Effect of EXAFS on the dosimetric related parameters

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ABSTRACT

Mass attenuation coefficients have been measured for rare earth compounds at photon energies 8.041, 8.907 and 13.347 keV. The measured values are compared with theoretical calculations. The agreement between experiment and theory is more than the experimental error when the incident photon energy is around the edge of the element present in the compound and agreeing with the theoretical values elsewhere. The difference in agreement between the theoretical values and experimental values is attributed to the EXAFS effects on the mass attenuation coefficient values.

Keywords: Mass Attenuation Coefficient;
Near Absorption Edge; Cross Section;
Resonance Raman Scattering; EXAFS

1. INTRODUCTION

In medical physics, it is important to measure the amount of radiation delivered by the ionizing radiation, in composite substances. For photon interactions in composite substances a single number cannot represent the atomic number uniquely across the entire energy region. This number in composite substances is called the effective atomic number and it varies with energy and is denoted here by Z_{eff}. On the other hand, the concept of z-dependence of photon attenuation has led to many applications in radiation studies. For example precise knowledge of effective atomic numbers is very important in medical radiation dosimetry and medical imaging, where the cross-sectional anatomy is generated by computer-assisted tomography (CAT) scans [1]. It is a common practice to verify the validity of calculation algorithms by comparing the generated doses with the measured doses in tissue equivalent phantom substances. Similarly, tissue-equivalent phantoms are specifically designed to study the image quality and performance of the CAT scanners. In both instances, a precise knowledge of the effective atomic number and electron density

of the composite substances is necessary in the low energy region and have proved to be a convenient parameter for interpretation of x-ray attenuation by a complex medium like a biological tissue and particularly for the calculation of dose in radiography and radiation dosimetry etc.

The x-ray mass attenuation coefficient, μ/ρ, for any material are usually estimated from Bragg's additivity law or more commonly called mixture rule. Thus μ/ρ for any chemical compound/material is given by

$$\mu/\rho = \sum \omega_i (\mu/\rho)_i,$$

where $(\mu/\rho)_i$ is the mass attenuation coefficient of the ith element and ω_i is the fraction by weight of the ith element. For a compound/material with chemical formula $(Z_1)_{a1}, (Z_2)_{a2}, \cdots, (Z_n)_{an}$ the weight factor for the ith element is given by

$$\omega_i = \left\{ (a_i A_i)/(\sum a_i A_i) \right\},$$

where A_i is the atomic weight of the ith element. Hence an attempt has been in this regard to determine the μ/ρ of x-rays for the dosimetric materials (sulphides of Mg, Ca, Mn Fe and Zn elements) and then determined the Z_{eff} of these materials by LSF method from $\ln(\mu/\rho)$ Vs $\ln Z$ graph. These values are compared with the theoretical values. The so determined value of Z_{eff} has been used in the expression

$$N_e = N_A Z_{eff} \sum n_i / A$$

to calculate the electron density.

In the present measurement the validity of Bragg's law is studied for rare earths compounds of L edges. The selection of the compounds was dictated by the incident photon energy and the by the limitations of our experimental facilities such that thin foils from the compounds. The former factor determined the region of the atomic numbers, wherein the absorption edges energy are close to the incident photon energy, and the latter determined the selection of particular compounds in this region. We have used ^{241}Am (VEC) radioactive x-ray source with weighted average energy of K_α of 8.041 and 13.347 keV energy respectively and the compounds of rare earths

having the elements in the region $57 \leq Z \leq 70$.

2. EXPERIMENTAL ARRANGEMENT

The good-geometry experimental arrangement used for the determination of the mass attenuation coefficient is similar to the one described in detail by us earlier [2]; and is shown in **Figure 1**. Briefly, photons from a variable energy x-ray source S passed through a collimator C1 and were incident on the specimen A in the form of a thin foil kept normal to the photon beam. The transmitted beam passed through another collimator C2 and reached a HPGe x-ray detector system D. The transmitted photon spectrum was recorded using a PC based multichannel analyzer.

