NUCL SCI TECH (2017) 28:63
DOI 10.1007/s41365-017-0220-0

A study on compatibility of experimental effective atomic numbers with those predicted by ZXCOM

Önder Eyecioğlu[1] · **A. M. El-Khayatt**[2,3] · **Yaşar Karabul**[4] · **Orhan İçelli**[4]

Received: 19 April 2016 / Revised: 15 August 2016 / Accepted: 15 September 2016 / Published online: 29 March 2017

Abstract In this study, effective atomic numbers (Z_{eff}) of materials determined at different experimental conditions by measuring the elastic-to-inelastic γ-ray scattering ratios are compared to ZXCOM predictions. It also presents the experimental data obtained via the transmission technique. The agreement and disagreement between ZXCOM and experimental values are investigated. The theoretical basics of determining Z_{eff} by scattering mode are outlined. The study shows that choosing appropriate experimental conditions can provide a good compatibility between the experimental results and theoretical ZXCOM calculations.

Keywords Effective atomic number · ZXCOM · Rayleigh scattering · Compton scattering

1 Introduction

The effective atomic number (Z_{eff}) is of significance in calculating the attenuation of X- and γ-ray in radiation dosimetry. Many physical characteristics of materials can be visualized by just the Z_{eff} [1]. It gives physical information about radiation interaction with matter and is used in many fields related to radiation shielding, absorbed dose and buildup factor [2]. The Z_{eff} value depends on energy of the incoming photons and the elements constituting the material. Briefly, it can be considered as an average of the number of electrons that joined to the photon–atom interaction [3].

Determination of Z_{eff} can be done by measuring attenuated or scattered photons by the materials. When photons penetrate matter, their intensities and energies change due to many interaction mechanisms. Calculations of photon attenuation are usually treated in terms of atomic mass attenuation coefficients. In fact, a variation of total mass attenuation coefficients with atomic numbers is generally employed for Z estimation. The theoretical basics of this method are described briefly elsewhere [4].

There are many programs to generate attenuation coefficients, total cross sections, partial cross sections for incoherent and coherent scattering, photoelectric absorption and pair production for any element, compound or mixture in different energy ranges, useful for different purposes, such as WinXCOM [5, 6], Xmudat [7] and NXCOM [8].

Although the measurements in transmission mode are widely applied for Z_{eff} determination [9–13], its sensitivity to detection of Z_{eff} of some materials is inadequate. For example, in low Z-materials (atomic number less than 10 such as tissue, polymers and dosimetric materials) the

---

This work was supported by the Yıldız Technical University (No. 2015-01-01-KAP06) and the Scientific and Technological Research Council of Turkey (TÜBİTAK) (No. 2015-115F311).

✉ Önder Eyecioğlu
onder.eyecioglu@nisantasi.edu.tr

[1] Department of Computer Engineering, Engineering and Architecture Faculty, Nisantasi University, Istanbul, Turkey

[2] Physics Department, College of Science, Al Imam Mohammad Ibn Saud Islamic University (IMSIU), Riyadh, Saudi Arabia

[3] Reactor Physics Department, Nuclear Research Centre, Atomic Energy Authority, Cairo 13759, Egypt

[4] Department of Physics, Science and Art Faculty, Yıldız Technical University, Istanbul, Turkey

photoelectric absorption has minor important than scattering in the energy range (>20 keV) required for transmission mode and in the photon energy range suitable for absorption measurements [14–16]. Therefore, in such cases, the scattering mode measurement may be carried out for Z_{eff} determination. Elastic (Rayleigh) and inelastic (Compton) scatterings, varying with energy, can be measured separately [17].

The Z_{eff} for different materials has been extensively investigated via the transmission mode, but the Z_{eff} determination via the scattering mode has been less investigated [17–20]. Manninen et al. [18] reported the problems that arise in comparison of the experimental results and theoretical predictions in scattering mode measurements. In this study, we attempted to compare the experimental results of the scattering measurements with those predicted by the ZXCOM program.

2 Physical background

Generally, the mathematical details of Z_{eff} and N_{eff} are explained by the transmission and elastic modes.

2.1 Computation of Z_{eff} and Z_{eff} via the transmission mode

The effective atomic number for any sample is given by:

$$Z_{\text{eff}} = \sigma_{\text{t-a}}/\sigma_{\text{t-e}}, \tag{1}$$

where $\sigma_{\text{t-a}}$ and $\sigma_{\text{t-e}}$ are the total effective atomic and total effective electronic cross section, respectively. One can find the formulation in detail in Ref. [21].

The effective electron density (in electrons g^{-1}) of the sample can be computed by Eq. (2)

$$N_{\text{eff}} = N_{\text{A}} n Z_{\text{eff}} / \sum N_i A_i = N_{\text{A}} Z_{\text{eff}} / \langle A \rangle, \tag{2}$$

where N_{A} is the Avogadro's constant; the total number, n, of atoms in the molecule; N_i and A_i are, respectively, the total number of atoms and the atomic mass of the ith elemental composition of the material; and □A□ is the average atomic mass of the sample. Therefore, using the Z_{eff} value obtained from logarithmic interpolation in Eq. (1), one can calculate the values of N_{eff} by using Eq. (2). The equations reveal that N_{eff} and Z_{eff} can be used interchangeably. The most important difference between them is the value of atomic weights that make up the compounds.

