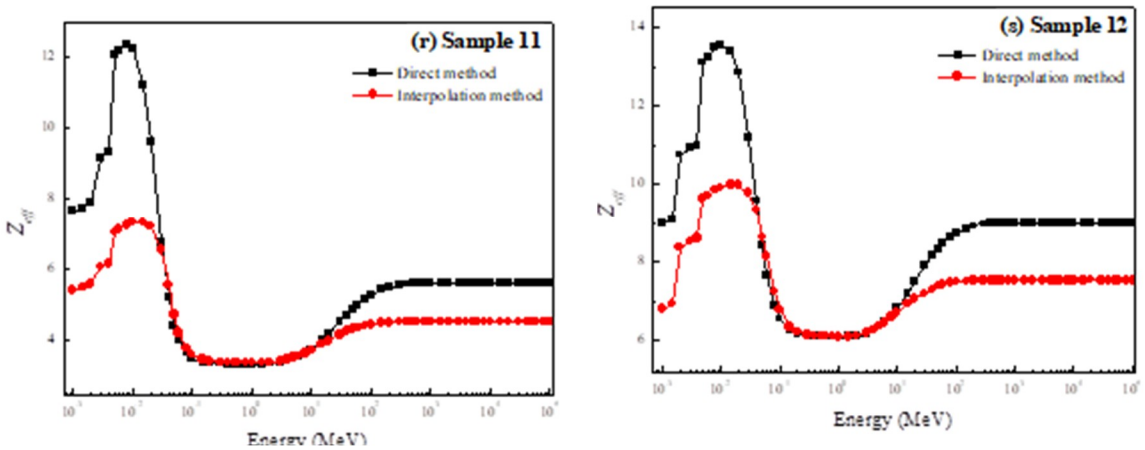


Figure 1 (a)-(f)Variation of Z_{eff} with incident photon energy for Pumice1-6 and (g)-(s) for Sample 1-12.

It was observed that the Z_{eff} has maximum values below 100 keV and has minimum values at intermediate energies. Generally, the all variations can be clearly explained by the Z dependence of total atomic cross sections thus effective atomic numbers as Z^{4-5} for photoelectric absorption, Z for Compton scattering and Z^2 for pair production.

One can distinguish three energy regions in Fig. 1 (a)-(s) for approximately all materials. The energy regions are approximately $E < 100$ keV where photoelectric process dominates and the difference in Z_{eff} for the two methods is large and differences in Z_{eff} are not uniform which may be due to the non-uniform variation of mass attenuation coefficients in this energy region. On the other hand, at the corresponding K absorption edge of high Z element present in the materials, the effective atomic number has more than a single value for the two methods. Thus revealing the non-availability of using Z_{eff} in this energy region and the methods are not in agreement for calculating Z_{eff}. The difference in Z_{eff} is negligible between $0.1 < E < 3$ MeV where the Compton scattering is predominating and the methods are in good agreement for calculating Z_{eff}, and $E > 100$ MeV where pair production process dominates and difference in Z_{eff} is less than the first region. Also, it can be clearly seen that for all materials the effective atomic numbers computed using direct method gives higher values as compared to the effective atomic numbers computed using the interpolation method both in the low and high energy regions in which photoelectric absorption and pair production dominate, respectively. Especially, the difference in the effective atomic number values in the low region (1-100 keV) are more than in the high energy region. At this point, it can be mentioned that the direct method yields a higher Z_{eff} value in the energy region in which variation in Z_{eff} has maximum value, especially near to the K(or L)-edges of constituent elements. The direct and interpolation methods give different weights to the individual atomic numbers when calculating the weighted average [17]. Thus, it can be mentioned that these discrepancies depend on to the strong energy and atomic number dependence of absorption processes.

The variations of N_{eff} with the incident photon energy for the all materials are shown respectively in Fig. 2 (a), (b), (c).