The collimators C1 and C2 were 40 mm thick lead discs that collimated respectively the incident and transmitted beam to 6 mm dia. The scatter acceptance angle equal to the sum of the incident beam divergence and acceptance angle at the detector is found to be $\leq 3°$ degrees. This thickness of the collimator would reduce the intensity of scattered photons of 300 keV by a factor of 10^{7}.

The variable energy x-ray source consisted of 10 mCi (370 MBq) ^{241}Am as the primary source of excitation radiation Copper and Rubidium targets were selected to produce fluorescence x-ray with characteristic energy of the target *i.e.*, 8.041 and 13.347 keV. The inner bremsstrahlung intensity was found to be negligible compared to the x-ray intensity in the region of interest. No noticeable impurities were found in the source spectra.

The Dosimetric compounds viz., rare earth sulphate compounds of 99.5% purity were obtained from SD fine chemicals Mumbai, India. The Dosimetric samples of required thickness in the range of 10 to 30 mg/cm^{2} were prepared by using blotting paper technique. The area density (mass per unit area) of each foil sample was determined by weighing it using a single pan electronic balance with an accuracy of 0.01 mg and measuring its dimensions using a traveling microscope with an accuracy of 0.001 cm. Thus the measured areal density expressed in mg/cm^{2} had an uncertainty.

The x-ray spectrometer consist of an n-type x-ray detector of area 500 mm^{2} × 100 mm thick High Purity Germanium detector connected to DSA-1000 16K MCA. The spectrometer was operated by Genie 2000 software. The detector is connected directly to a preamplifier through a cooled FET device, and mounted over a rigid cryostat with Dewar to accommodate the liquid Nitrogen. DSA-1000 allows independent of rise time and flat top selection, which optimizes the performance of the detector, spectral energy, count rate and resolution. HPGe detector along with DSA-1000 has resulted with a resolution of 191 eV at 5.895 keV as against 200 eV by the
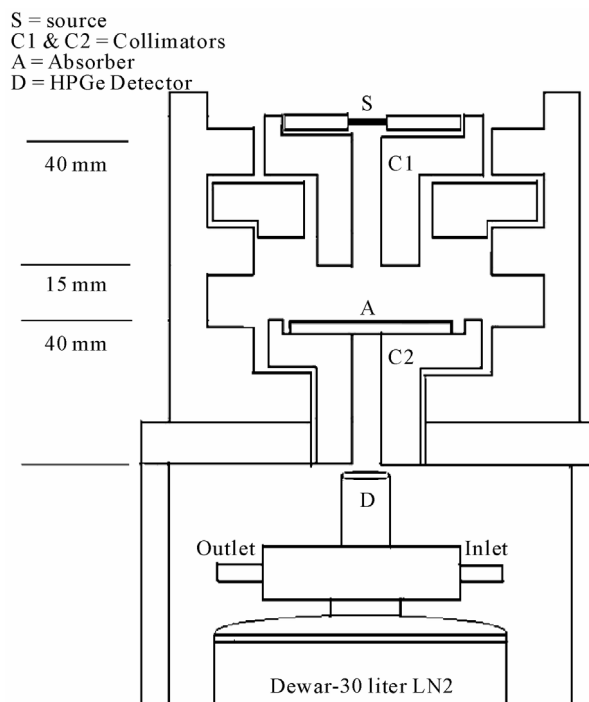

Figure 1. Experimental arrangement.

manufacturers.

The advantage of the high resolution HPGe detector system is its wide operating energy range from 3 keV to 500keV and very good energy resolution, ^{241}Am source with different target the photo peaks of K_{α} and K_{β} of were well resolved. As a result of this, the energies of the photons with degrade in energy due to small angle scattering and multiple scattering, if at all present, could be observed in the source spectrum, but in the present case no such degraded photo peak were observed except the K_{β} and K_{β} and gamma photons of ^{241}Am source. Therefore, μ/ρ value obtained in such configuration is purely corresponding to the respective energies only *i.e.*, K_{α} and K_{β} gamma-rays.