2.2 Computation of Z_{eff} and N_{eff} via the elastic mode

If the photon energy and scattering angle are high enough to produce all interatomic interference phenomena negligible, the photon energy is not too high to produce the addition of pair production and nuclear-scattering interactions necessary. This roughly means that $\sin(\theta/2)/\lambda_0 \geq 20\ \text{nm}^{-1}$, where λ_0 is the wavelength of the primary photons, and $E_0 < 1$ MeV. In this case, elastic scattering can be viewed as a scattering through free atoms whatever configuration of the sample, and the differential cross section of the Rayleigh scattering is given by [18]:

$$(\text{d}_{\text{a}}\sigma/\text{d}\Omega)_{\text{R}} = (\text{d}_{\text{e}}\sigma/\text{d}\Omega)_{\text{T}} F^2(x, Z), \tag{3}$$

where index a stands for the whole atom, index e stands for a unique electron, index T refers to the Thomson differential cross sections, which are given as:

$$(\text{d}_{\text{e}}\sigma/\text{d}\Omega)_{\text{T}} = \left(1 + \cos^2\theta\right) r_0/2, \tag{4}$$

where r_0 is the classical electron radius, and θ is the scattering angle.

Similarly, the atomic differential cross sections for Compton process for a bounded electron can be written as [22, 23]:

$$(\text{d}_{\text{a}}\sigma/\text{d}\Omega)_{\text{C}} = (\text{d}_{\text{e}}\sigma/\text{d}\Omega)_{\text{K-N}} S(x, Z), \tag{5}$$

where "K–N" stands for the Klein–Nishina cross section and $S(x, Z)$ is the inelastic scattering function:

$$\left(\frac{\text{d}_{\text{e}}\sigma}{\text{d}\Omega}\right)_{\text{K-N}} = \frac{r_0}{2}\left(\frac{\omega_2^0}{\omega_1}\right)^2\left(\frac{\omega_1}{\omega_2^0} + \frac{\omega_2^0}{\omega_1} - \sin\theta\right), \tag{6}$$

where ω_1 and ω_2^0 are the angular frequencies of the incident and scattered photons, respectively.

In Eqs. (3) and (5), the elastic-to-inelastic cross-sectional ratio is then, for one atom, given by:

$$\frac{(\text{d}_{\text{a}}\sigma/\text{d}\Omega)_{\text{R}}}{(\text{d}_{\text{a}}\sigma/\text{d}\Omega)_{\text{C}}} = \frac{(\text{d}_{\text{e}}\sigma/\text{d}\Omega)_{\text{T}} F^2(x, Z)}{(\text{d}_{\text{e}}\sigma/\text{d}\Omega)_{\text{K-N}} S(x, Z)}, \tag{7a}$$

and therefore, the F^2/S factor

$$\frac{F^2(x, Z)}{S(x, Z)} = \frac{(\text{d}_{\text{e}}\sigma/\text{d}\Omega)_{\text{K-N}}}{(\text{d}_{\text{e}}\sigma/\text{d}\Omega)_{\text{T}}} \frac{(\text{d}_{\text{a}}\sigma/\text{d}\Omega)_{\text{R}}}{(\text{d}_{\text{a}}\sigma/\text{d}\Omega)_{\text{C}}}. \tag{7b}$$

The multiplication of $(\text{d}_{\text{e}}\sigma/\text{d}\Omega)_{\text{K-N}}$ and $(\text{d}_{\text{e}}\sigma/\text{d}\Omega)_{\text{T}}$ by $S(x, Z)$ and the atomic form factor $F(x, Z)$, respectively, allows us to include the effect of electron binding into the accounts. The values of $S(x, Z)$ and $F(x, Z)$ functions are extending from zero to Z. Also, they depend on the momentum transfer parameter x (in Å^{-1});

$$x = \sin(\theta/2)/\lambda_0 = \sin(\theta/2) E_0/12400, \tag{8}$$

where λ_0 and E_0 are the wavelength (in Å^{-1}) and energy (in eV) of the primary photons, respectively. The number of atoms scattered to the detector is given in Eq. (9). It takes into account the experimental setup, photon flux of the source and atomic density of the sample $\eta_{\text{a}} = N_{\text{A}}\rho/M_{\text{A}}$; where ρ is the target density and M_{A} is the atomic mass [20].

$$N = \frac{\mathrm{d_a}\sigma}{\mathrm{d}\Omega}\Delta\Omega\eta_{\mathrm{a}} V N_0 A, \tag{9}$$

where $\mathrm{d_a}\sigma/\mathrm{d}\Omega$ is the atomic differential cross section, the probability of a photon to be scattered at an angle θ by one atom of the material, within an elementary solid angle $\mathrm{d}\Omega$; N_0 is the initial fluency; A is the self-attenuation factor for photons; V is the scattered volume; and $\Delta\Omega$ is the solid angle.

