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Effective atomic numbers of some H-, C-, N- and O-based composite materials derived from differential incoherent scattering cross-sections

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Abstract. In this work, we have made an effort to determine whether the effective atomic numbers of H-, C-, N- and O-based composite materials would indeed remain a constant over the energy grid of 280–1200 keV wherein incoherent scattering dominates their interaction with photons. For this purpose, the differential incoherent scattering cross-sections of Be, C, Mg, Al, Ca and Ti were measured for three scattering angles 60°, 80° and 100° at 279.1, 661.6 and 1115.5 keV using which an expression for the effective atomic number was derived. The differential incoherent scattering cross-sections of the composite materials of interest measured at these three angles in the same set-up and substituted in this expression would yield their effective atomic number at the three energies. Results obtained in this manner for bakelite, nylon, epoxy, teflon, perspex and some sugars, fatty acids as well as amino acids agreed to within 2% of some of the other available values. It was also observed that for each of these samples, Z_{eff} was almost a constant at the three energies which unambiguously justified the conclusions drawn by other authors earlier [Manjunathaguru and Umesh, *J. Phys. B: At. Mol. Opt. Phys.* **39**, 3969 (2006); Manohara *et al*, *Nucl. Instrum. Methods* **B266**, 3906 (2008); Manohara *et al* *Phys. Med. Biol.* **53**, M377 (2008)] based on total interaction cross-sections in the energy grid of interest.

Keywords. Differential incoherent scattering cross-sections; effective atomic number; average atomic number; composite materials.

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1. Introduction

Recently, in our laboratory [1,2], the effective atomic numbers of several H-, C-, N- and O-based samples were determined by a method which employs the measured total interaction cross-sections in the energy region 5–1500 keV. One of the findings of this work [1] was that the photon interaction of low Z composite materials such as H-, C-, N- and O-based samples in the energy region 200–1500 keV was characterized by an average atomic number which was energy-independent but

composition-dependent. This could be attributed to the fact that such samples would essentially behave as pure incoherent scatterers.

In a recent work by Gerward group (Manohara *et al* [3,4]), it has been suggested that at intermediate energies (0.05 MeV $< E <$ 5 MeV), Z_{eff} of most of the composite materials such as fatty acids and carbohydrates would be constant and energy independent because incoherent or Compton scattering practically accounts for all photon interactions with low Z composite materials. Since most of the samples of biological interest (particularly the H-, C-, N- and O-based) are of low Z, it will be practically very useful to represent them by an average atomic number during applications of radiation dosimetry. In view of the above, we felt it worthwhile to verify these recent conclusions [1,3,4] by determining the effective atomic number of any such H-, C-, N- and O-based composite material by making use of their differential incoherent scattering cross-sections at some typical energies in the above energy grid and then studying the energy dependence. However, for this purpose, we must choose only such scattering angles (momentum transfer q) at which the incoherent scattering function $S(q, Z)$ to a very good approximation equals the atomic number Z pointing to negligible electron binding effects. With this in view, we have experimentally measured the differential incoherent scattering cross-sections at three scattering angles 60°, 80° and 100° for three incident photon energies, viz., 279.1, 661.6 and 1115.5 keV for beryllium, carbon, magnesium, aluminum, calcium and titanium as well as for fourteen H-, C-, N- and O-based composite materials. The measured incoherent scattering cross-sections have been further used to evaluate Z_{eff} of these composite materials by a novel method.

2. Experimental procedure

In this method, first the differential incoherent scattering cross-sections of Be, C, Mg, Al, Ca and Ti, composite materials such as bakelite, perspex, nylon, epoxy, teflon and sugars like glucose, melibiose and raffinose, fatty acids like lauric acid, myristic acid and palmitic acid and amino acids like alanine, leucine and tryptophan were measured at three scattering angles 60°, 80° and 100° on a goniometer assembly for 661.6 keV energy γ-rays emitted by ^{137}Cs source which was procured in the form of a radiographic capsule from M/S Amersham, U.K. A schematic diagram of the experimental set-up is shown in figure 1. The well-collimated beam of photons from the source S was made to fall on the target T mounted on the target holder. The detector D received the scattered γ-rays. The γ-ray beam was properly shielded by lead throughout its journey from the source to the detector and care was taken to minimize the background radiation. An ORTEC model 23210 gamma-x high purity germanium detector has been used to record the data along with a personal computer-based multichannel analyzer. The counts under the peak were determined accurately after subtracting the background counts by applying Gaussian fitting. The entire experiment was carried out in an air-conditioned room wherein the mains' voltage was stabilized in order to minimize the channel drift. The thickness of the elemental samples, which were in the form of thin cylinders of uniform thickness, ranged from 9 to 14 g/cm^2. The thickness of the composite materials ranged from 39 to 42 g/cm^2, while the purity of the samples was better than 99.9% as mentioned by the suppliers.