The error involved in each measurement is taken care by following the procedure counting time conditions as stated in [3]; viz., background to signal background to foil thickness and signal to foil thickness, systematic errors due to the detection of forward scattered radiation, beam hardening when higher atomic number absorber is used. Ray-sum method has been adopted in the present measurement for calculation for the random errors which arises from all aspects of the measurement, further is has also suggested a method for the calculation called the ray-sum error. In the present measurements ray-sum method is applied to all the observation since the random errors arises from all aspects of measurement, in the exponential law of attenuation. The errors are calculated by using the formula provided by [4]; and are presented in

the tables.

No dead time corrections are found for photon intensity measurements considered area under photopeak. However, in the present case we have selected the live time of the MCA for sources. With these conditions, the transmitted intensity of x-rays for various combinations of specimen thickness is recorded and corrected for background intensity [5,6]. A plot of logarithm of transmission as a function of specimen thickness yielded a straight line for the entire transmission region, verifying the validity of the Beer-Lambert's law. This is confirmed for different materials also.

3. RESULTS AND DISCUSSION

The plots of the logarithm of transmitted intensity versus specimen thickness were linear for all the samples and the μ/ρ was obtained from the plots by linear regression over the 50% - 2% transmission range [7]. The μ/ρ obtained for the all dosimetric compounds at three different photon energies are presented in **Table 1**.

The theoretical estimated errors are between 1% and 2% taken from the WinXCom. The error involved in over all experimental values is about 2% to 3% for the dosimetric samples.

In **Table 1** the second column represent L shell Bind-

ing energies E_L of the element present in the compound, third column represents difference, $(E_x − E_L)$ between the incident photon energy E_x (viz., 8.041, 8.907 and 13.347 keV) and L shell binding energy E_L. The fourth column represents experimental μ/ρ value, fifth column represents theoretical μ/ρ value (WinXom), and the percentage difference (PD) between experiment and theory is given in the last column of the table. The positive and negative sign indicates that the interested element L shell binding energy is above or below the incident photon energy, and the binding energies are taken from Kortright *et al.* [8].

Further from **Table 1**, there is a good agreement between theoretical and experimental value for all the compounds at 13.347 keV, it is confirmed fact that when the incident photon energy is far away from the absorption edge, there is good agreement between experimental value with theoretical value within 4%. On the other hand, the same mixture rule can't be applicable for Neodymium and Europium sulphate with E_x-E_L ranging from 0.915 to 0.429. Here, the experimental value deviates from the theoretical value by −7.7% and −16.2% and next, in case of Europium and Terbium sulphate at 8.907 keV with E_x-E_L in range from 1.295 and 0.655 keV for L edge shows a deviation in the mass attenuation

Table 1. Experimental and theoretical mass attenuation coefficient.

Name of the Sample	E_L binding energy in keV	$\Delta E = E_x − E_L$ (keV)	Mass attenuation coefficient (cm^2/kg)		P.D in %
			Expt. value	*WinXcom*	
E_x = 8.041 keV					
$Nd_2(SO_4)_3 \cdot 8H_2O$	7.126	0.915	165.3 ± 1.7	179.2	−7.7
$Eu_2(SO_4)_3 \cdot 8H_2O$	7.612	0.429	150.5 ± 1.5	179.6	−16.2
$Tb_2(SO_4)_3 \cdot 8H_2O$	8.252	−0.211	152.8 ± 1.6	147.8	+3.3
$Yb_2(SO_4)_3 \cdot 8H_2O$	9.978	−1.937	80.32 ± 0.9	79.62	+0.8
E_x = 8.907 keV					
$Nd_2(SO_4)_3 \cdot H_2O$	7.126	1.781	140.2 ± 1.6	137.2	+2.2
$Eu_2(SO_4)_3 \cdot H_2O$	7.612	1.295	168.4 ± 1.8	157.8	+6.7
$Tb_2(SO_4)_3 \cdot H_2O$	8.252	0.655	193.4 ± 2.0	171.6	+12.7
$Yb_2(SO_4)_3 \cdot H_2O$	9.978	−1.071	59.76 ± 0.8	60.97	−1.6
E_x = 13.347 keV					
$Nd_2(SO_4)_3 \cdot H_2O$	7.126	6.221	47.21 ± 0.5	46.89	+0.8
$Eu_2(SO_4)_3 \cdot H_2O$	7.612	5.735	55.43 ± 0.6	54.62	+1.5
$Tb_2(SO_4)_3 \cdot H_2O$	8.252	5.095	59.01 ± 0.7	59.84	−1.3
$Yb_2(SO_4)_3 \cdot H_2O$	9.978	3.369	75.23 ± 0.6	74.81	+0.5