Using Eqs. (4) and (5) in Eq. (9), the recorded photon numbers for Rayleigh (N_R) and Compton (N_C) by a detector of efficiency ε can be expressed as:

$$N_\mathrm{R} = \left(\frac{\mathrm{d_e}\sigma}{\mathrm{d}\Omega}\right)_\mathrm{T} F^2(x,Z)\Delta\Omega\eta_\mathrm{a} V N_0 \varepsilon(E_0) A_\mathrm{R}, \tag{10}$$

$$N_\mathrm{C} = \left(\frac{\mathrm{d_e}\sigma}{\mathrm{d}\Omega}\right)_\mathrm{K-N} S(x,Z)\Delta\Omega\eta_\mathrm{a} V N_0 \varepsilon(E_\mathrm{C}) A_\mathrm{C}. \tag{11}$$

where $A_\mathrm{R} = \exp[-\mu(E_0)L_\mathrm{i} + \mu(E_0)L_\mathrm{s}]$ and $A_\mathrm{C} = \exp[-\mu(E_0) L_\mathrm{i} + \mu(E_\mathrm{C})L_\mathrm{s}]$ are self-attenuation factors for the Rayleigh and Compton, respectively, with E_C being energy of the photons after a Compton scattering, μ is the linear attenuation coefficient, and L_i and L_s are the path lengths through the sample, along the incident and scattered beams, respectively. The self-attenuation correction factor can be estimated by: $\mathrm{e}^{[\mu(E_\mathrm{C})-\mu(E_0)]L_\mathrm{s}}$

$$\mathrm{SCF} = A_\mathrm{R}/A_\mathrm{C} = \mathrm{e}^{[\mu(E_\mathrm{C})-\mu(E_0)]L_\mathrm{s}}. \tag{12}$$

The Rayleigh N_R to Compton photons N_C ratio, R, can be written as the ratio of the net peak areas under the elastic and inelastic peaks, corrected for detector efficiency and pulse losses

$$R(x,Z) = N_\mathrm{R}/N_\mathrm{C} = C\left[F^2(x,Z)/S(x,Z)\right]\mathrm{SCF}, \tag{13}$$

where C holds for the ratio $C = (\mathrm{d_e}\sigma/\mathrm{d}\Omega)_\mathrm{T}/(\mathrm{d_e}\sigma/\mathrm{d}\Omega)_\mathrm{K-N}$.

Thus, for a specific experimental condition characterized by x

$$R_x(Z) = Cf_x^\mathrm{D}\left[F^2(x,Z)/S(x,Z)\right]\mathrm{SCF}. \tag{14}$$

For some experimental conditions (E_0, θ), in which E_0 and E_C are roughly equal: This is true for a relatively low scattering angle θ; Eqs. (13) and (14) can be drawn without making self-attenuation corrections [$A_\mathrm{R} \approx A_\mathrm{C}$]. Also, R_x and Z can be determined by the following relations:

$$R_x(Z) = Cf_x^\mathrm{D}\left[\left(\frac{F^2(Z)}{S(Z)}\right)\right] = f_x^\mathrm{D}(Z), \tag{15}$$

$$(Z)_x = f_x^D\left[\left(\frac{F^2}{S}\right)\right]. \tag{16}$$

where $f_x^\mathrm{D}(F^2/S)$ is a discrete function at certain momentum transfer parameter (x), which gives Z as a function of F^2/S factor. The points of the discrete function $R = f_x^\mathrm{D}(Z)$ for the elements can be calculated by Eq. (15) from the knowledge of $F(x, Z)$ and $S(x, Z)$ using suitable tabulations such as those in Ref. [22].

Figure 1 shows the discrete points of the functions $R_{1.5} = f_{1.5}^\mathrm{D}(Z_\mathrm{eff})$ and $Z_{1.5} = f_{1.5}^\mathrm{D}(F^2/S)$, obtained by theoretical values of F^2/S, for elements of atomic number 1–100. Equation (15) is the basis for the atomic number measurement method by the Rayleigh to Compton scattering ratio, where the R ratio is independent of the attenuation in the sample. It should be stressed that as long as ω_2^0 describes the average photon energy of Compton scattered photons, Eq. (15) can be successfully applied [18, 24].

For compounds and homogenous mixtures containing various elements, we can generalize Eqs. (15) and (16) as follows,

$$R_x = \left(\frac{N_R}{N_C}\right)_x = Cf_x\left[\left(\frac{F^2(Z)}{S(Z)}\right)_\mathrm{eff}\right] = f_x(Z_\mathrm{eff}), \tag{17}$$

$$(Z_\mathrm{eff})_x = f_x\left[\left(\frac{F^2}{S}\right)_\mathrm{eff}\right] = f_x\left[\left(\frac{\sum_{i=0}^n \alpha_i^\mathrm{at} F^2(Z_i)}{\sum_{i=1}^n \alpha_i^\mathrm{at} S(Z_i)}\right)\right]. \tag{18}$$

where α_i^at is defined by the mass percentage ω_i and the atomic mass M_i of the ith element:

$$\alpha_i^\mathrm{at} = \frac{\omega_i/M_i}{\sum_{i=1}^n \omega_i/M_i}. \tag{19}$$

Here the function $R = f_x(Z_\mathrm{eff})$ is a continuous function, which can be deduced by fitting the discrete f_x^D function. The last relationships enable us to determine theoretical values for R_x and Z_eff from the calculated values of $(F^2/S)_\mathrm{eff}$ for any material under consideration [19]. Thus, for any element, R_x can be calculated via Eq. (15) at a certain experimental condition. Hence, these values can be referred to as "point-wise data," which can be plotted as continuous functions to determine R_x and $(Z_\mathrm{eff})_x$ for any material with an adequate interpolation method. Under correct experimental conditions, we expect that a good agreement can be achieved between the measured and calculated values.