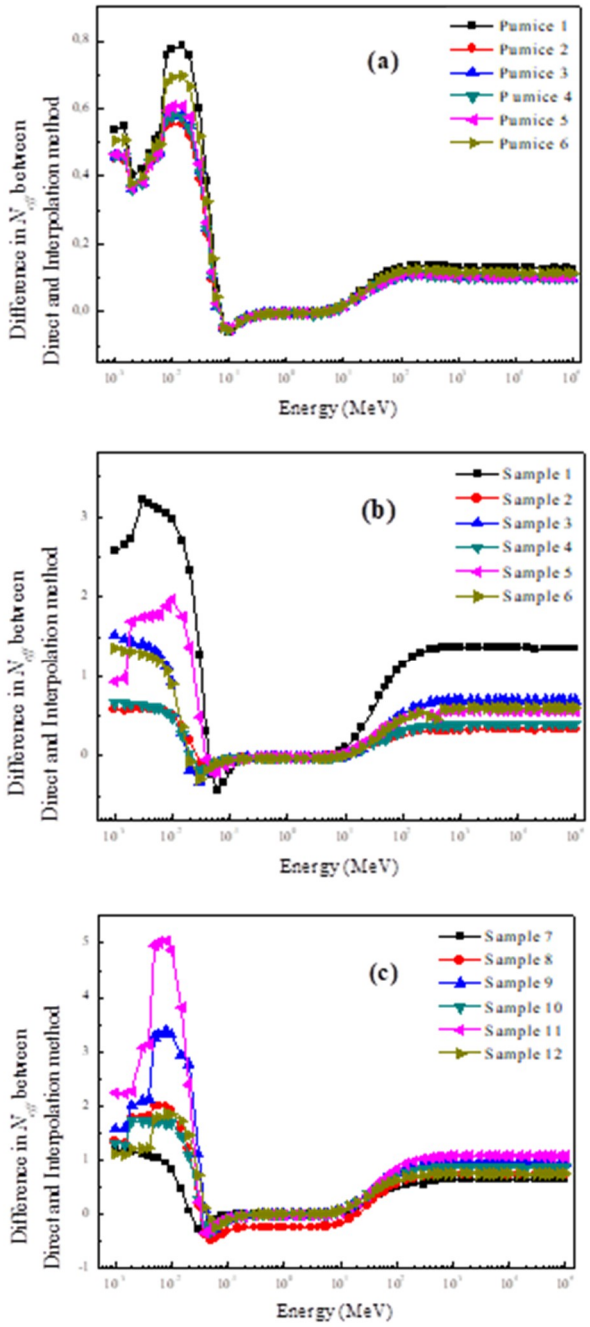


Figure 2 (a) Differences between the direct and interpolation methods with respect to N_{eff} with incident photon energy for Pumice 1-6, (b) for Sample 1-6 and (c) for Sample 7-12.

It can be seen from Fig. 2 (a)-(c) the variations of Z_{eff} and N_{eff} with the incident photon energy are similar, because these two quantities are related by the Eq. (5).

4. CONCLUSIONS

In this work, the effective atomic number (Z_{eff}) and the electron density (N_{eff}) for different types of materials have been calculated by using a direct method and an interpolation method for total photon interaction in the energy region from 1 keV - 100 GeV using WinXCom program [19, 20]. The results obtained from this study show that effective atomic number depends strongly on the chemical composition of the interacting material in the lower as well as higher energy region, but in the intermediate energy region, the chemical composition dependence becomes very weak. Also at the absorption edge energies of the constituent elements of materials the atomic number is not single-valued function of the total atomic cross section, thus the interpolation method could give more than a value of Z_{eff} at the same energy. Thus the direct method gives better agreement than the other method at some available photon energies as mentioned earlier [3]. The variations of N_{eff} with the incident photon energy have same properties because N_{eff} is closely related to the Z_{eff}. The two methods are in good agreement for calculating Z_{eff} between $0.1 < E < 3$ MeV where the Compton scattering is predominating for both new materials (Sample 5-12) or well known materials (Sample 1-4), but in the low and high energy region the methods are disagreed. And, we have shown the agreement and disagreement between the methods in the continuous energy region. Hence, especially experimental verification of effective atomic number is required in the lower energy region. However, it is believed that obtained results may be useful for engineering in application and manufacture of the new types of materials.

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