PD = Percent difference = [(Experimental mean μ/ρ − Computed μ/ρ)/Computed μ/ρ] × 100
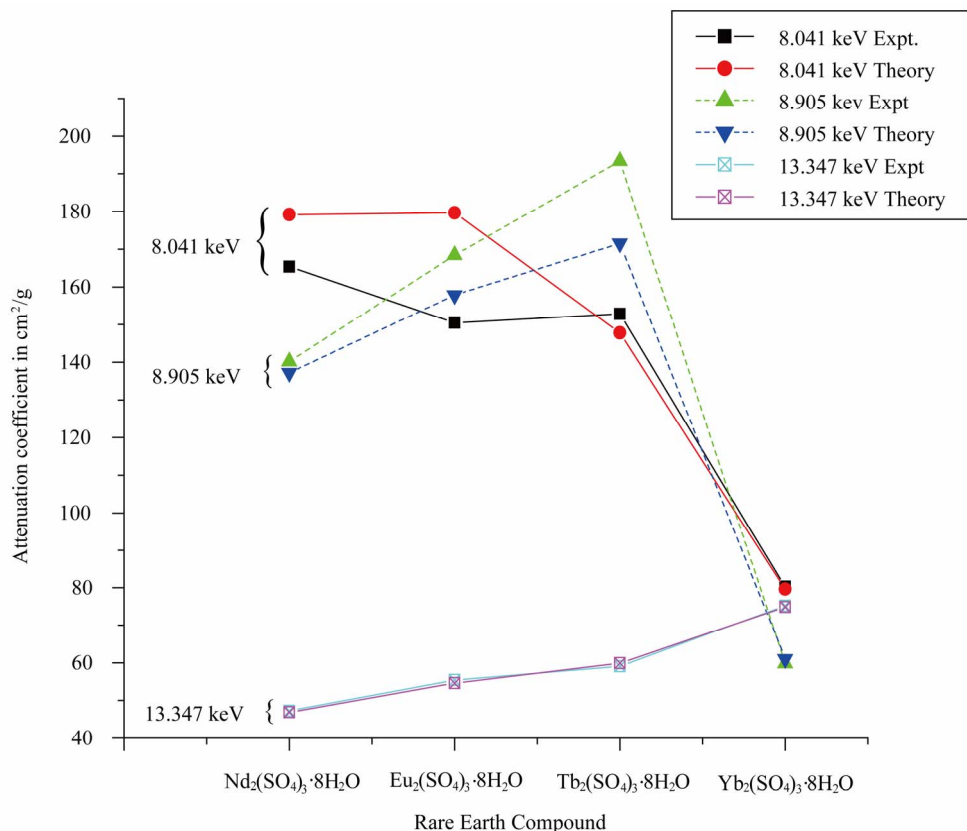
Figure 2. Experimental and Theoretical estimated values of mass attenuation coefficient of rare earth sulphates.

coefficient between the experimental and theoretical by 6.7%, and 12.7% respectively. Thus mixture rule cannot be applicable for the rare earths compounds where L edge energy is close to the incident photon energy. This deviation is also shown in **Figure 2** by plotting mass attenuation coefficient (Experimental and Theoretical) Vs rare earths compound. The experimental and theoretical mass attenuation coefficient value for Neodymium and Europium sulphates at 13.347 shows a good agreement within the 2% and other hand the same compound at 8.041 and 8.907 keV shows a deviation with theoretical value. This results purely the mixture rule can't be applicable in both the cases otherwise it can be applicable provided that the edge effects/chemical effects are taken into account.

In the **Table 2** effective atomic number are estimated using the least squares formula by ploting the mass attenuation coefficient versus the elements for each energies. From the said graph the estimated value of effective atomic number of the dosimetric materials found to vary from 10% to 18% for all the suphides. The theoretical values of the Z_{eff} are also calculated using the formula given by Jackson and Hawkes [1] and these values are discussed in the light of the dosimetry point of view and as discussed in the introduction. The experimental

Table 2. Determined and estimated values of effective atomic number and electron density of the rare earths compounds.