Practically, details of right experimental compromise for E_0 and θ values were given by many researchers. For example, Duvauchelle et al. showed that E_0 and θ values should be carefully chosen when (1) neglecting the correction factors mentioned in Eq. (12), (2) obtaining a good counting statics for both Rayleigh and Compton components, and (3) achieving a good separation between them. They considered that, for example, the choice of photon energy of 59.53 keV and a scattering angle of 35° lead to an acceptable compromise between parameters influencing the measurement [19]. Finally, the effective electron density at certain momentum transfer parameter (x), $(N_\mathrm{eff})_x$ of the sample can be calculated by Eq. (2).

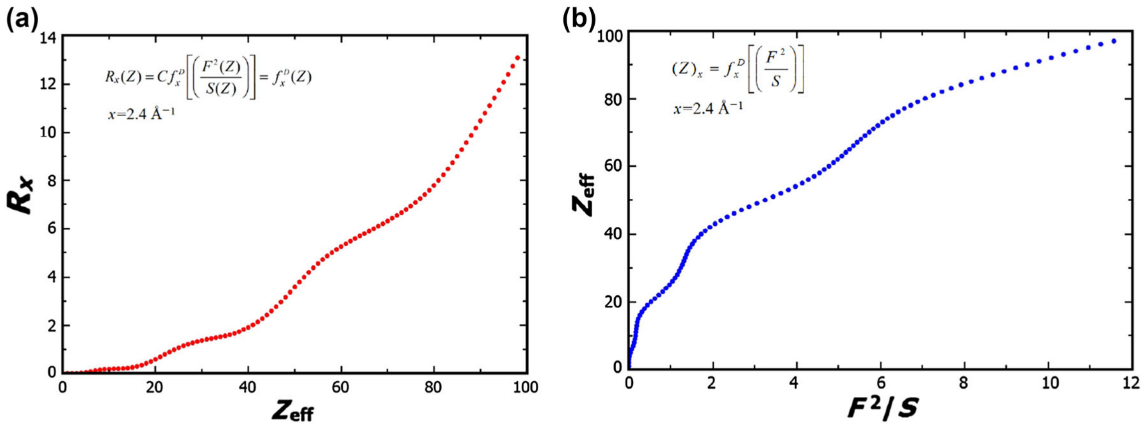

Fig. 1 Variation of Rayleigh to Compton ratio $R_{1.5}$ as a function of Z_{eff} (**a**) and F^2/S (**b**), for $x = 1.5$ Å^{-1} calculated by ZXCOM

We compared the calculated Z_{eff} with the Z_{eff} for some materials measured under different conditions.

2.3 ZXCOM: Windows-based program for calculating Z_{eff}

Based on the above theoretical treatment, a computer program called ZXCOM has been constructed. It is a MS Windows-based program to calculate Z_{eff} and N_{eff} using R ratio for any element, compound or mixture, of $\theta = 1°$–$180°$ and photon energy of $E_0 = 1$ keV–1 MeV.

2.4 Database

A database file for F and S for 100 elements over the studied energy range has been compiled from the tabulation in Ref. [23]. The R and Z_{eff} are calculated from F^2/S factors, which depend on the momentum transfer parameter, $x(E_0, \theta)$, as mentioned in the previous section. The continuous functions of R and Z_{eff} for any materials are obtained by interpolation of the discrete values of F^2/S for the 100 elements.

2.5 Input and output

ZXCOM has a graphical user interface (GUI). The GUI facilitates define and redefine the elements, compounds and mixtures. In addition, each variable can be redefined within the ongoing run. The main output calculations of ZXCOM are the variation of R with incident photon energy E_0 (in keV), at a certain scattering angle θ in degrees, and the variation of R with θ at constant E_0. The calculated data are listed in "DataGridView object" to a predefined MS Excel template or simple data file. Graphics of the data can be drawn. The execute version of this program can be downloaded via http://photon.yildiz.edu.tr/zxcom.php and http://photon.gelisim.edu.tr/zxcom.php.

3 Results and discussion

3.1 Comparison with values determined by *R* measurement

Z_{eff} measured using the elastic-to-inelastic scattering ratio is collected from Refs. [25–29]. Tables 1, 2 and 3 provide comparisons with experimental results. Table 1 lists the calculated and measured Z_{eff} for low Z-materials ($Z < 10$) at experimental conditions of (1) $E_0 = 17.44$ keV, $\theta = 90°$, $x = 0.99$ Å^{-1} and $\Delta E = 0.58$ keV, and (2) $E_0 = 59.54$ keV, $\theta = 60°$, $x = 2.4$ Å^{-1} and $\Delta E = 3.28$ keV.