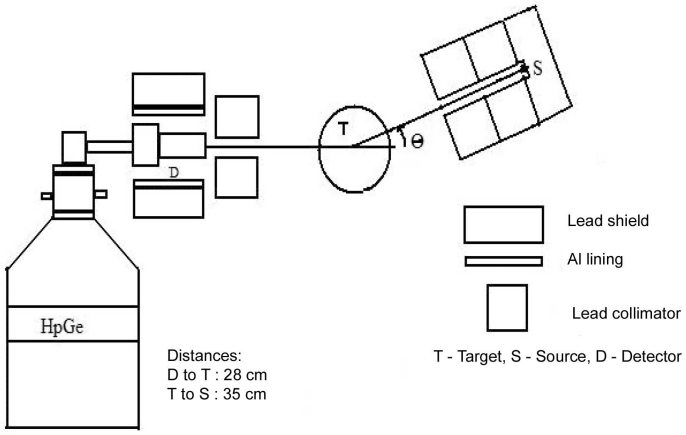

Figure 1. Schematic diagram of the experimental set-up.

In the present measurements, although the mass per unit area of the composite material samples were 3–4 times more than that of the elemental samples, care was taken to maintain the same diameter for all the cylindrical sample containers. They differed only in their heights. Therefore, the angle of acceptance was almost the same in each measurement. It may be argued that multiple scattering of photons occurs whenever thick samples are used because such samples offer a larger mean free path for the incident photons to scatter and rescatter inside the target material. Thus, the multiple scattering can result in energy degraded photons which may contribute to the lower energy side of the photopeak thus overestimating the scattered intensity. However, in the present study, the intensity under the scattered peak was determined from the background subtracted scattered photopeak by a suitable peak fitting routine. Also, a high resolution detector as well as low Z targets of optimum thickness were employed. Hence, it is felt that the multiple scattering effects were negligible during the present study.

The experiment was then repeated with the ^{203}Hg and ^{65}Zn sources, which emit 279.1 and 1115.5 keV γ-rays respectively. These two sources were procured in the form of radiographic capsules from the Bhabha Atomic Research Centre, Mumbai, India. The error analysis and the evaluation of differential incoherent scattering cross-sections of the experimental samples were performed by following a procedure similar to an earlier work carried out in our laboratory [5]. It was estimated that the errors in the present work were expected to impart an uncertainty to the extent of 2–3% of the measured values. The measured cross-sections of composite materials are listed in table 1.

3. Results and discussion

To evaluate the effective atomic number, the measured differential incoherent scattering cross-sections, σ_i, of the elements were plotted vs. their atomic number Z. This was done separately at all the three scattering angles (momentum transfers)

Table 1. Differential incoherent scattering cross-sections σ_i (millibarn/atom/steradians), mol. wt, A (in g), A_{eff} (in g) and Z_{eff} of composite materials.