Name of the Sample	Effective Atomic Number (Z_{eff})		Electron Density N_e (10^{24} elec g^{-1})
	Expt	*Jackson* 1981	
8.041 keV			
$Nd_2(SO_4)_3 \cdot 8H_2O$	48.14	41.41	1.649
$Eu_2(SO_4)_3 \cdot 8H_2O$	46.58	43.79	1.562
$Tb_2(SO_4)_3 \cdot 8H_2O$	46.83	45.63	1.542
$Yb_2(SO_4)_3 \cdot 8H_2O$	37.37	49.91	1.185
8.907 keV			
$Nd_2(SO_4)_3 \cdot 8H_2O$	45.44	41.41	1.557
$Eu_2(SO_4)_3 \cdot 8H_2O$	48.45	43.79	1.625
$Tb_2(SO_4)_3 \cdot 8H_2O$	50.87	45.63	1.674
$Yb_2(SO_4)_3 \cdot 8H_2O$	37.69	49.91	1.196
13.347 keV			
$Nd_2(SO_4)_3 \cdot 8H_2O$	31.02	41.41	1.063
$Eu_2(SO_4)_3 \cdot 8H_2O$	32.82	43.79	1.101
$Tb_2(SO_4)_3 \cdot 8H_2O$	33.55	45.63	1.104
$Yb_2(SO_4)_3 \cdot 8H_2O$	36.53	49.91	1.159

and theoretical Z_{eff} values are agreeing within 5% except the edge region. It is important to mention that the theoretical/calculated values have not considered the edge effects and since the effective atomic numbers are under/over estimated when any element falls below the absorption edge.

In the present work, there is a good indication that even in the low photon energy region say that up to 15 keV the effective atomic number can be determined with greater accuracy but one should take into account of edge effects.The electron density of the dosimetric materials is calculated using the experimental Z_{eff} values and found to vary 0.478 to 0.676 (10^{24} electrons g^{-1}). In conclusion, the determined Z_{eff} value is agreeing with the theoretical values within 5% at this energy range and one should also take care of effects if high atomic number dosimeters are involved.

4. ACKNOWLEDGEMENTS

REFERENCES

[1] Jackson, D.F and Hawkes, J.D. (1981) X-ray attenuation coefficients of elements and mixtures. *Physics Reports*, **70**, 169. doi:10.1016/0370-1573(81)90014-4

[2] Nagabhushan, N.M., Kerur, B.R., Lagare, M.T., Nathuram, R., Abani, M.C., Thontadarya, S.R. and Hanumaiah, B. (2004) Technique for measurement of photon intensity for the determination of μ in the low photon energy region. *Journal of X-Ray Science and Technology*, **12**, 161-168.

[3] Rose, E.M. and Shapiro, M.M. (1948) Statistical error in absorption experiments. *Physical Review A*, **74**, 1853-1864. doi:10.1103/PhysRev.74.1853

[4] Pearson, J.J. and Osborne, R.R. (1960) Practicle nucleonics; a course of experiments in nuclear physics. E & F.N. Spon, London.

[5] Sharnabasappa, K.B.R., Anilkumar, S. and Hanumaiahm, B. (2010) Determination of X-ray mass attenuation coefficients using HPGe detector. *Applied Radiation and Isotopes*, **68**, 76-83. doi:10.1016/j.apradiso.2009.08.004

[6] Kerur, B.R., Thontadarya, S.R. and Hanumaiah, B. (1993) Measurement of x-ray mass attenuation coefficients using mixed radiation emitters. *Indian Journal of Physics*, **67**, 163.

[7] Gerward, L., Guilbert, N., Jensen, K.B. and Levring, H. (2001) X-ray absorption in matter Reengineering XCOM. *Radiation Physics and Chemistry*, **60**, 23-24. doi:10.1016/S0969-806X(00)00324-8

[8] Kortright, J.B. (1986) Characteristic X-ray energies, X-ray data booklet. In: Vaughan, D. Ed., *Lawrence Berkeley Laboratory*, University of California, Berkeley.