Table 1 includes the columns of corrected ZXCOM results for self-attenuation corrections of primary and scattered photons. The corrections are calculated with Eq. (12) using attenuation coefficients tabulated in Ref. [32]. The corrections improve the agreement between measured and calculated values, as given in Table 1. Experimentally, self-attenuation correction factor is dependent on the relative transmission of radiation at various energies as a ratio of photo-peak count rate passing through the reference standard and other materials to that through the air or water of the same geometry [30].

A closer study of Table 1 shows a considerable agreement (differences up to 9.6%) between the calculated and measured Z_{eff} under experimental conditions of (1), and a good agreement, too, under experimental conditions of (2).

Generally, the theoretical and experimental results agree with each other better for incident photon energies of >20 keV (see the example of $E_0 = 17.44$ and $E_0 = 17.4459.54$ keV in Table 1). This is a natural result for employing photons in an energy range of scattering dominance, since the relative interaction probabilities for elastic scattering and photoelectric process are roughly comparable for energies of >20 keV in a matter with atomic numbers of <10 (similar to our studied materials) [17]. Therefore, when determining the Z_{eff} for low Z-

Table 1 Calculated and measured Z_{eff} of low Z-materials at experimental conditions (1) Antoniassi et al. [25] and (2) Del Lama et al. [26]

Material	(1) $E_0 = 17.44$ keV, $\theta = 90°$, $x = 0.99$ Å^{-1}, $\Delta E = 0.58$ keV						(2) $E_0 = 59.54$ keV, $\theta = 60°$, $x = 2.4$ Å^{-1}, $\Delta E = 3.28$ keV					
	Uncorrected			Corrected			Uncorrected			Corrected		
	Cal.	Exp.	Dev.%	Cal.	Exp.	Dev.%	Cal.	Exp.	Dev.%	Cal.	Exp.	Dev.%
Water (H_2O)	6.41	5.85	−9.57	5.99	5.85	−2.34	7.43	7.2	−3.25	7.34	7.2	−1.89
Ethanol (C_2H_6O)	5.71	5.26	−8.56	5.64	5.26	−7.25	6.32	5.98	−5.70	6.30	5.98	−5.42
Isopropanol (C_3H_8O)	5.64	5.21	−8.25	5.57	5.21	−6.89						
Glycerol ($C_3H_8O_3$)	6.06	5.64	−7.45	5.97	5.64	−5.85	6.75	6.45	−4.65	6.70	6.45	−3.94
Dimethylformamide (C_3H_7NO)	5.86	5.36	−9.33	5.79	5.36	−7.99						
Acrylic ($C_5H_8O_2$)	5.91	5.53	−6.80	5.84	5.53	−5.67	6.395	6.16	−3.80	6.38	6.16	−3.53
Nylon ($C_6H_{11}NO$)	5.76	5.34	−7.87	5.71	5.34	−6.89	6.15	5.91	−3.98	6.13	5.91	−3.76

Table 2 Calculated and measured Z_{eff} of some compounds under different experimental conditions

A[a] ($E_0 = 59.54$ keV, $\theta = 90°$, $x = 3.4$ Å^{-1}, $\Delta E = 6.21$ keV)				B[b] ($E_0 = 59.54$ keV, $\theta = 60°$, $x = 2.41$ Å^{-1}, $\Delta E = 3.28$ keV)			
Materials	Cal.	Exp.	Dev.%	Materials	Cal.	Exp.	Dev.%
Pr_2O_3	52.22	55.11	5.25	BaO	53.60	53.84	0.46
Eu_2O_3	57.31	58.88	2.66	La_2O_3	53.59	54.33	1.35
Lu_2O_3	66.78	63.56	−5.06	CeO_2	53.61	54.68	1.96

[a] Taken from Singh et al. [28]

[b] Taken from İçelli [29]

Table 3 Calculated and measured Z_{eff} of two alloys at $E_0 = 145$ keV, $\theta = 70°$ and $x = 6.71$ Å^{-1} [27]

Materials	Uncorrected			Corrected		
	Cal.	Exp.	Dev.%	Cal.	Exp.	Dev.%
$Cu_{0.7}Zn_{0.3}$	29.30	29.1	−0.69	29.30	29.1	−0.69
$Cu_{0.6}Sn_{0.4}$	38.29	40.3	5.00	41.42	40.3	−2.78

materials by the R ratio measurement, the photon energy should not be too low (>20 keV) in order to depart the photoelectric dominance energy region. If the measurement is performed at lower energies, where the scattering contributions are minor, the R determination becomes a difficult problem, with high uncertainties, especially for low-intensity radioactive sources. So the primary photon energy of 59.54 keV is more convenient for scattering measurements, with more reliable results than those of photon energies below 20 keV (Table 1).

Also, we noticed that the deviations between theoretical and experimental results in Table 1 are always negative, which means that the experimental results are constantly lower than those calculated (as Dev. = (Exp. − Theo.)/Exp. × 100%); this can be attributed to overestimate of Compton scattering contribution as discussed in the following statements.