		$\theta = 60^\circ$			$\theta = 80^\circ$			$\theta = 100^\circ$			
Composite material	Mol. weight A and A_{eff}	279.1 keV	661.6 keV	1115.5 keV	279.1 keV	661.6 keV	1115.5 keV	279.1 keV	661.6 keV	1115.5 keV	Mean Z_{eff}
Bakelite	330.37[a]	127.1[c]	84.1[c]	67.6[c]	87.3[c]	58.2[c]	47.4[c]	75.3[c]	47.8[c]	36.8[c]	4.1[e]
$C_{22}H_{18}O_3$	7.68[b]	4.0[d]	3.9[d]	3.9[d]	3.9[d]	4.0[d]	3.9[d]	4.0[d]	4.3[d]	4.0[d]	4.0[f]
Nylon	113.17[a]	98.5[c]	64.5[c]	52.3[c]	65.9[c]	44.4[c]	36.7[c]	56.6[c]	36.5[c]	28.5[c]	3.2[e]
$C_6H_{11}NO$	5.96[b]	3.1[d]	2.9[d]	2.9[d]	3.0[d]	3.1[d]	3.0[d]	3.1[d]	3.3[d]	3.1[d]	3.1[f]
Teflon	100.02[a]	282.4[c]	184.5[c]	146.6[c]	193.8[c]	128.1[c]	102.8[c]	165.5[c]	106.0[c]	79.8[c]	8.9[e]
C_2F_4	16.7[b]	8.9[d]	8.6[d]	8.5[d]	8.5[d]	8.9[d]	8.7[d]	8.6[d]	8.9[d]	8.7[d]	8.8[f]
Epoxy	284.35[a]	115.6[c]	75.7[c]	61.1[c]	78.5[c]	52.2[c]	42.8[c]	66.8[c]	43.0[c]	33.3[c]	3.7[e]
$C_{18}H_{20}O_3$	6.94[b]	3.6[d]	3.5[d]	3.4[d]	3.5[d]	3.6[d]	3.5[d]	3.6[d]	3.7[d]	3.6[d]	3.6[f]
Perspex	100.12[a]	113.3[c]	73.6[c]	59.4[c]	76.4[c]	50.7[c]	41.7[c]	64.9[c]	41.8[c]	32.4[c]	3.6[e]
$C_5H_8O_2$	6.67[b]	3.6[d]	3.4[d]	3.3[d]	3.4[d]	3.5[d]	3.4[d]	3.5[d]	3.6[d]	3.5[d]	3.5[f]

Glucose	180.14[a]	124.1[c]	82.0[c]	66.5[c]	86.5[c]	56.6[c]	46.7[c]	73.5[c]	46.6[c]	36.2[c]	4.0[e]
$C_6H_{12}O_6$	7.51[b]	3.9[d]	3.9[d]	3.8[d]	3.8[d]	3.9[d]	3.8[d]	3.9[d]	4.0[d]	3.9[d]	3.9[f]
Melibiose	342.30[a]	123.7[c]	84.1[c]	67.3[c]	87.3[c]	58.1[c]	47.2[c]	74.4[c]	47.8[c]	36.4[c]	4.1[e]
$C_{12}H_{22}O_{11}$	7.61[b]	3.9[d]	3.9[d]	3.8[d]	3.9[d]	4.0[d]	3.9[d]	4.0[d]	4.1[d]	4.0[d]	4.0[f]
Raffinose	594.50[a]	120.3[c]	80.7[c]	64.9[c]	83.5[c]	55.7[c]	45.5[c]	70.2[c]	45.9[c]	35.3[c]	3.9[e]
$C_{18}H_{32}O_{16}{\cdot}5H_2O$	7.34[b]	3.8[d]	3.7[d]	3.6[d]	3.7[d]	3.9[d]	3.8[d]	3.8[d]	4.0[d]	3.8[d]	3.8[f]
Lauric acid	200.32[a]	82.1[c]	57.2[c]	47.0[c]	57.6[c]	39.3[c]	33.0[c]	48.9[c]	31.3[c]	25.6[c]	2.8[e]
$C_{12}H_{24}O_2$	5.27[b]	2.6[d]	2.6[d]	2.5[d]	2.6[d]	2.7[d]	2.6[d]	2.8[d]	2.9[d]	2.8[d]	2.7[f]
Myristic acid	228.38[a]	80.1[c]	56.3[c]	46.2[c]	56.3[c]	38.7[c]	32.4[c]	47.7[c]	31.8[c]	25.2[c]	2.7[e]
$C_{14}H_{28}O_2$	5.19[b]	2.5[d]	2.5[d]	2.5[d]	2.6[d]	2.7[d]	2.6[d]	2.7[d]	2.8[d]	2.7[d]	2.6[f]
Palmitic acid	256.43[a]	80.2[c]	55.5[c]	45.4[c]	55.0[c]	38.1[c]	31.8[c]	47.2[c]	30.3[c]	24.7[c]	2.7[e]
$C_{16}H_{32}O_2$	5.13[b]	2.5[d]	2.5[d]	2.4[d]	2.6[d]	2.6[d]	2.5[d]	2.7[d]	2.7[d]	2.7[d]	2.6[f]
Alanine	89.10[a]	112.9[c]	74.6[c]	60.9[c]	76.8[c]	51.6[c]	42.7[c]	65.3[c]	42.5[c]	33.2[c]	3.7[e]
$C_3H_7NO_2$	6.85[b]	3.6[d]	3.4[d]	3.4[d]	3.4[d]	3.6[d]	3.5[d]	3.6[d]	3.7[d]	3.6[d]	3.6[f]
Leucine	131.20[a]	95.6[c]	64.8[c]	52.7[c]	65.8[c]	44.6[c]	36.9[c]	55.7[c]	36.7[c]	28.7[c]	3.2[e]
$C_6H_{13}NO_2$	5.96[b]	3.0[d]	2.9[d]	2.9[d]	3.0[d]	3.1[d]	3.0[d]	3.1[d]	3.2[d]	3.1[d]	3.1[f]
Tryptophan	204.20[a]	124.0[c]	83.2[c]	66.5[c]	86.8[c]	57.5[c]	46.7[c]	74.1[c]	47.4[c]	36.2[c]	4.0[e]
$C_{11}H_{12}N_2O_2$	7.56[b]	3.9[d]	3.9[d]	3.8[d]	3.8[d]	4.0[d]	3.9[d]	3.9[d]	4.0[d]	3.9[d]	3.9[f]