The origin of differences between theoretical and experimental results comes from the fact that ω_2^0, in Eq. (6), corresponds to the radiation energy after scattering by a stationary free electron. But the electrons in a real matter are neither stationary nor free. The electron velocities cause the broadening in the energy distribution of scattered photons [so-called Compton profile]. As long as ω_2^0 describes the average energy of the Compton profile, then the general Eq. (7) can be successfully applied for estimating the elastic-to-inelastic cross-sectional ratio, the (F^2/S) factor and Z_{eff}. In fact, if the binding energy of a particular electron shell, especially K- or L-shells, is of the order of the energy difference of ($\omega_1 - \omega_2^0$), ω_2^0 is no longer the average photon energy after scattering from those electrons [18]. The actual ω_2 (average) is smaller, and therefore, $(d_e\sigma/d\Omega)_{K\text{–}N}$ overestimates the Compton scattering contribution, and as a result, the obtained values of F^2/S and Z_{eff} are overestimated, as given in Eqs. (7b) and (18), respectively. The $(d_e\sigma/d\Omega)_{K\text{–}N}$ overestimate is due to the factor $(\omega_2^0/\omega_1)^2$ in Eq. (6). As given in Table 1, the energy difference $\omega_1 - \omega_2^0$ (about 0.58 keV) is of the order of the K-shell binding energy of the oxygen (about 0.55 keV), and ω_2^0 is no longer the average photon energy after scattering from oxygen K-shell electrons. So Eq. (18) assigns too much value to the calculated Z_{eff}. İçelli and Erzeneoğlu [31] showed that the differential cross-

Table 4 Calculated and measured Z_{eff} of low Z-materials at $E_0 = 59.5$ keV, $\theta = 90°$, $x = 3.4$ Å^{-1} and $\Delta E = 6.21$ keV [34]

Materials	Cal.	Exp.	Dev.%	Materials	Cal.	Exp.	Dev.%	Materials	Cal.	Exp.	Dev.%
$AlCl_3$	16.02	14.83	−8.02	$FeCl_2$	21.25	22.13	3.94	Na_2CO_3	9.37	9.45	0.79
$Al(NO_3)_3$	8.73	8.54	−2.29	$FeCl_3$	20.21	20.54	1.57	NaF	10.16	9.90	−2.70
CaF_2	13.78	14.57	5.41	$Fe_2(SO_4)_3$	13.92	15.66	11.14	$NaNO_3$	8.88	8.09	−9.81
$CaHPO_4$	12.82	12.29	−4.35	$Mg(NO_3)_2$	8.73	7.92	−10.19	Na_2SO_3	11.31	12.36	8.50
$CaO_6C_6H_{10}$	10.01	6.47	−54.61	MgO	10.65	10.04	−6.06	Na_2SO_4	11.02	11.65	5.43
$CaSO_4$	13.07	15.70	16.75	$NaO_2C_2H_3$	8.62	5.88	−46.58	NaCl	14.32	14.23	−0.64

sectional ratios decreased with increasing scattering angle. The Z_{eff} values at 60° are higher than those calculated at 90° (Table 1).

While Z increases, the contributions of K- and L-shell electrons, in Compton scattering, become negligible, and this error does not provide any observable impact on the cross-sectional ratio, hence no overestimate for calculated values of R or Z and no negative deviation between the calculated and measured values (Table 2). The negative deviation value of Lu_2O_3 results from the effect of anomalous scattering. As the energy of the incident radiation (about 60 keV) is close to the absorption edge of electron K-shell of Lu (63 keV), the true atomic scattering factor deviates from that employed in ZXCOM program, which is taken from Ref. [32]. Finally, in Table 2, it was noticed that the deviation is significantly lowered by lowering the scattering angle. Also, Table 3 lists the experimental [27] and the ZXCOM results for two alloys. A good agreement is achieved.

Another source of discrepancies arises between the calculation and measurement results because of the electron charge distribution in the molecule due to the effect of binding between different types of atoms. This distortion leads to inaccurate Rayleigh cross-sectional estimation as a result of limited range of validity of the form factor approximation, which was originally derived to correct the Thomson formula for scattering by a charge distribution rather than a point charge. Specifically, the form factor approximation is not valid for momentum transfers that are higher than the electron binding, and therefore, the independent atomic model, in which each atom in a material scatters independently of the others, cannot be successfully applied. The effects of interatomic bonding within a molecule, especially for large scattering, should be considered [33].

The deviations may be also originated by experimental errors such the counting statistics errors at the lower counting rates and the error in designating the scattering angle. The overlap between the signals of coherently and incoherently scattered photons will result in a wrong number of counts, especially at small angles.

3.2 Comparison with experimental values determined by transmission technique

Table 4 shows the experimental $Z_{\mathrm{eff,T}}$ values deduced from transmission technique based on measuring the total attenuation coefficients [34] and ZXCOM results (Z_{eff}) for low Z-materials. One can see that the $Z_{\mathrm{eff,T}}$ and Z_{eff} for the most majority of listed materials are in good agreement. However, this agreement is not upon any physical principles, since the $Z_{\mathrm{eff,T}}$ and Z_{eff} are independent parameters used for characterizing the material uniquely for different photon interaction processes of attenuation and scattering [26]. Moreover, in some cases large deviations were noted, for example, up to 55% for $CaO_6C_6H_{10}$ and 47% for $NaO_2C_2H_3$. Del Lama et al. [26] reported a similar large deviation between $Z_{\mathrm{eff,T}}$ and Z_{eff} values. Therefore, these parameters are not directly related. Consequently, the ZXCOM predictions are principally limited to the scattering mode of measurement.

4 Conclusion

We have presented a comprehensive comparison between the ZXCOM predications and the experimental results of transmission and scattering measurements. For the scattering technique, the noticed deviations between the experimental and calculated values are resolved in the studied cases. The overestimate of Z_{eff} values for substances with low and high atomic numbers is explained. The effect of the self-attenuation correction factor is studied. ZXCOM predictions are improved when the attenuation correction factors are considered. The results indicate that as long as ω_2^0 describes the average photon energy of Compton profile, Eq. (7) can be applied, and then, a good matching can be obtained between the experiment and theory.

The deviation between the transmission technique data and those predicted by ZXCOM program is attributed to the different natures of photon interactions in the transmission and scattering mode measurements. Right experimental compromise for E_0 and θ values should be taken into account when measuring or calculating Z_{eff} via scattering mode. On the other hand, the requirements of the fine beam geometry must be fulfilled in the transmission mode.