[a]Molecular weight, [b]A_{eff}, [c]differential incoherent scattering cross-sections, [d]Z_{eff} (present values), [e]mean Z_{eff} (ref. [1]), [f]mean Z_{eff} (present values).

Table 2. Best-fit values of the coefficients used in eq. (1) with uncertainties, χ^2 and standard deviation (number of data points used = 6).

Energy (keV)	Scattering angle	Coefficient		χ^2	Standard deviation
		m_i	Error		
279.1	60°	31.643	0.008	1.000	0.301
	80°	22.182	0.007	1.000	0.275
	100°	19.000	0.000	1.000	0.000
661.6	60°	21.407	0.007	1.000	0.337
	80°	14.236	0.007	1.000	0.254
	100°	11.907	0.008	0.999	0.286
1115.5	60°	16.907	0.008	1.000	0.286
	80°	10.854	0.008	0.999	0.309
	100°	08.966	0.009	0.999	0.342

and the three energies of interest. These angles were chosen because at the momentum transfers corresponding to these scattering angles the incoherent scattering function $S(q, Z)$ to a good approximation equalled the Z values at the energy of interest due to minimum electron binding effects in the atom. This would also mean that the scattering at these momentum transfers was almost like incoherent scattering by free electrons. A typical plot obtained at 661.6 keV is shown in figure 2. It was noticed that the measured elemental cross-sections were in good agreement with the interpolated theoretical values of Hubbell *et al* [6] and Kahane [7] at all the three scattering angles (momentum transfers) and the three energies of interest.

It was observed that the plots were straight lines (passing through origin) at all the three scattering angles for all the three incident energies. Hence we could construct relations of the form

$$\sigma_i = m_i Z, \tag{1}$$

where σ_i are the measured differential scattering cross-sections in millibarn/steradian/atom, m_i are the slopes determined at the three scattering angles, θ. Here $i = 1, 2$ and 3 represent $\theta = 60°$, 80° and 100° respectively. Further, a suitable linear regression analysis was performed and the best-fit values of m_i were determined. These coefficients are shown in table 2 along with the corresponding uncertainties, χ^2, standard deviation and the actual number of data points used. The errors shown in table 2 on m are those incurred during the fitting procedure (as indicated in the script window of the ORIGIN software used for the purpose).

Equation (1) can be rewritten as

$$Z_{\text{eff}} = \frac{\sigma_i}{m_i}. \tag{2}$$

Here, $Z_{\text{eff}} = Z$, for a pure element and for a composite material it is the effective atomic number.