References

1. K. Singh, R. Kaur, V. Kumar, Study of effective atomic numbers and mass attenuation coefficients in some compounds. Radiat. Phys. Chem. **47**, 535–541 (1996). doi:10.1016/0969-806X(95)00057-5
2. S.R. Manohara, S.M. Hanagodimath, L. Gerward, Studies on effective atomic number, electron density and kerma for some fatty acids and carbohydrates. Phys. Med. Biol. **53**, N377–N386 (2008). doi:10.1088/0031-9155/53/20/N01
3. V. Manjunathaguru, T.K. Umesh, Simple parametrization of photon mass energy absorption coefficients of H-, C-, N- and O-based samples of biological interest in the energy range 200–1500 keV. Pramana **72**, 375–387 (2009). doi:10.1007/s12043-009-0033-8
4. A.M. El-Khayatt, İ. Akkurt, Photon interaction, energy absorption and neutron removal cross section of concrete including marble. Ann. Nucl. Energy **60**, 8–14 (2013). doi:10.1016/j.anucene.2013.04.021
5. L. Gerward, N. Guilbert, K. Bjorn Jensen et al., X-ray absorption in matter. Reengineering XCOM. Radiat. Phys. Chem. **60**, 23–24 (2001). doi:10.1016/S0969-806X(00)00324-8
6. M.J. Berger, J.H. Hubbell, XCOM: Photon Cross Sections on a Personal Computer NBSIR 87-3597 (1987). http://www.iaea.org/inis/collection/NCLCollectionStore/_Public/19/009/19009871.pdf
7. R. Nowotny, XMuDat: Photon Attenuation Data on PC, in IAEA-NDS-195 (1998). http://www.iaea.org/inis/collection/NCLCollectionStore/_Public/30/022/30022813.pdf
8. A.M. El-Khayatt, NXcom—a program for calculating attenuation coefficients of fast neutrons and gamma-rays. Ann. Nucl. Energy **38**, 128–132 (2011). doi:10.1016/j.anucene.2010.08.003
9. T.K. Kumar, K.V. Reddy, Effective atomic numbers for materials of dosimetric interest. Radiat. Phys. Chem. **50**, 545–553 (1997). doi:10.1016/S0969-806X(97)00089-3
10. H. Singh, K. Singh, G. Sharma et al., Barium and calcium borate glasses as shielding materials for X-rays and gamma-rays. Phys. Chem. Glasses Eur. J. Glass Sci. Technol. Part B **44**, 5–8 (2003)
11. H. Singh, K. Singh, L. Gerward et al., ZnO–PbO–B_2O_3 glasses as gamma-ray shielding materials. Nucl. Instrum. Methods Phys. Res. Sect. B **207**, 257–262 (2003). doi:10.1016/S0168-583X(03)00462-2
12. K. Singh, H. Singh, G. Sharma et al., Gamma-ray shielding properties of CaO–SrO–B_2O_3 glasses. Radiat. Phys. Chem. **72**, 225–228 (2005). doi:10.1016/j.radphyschem.2003.11.010
13. I. Akkurt, A.M. El-Khayatt, Effective atomic number and electron density of marble concrete. J. Radioanal. Nucl. Chem. **295**, 633–638 (2013). doi:10.1007/s10967-012-2111-5
14. V.P. Singh, N.M. Badiger, N. Kucuk, Determination of effective atomic numbers using different methods for some low-Z materials. J. Nucl. Chem. (2014). doi:10.1155/2014/725629
15. R. Shivaramu, L. Vijayakumar, N. Rajasekaran, Ramamurthy, effective atomic numbers for photon energy absorption of some low-Z substances of dosimetric interest. Radiat. Phys. Chem. **62**, 371–377 (2001). doi:10.1016/S0969-806X(01)00221-3
16. V.P. Singh, N.M. Badiger, Effective atomic numbers of some tissue substitutes by different methods: a comparative study. J. Med. Phys. **39**, 24–31 (2014). doi:10.4103/0971-6203.125489
17. H.P. Schätzler, Basic aspects on the use of elastic and inelastic scattered gamma radiation for the determination of binary systems with effective atomic numbers of less than 10. Int. J. Appl. Radiat. Isot. **30**, 115–121 (1979). doi:10.1016/0020-708X(79)90143-1
18. S. Manninen, T. Pitkänen, S. Koikkalainen et al., Study of the ratio of elastic to inelastic scattering of photons. Int. J. Appl. Radiat. Isot. **35**, 93–98 (1984). doi:10.1016/0020-708X(84)90190-X
19. P. Duvauchelle, G. Peix, D. Babot, Effective atomic number in the Rayleigh to Compton scattering ratio. Nucl. Instrum. Methods Phys. Res. Sect. B **155**, 221–228 (1999). doi:10.1016/S0168-583X(99)00450-4
20. P. Duvauchelle, G. Peix, D. Babot, Rayleigh to Compton ratio computed tomography using synchrotron radiation. NDT E Int. **33**, 23–31 (2000). doi:10.1016/S0963-8695(99)00014-6
21. O. İçelli, Z. Yalçın, M. Okutan et al., Determination of photon energy absorption parameters for pellet waste, trommel sieve waste and original tincalconite. Ann. Nucl. Energy **47**, 38–45 (2012). doi:10.1016/j.anucene.2012.03.028
22. J.H. Hubbell, W.J. Veigele, E.A. Briggs et al., Atomic form factors, incoherent scattering functions, and photon scattering cross sections. J. Phys. Chem. Ref. Data **4**, 471–538 (1975). doi:10.1063/1.555523
23. F.H. Attix, W.C. Roesch, E. Tochilin, *Radiation Dosimetry*, 2nd edn. (Academic Press, New York, 1968). doi:10.1016/B978-0-12-066401-6.50001-4
24. B. Williams, *Compton Scattering. The Investigation of Electron Momentum Distribution* (McGraw-Hill Inc., London, 1977)
25. M. Antoniassi, A.L.C. Conceição, M.E. Poletti, Study of effective atomic number of breast tissues determined using the elastic to inelastic scattering ratio. Nucl. Instrum. Methods Phys. Res. Sect. A **652**, 739–743 (2011). doi:10.1016/j.nima.2010.09.110
26. L.S. Del Lama, L.D.H. Soares, M. Antoniassi et al., Effective atomic numbers for materials of medical interest at low photon energy using the Rayleigh to Compton scattering ratio. Nucl. Instrum. Methods Phys. Res. Sect. A **784**, 597–601 (2015). doi:10.1016/j.nima.2014.12.046
27. M.P. Singh, B.S. Sandhu, B. Singh, Measurement of effective atomic number of composite materials using scattering of γ-rays. Nucl. Instrum. Methods Phys. Res. Sect. A **580**, 50–53 (2007). doi:10.1016/j.nima.2007.05.037
28. M.P. Singh, A. Sharma, B. Singh et al., A non-destructive technique for assigning effective atomic number to scientific samples by scattering of 59.54 keV gamma photons. Nucl. Instrum. Methods Phys. Res. Sect. A **619**, 63–66 (2010). doi:10.1016/j.nima.2010.01.012
29. O. Içelli, Practical method for experimental effective atomic number in the coherent to Compton scattering ratio. J. Quant. Spectrosc. Radiat. Transf. **101**, 151–158 (2006). doi:10.1016/j.jqsrt.2005.11.014
30. A.E.M. Khater, Y.Y. Ebaid, A simplified gamma-ray self-attenuation correction in bulk samples. Appl. Radiat. Isot. **66**, 407–413 (2008). doi:10.1016/j.apradiso.2007.10.007
31. O. Içelli, S. Erzeneoğlu, Experimental study on ratios of coherent scattering to Compton scattering for elements with atomic numbers $26 \leq Z \leq 82$ in 59.5 keV for 55° and 115°. Spectrochim. Acta Part B At. Spectrosc. **57**, 1317–1323 (2002). doi:10.1016/S0584-8547(02)00050-2
32. J.H. Hubbell, S.M. Seltzer, Tables of X-ray Mass Attenuation Coefficients and Mass Energy-Absorption Coefficients (Version 1.4) (2004). http://physics.nist.gov/xaamdi

33. M.A. Abdel-Rahman, N. Kamel, Measurement of coherent plus incoherent differential scattering cross section of 59.54 keV γ-ray from anthracene and POPOP. Nucl. Instrum. Methods Phys. Res. Sect. A **416**, 64–69 (1998). doi:10.1016/S0168-9002(98)00652-4
34. B. Akça, S.Z. Erzeneoğlu, The mass attenuation coefficients, electronic, atomic, and molecular cross sections, effective atomic numbers, and electron densities for compounds of some biomedically important elements at 59.5 keV. Sci. Technol. Nucl. Install. (2014). doi:10.1155/2014/901465