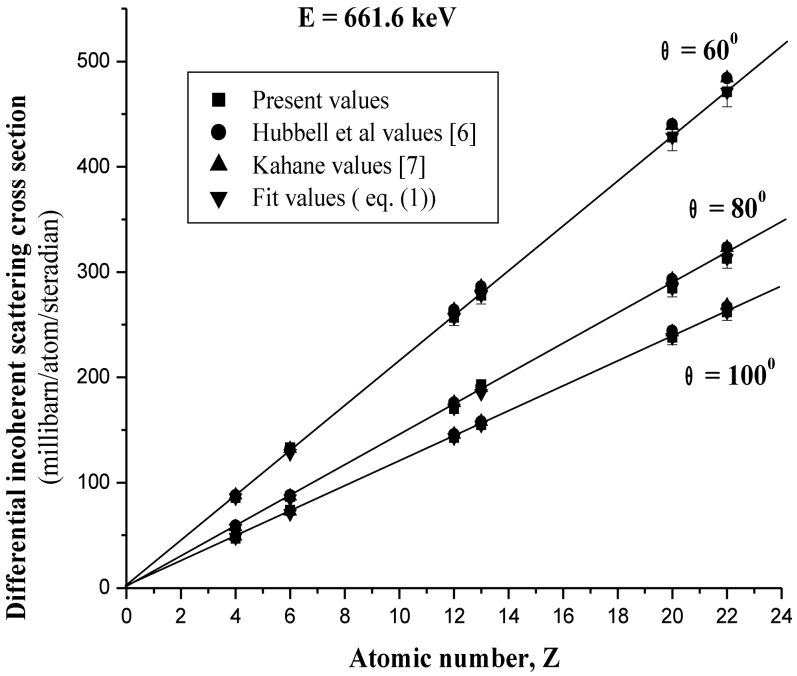

Figure 2. Typical plot of differential incoherent scattering cross-sections of elements in millibarn/atom/steradian vs. atomic number Z measured at 661.6 keV.

The advantage of eq. (2) is that it can be used to calculate Z_{eff} of any sample from its differential incoherent scattering cross-sections measured at any angle in the range 60°–100° for any incident photon energy (keV) in the range 279.2–1115.5 keV. The measured differential incoherent scattering cross-sections of the composite materials shown in table 1 were used in eq. (2) and Z_{eff} values for the composite materials were calculated. These values are also listed in table 1. It can be observed from table 1 that Z_{eff} values for a composite material remain almost constant at the three angles and energies identical to the case of elements. Hence the mean value $Z_{\text{eff}}^{\text{mean}}$ was calculated for each sample. While $Z_{\text{eff}}^{\text{mean}}$ values for palmitic acid and myristic acid were the lowest (2.6), teflon showed the highest value of 8.8. Hence, we can conclude that all the composite materials studied in the present work were low Z materials.

Further, the effective atomic weight, A_{eff}, which is simply the molecular weight divided by the total number of all types of atoms present in it, was also calculated (table 1). The mean value $Z_{\text{eff}}^{\text{mean}}$ was then plotted vs. the effective atomic weight A_{eff} of the composite materials (figure 3). The plot was a straight line passing through the origin (0,0). The best-fit value of the slope was found to be nearly 0.522. This was within 2% of the value of 0.533 reported by two of the present authors in a recently published work which used data on total attenuation cross-sections [1]. Since the present values were based on incoherent scattering cross-sections and the other values used for comparison [1] were based on total attenuation cross-sections,

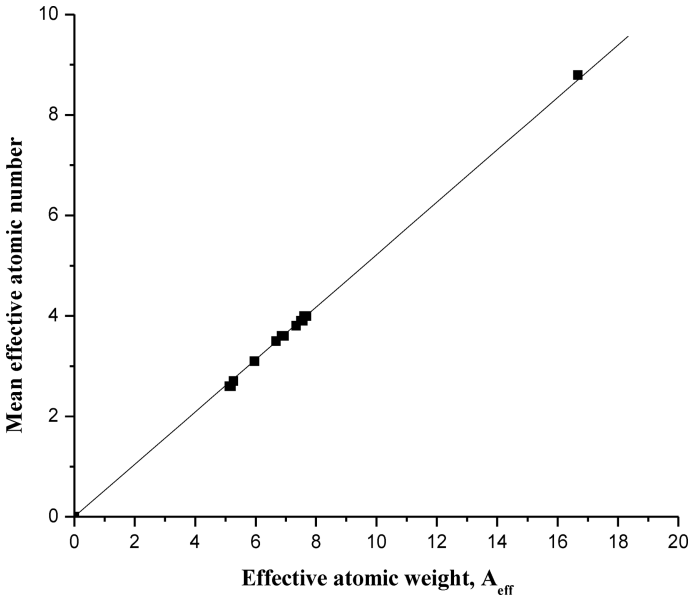

Figure 3. Plot of mean effective atomic number vs. effective atomic weight of samples.

it is clear that the low Z composite materials of present interest were essentially pure incoherent scatterers.

4. Conclusions

Thus, the results obtained in the present work have justified the contention of the earlier reports [1,3,4] that low Z composite materials behave as pure incoherent scatterers and hence such samples can indeed be represented by an average (single) energy-independent but composition-dependent effective atomic number at least in the energy grid of 280–1200 keV.

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