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Atomic Form Factor of Some Tissue- Equivalent Materials at 25.2keV Photon Energy Using Geant4 Toolkit

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Abstract: Using Geant4 toolkit, the differential cross-section and the atomic form factor for coherent scattering of 25.2 keV photons in some tissue- equivalent compounds at 90° were calculated. The results gave good agreement with those calculated theoretically. **PACS:** 87.50.-a, 87.53.-j

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Introduction

At low energies, as in diagnostic radiology or nuclear medicine, coherent and incoherent scattering play an important role in the interaction of photons with matter.

Coherent and incoherent scattering are subject to some limitations, mainly selfattenuation of the primary and scattered radiations within the material and the multiple scattering of the radiation. But this doesn't limit the interest increase of using them in the public safety sector, detection of explosives in the passenger luggage and food inspection [1-3]. The unique scattering signature they gave, which is characteristic of the material, enhanced their use in the field of tissue characterization in the medical environment and other industrial in applications [4].

In diagnostic problems, using of tissue equivalent materials is recommended to detect any change in the radiological properties of tissues, because of the similar density and elemental composition to real human tissues. Also, other studies support the close match with its scattering characteristics [5-7]. Experimentally, the intensity fluctuations of x-ray tubes limit their use as a photon source, and instead of that many measurements in this field were performed during the past (50) years using a narrow beam of γ -rays emitted by radioactive isotopes. However, these sources suffer from weak intensities and high energy backgrounds [8-11].

In this work, the coherent scattering crosssection and the atomic form factor of 25.2 keV photons from a set of low and close Z tissue - equivalent materials (5.4<Z<7.6) were calculated by simulation using CERN's toolkit "Geant4" as introduced by Gupta et al. [12] and compared with values obtained theoretically. The atomic form factor provides information about the inner structure of the atoms and macro - molecules which can be widely utilized in medical diagnostics and imaging.

Many measurements were conducted to obtain this scattering cross - section, but for larger energy and for other atomic number materials [13-14]. At 25.2 keV, we cannot resolve experimentally the coherent peak from the incoherent one, but this can be achieved in simulation.

Theoretical Concepts

The scattering spectrum from the scattering material can be analyzed in such a way that one can obtain the coherent and the incoherent peaks separately. So, one can obtain the coherent scattering cross-section by comparing the area of the coherent peak with that of the incoherent peak in the spectrum and using the relation [12];

$$\frac{\frac{(d\sigma(\theta)}{d\Omega}_{coh}}{\binom{d\sigma(\theta)}{d\Omega}_{inc}} = \frac{N(\theta)_{coh}}{N(\theta)_{inc}} \frac{f_s(\theta)}{f_p(\theta)} \frac{\epsilon_{inc}}{\epsilon_{coh}} \quad (1)$$

where:

 $N(\theta)_{coh}$ and $N(\theta)_{inc}$ are the photo-peak area of the coherent and incoherent spectrums, respectively, at an angle θ from the scatterer.

 $f_s(\theta)$ is the attenuation factor for the incoherently scattered photons.

$$f_{s}(\theta) = \frac{I}{I_{0}} = \exp[-\mu_{inc}x]$$

$$= \exp[-\sigma_{inc}\rho x]$$
(2)

 $f_p(\theta)$ is the absorption factor for the coherently scattered photons.

$$f_{p}(\theta) = \frac{I_{abs}}{I_{0}} = \frac{I_{0} - I}{I_{0}}$$
$$= 1 - \exp[-\mu_{coh}x]$$
$$= 1 - \exp[-\sigma_{coh}\rho x]$$
(3)

 \in_{coh} and \in_{inc} are the photo-peak efficiencies of the detector for the coherently and incoherently scattered photons, respectively.

The incoherent scattering cross-section is governed by Klein Nishina cross-section in the relation:

$$\left(\frac{d\sigma(\theta)}{d\Omega}\right)_{inc} = S(x,Z)\left(\frac{d\sigma(\theta)}{d\Omega}\right)_{KN} \tag{4}$$

S(x, Z) is the incoherent atomic scatter function that represents the effect of the electron binding energy, Z is the effective atomic number of the scatterer and x is the photon momentum transfer (= $(\sin(\theta/2))/\lambda$), where θ is the angle of scattering and λ is the wavelength of the incident radiation. In our case, all the samples were low Z materials, so the coupling between electrons and between electrons and nuclei is small compared to the photon energies used; i.e. $S(q, Z) \approx Z$. And

$$\left(\frac{d \sigma(\theta)}{d \Omega}\right)_{KN} = \frac{r_0^2}{2} \frac{1}{\left[1 + Y \left(1 - \cos \theta\right)\right]^2} \times \left[1 + \cos^2 \theta + \frac{Y^2 \left(1 - \cos \theta\right)^2}{1 + Y \left(1 - \cos \theta\right)}\right]\right\},$$

 $Y = \frac{E_0}{m_0 c^2}$, r_0 is the classical electron radius.

Substituting these values for Y, $\left(\frac{d\sigma(\theta)}{d\Omega}\right)_{KN}$ and $\in_{inc} < _{coh}$, one can simplify Eq. 1 to be:

$$\left(\frac{d \,\sigma(\theta)}{d \,\Omega}\right)_{coh} = \left\{ K \times Z \, \frac{(\exp[-\sigma_{inc} \,\rho x \,])}{(1 - \exp[-\sigma_{coh} \,\rho x \,])} \frac{N(\theta)_{coh}}{N(\theta)_{inc}} \right\}$$
(5)

K is the system constant that depends on the geometry of the experiment, the probability of scattering of photons and on the system parameters and can be calculated from the previous relations.

With such ratio method, the effect of multiple scattering within the sample is illuminated.

F(x, Z) can be calculated from the relation:

$$F(x,Z) = \left[\frac{(d\sigma(\theta)/d\Omega)_{coh}}{(d\sigma/d\Omega)_T}\right]^{\frac{1}{2}}$$
(6)

where $(d\sigma/d\Omega)_T$ is Thomson scattering cross - section.

There are three main atomic form factor theories used in the literature; the non relativistic form factor (NRFF), the relativistic form factor (RFF) and the relativistic modified form factor (RMFF) which give different theoretical values extending over a wide momentum transfer range for many elements. There are small discrepancies between their values, but all of them show a direct increase with increasing the atomic number of the sample and an indirect relationship with momentum transfer increase, as represented in Fig. 1. Extracting the results to $1.4344A^{-1}$ gives values which can be used for comparison.



FIG. 1. The atomic form factor vs. momentum transfer for different atomic number elements as obtained from (RFF) theory [15].

Geant4 and the Modeled Experiment

Geant4 is a free Monte Carlo toolkit written in C++ for the simulation of the passage of particles in matter designed and developed at CERN by world wide collaboration [16]. It has a very rich set of physics models for a wide energy range to handle the interaction of particles with matter. Geant4 provides a diverse, wide-ranging, comprehensive toolkit that includes a powerful kernel for tracking, geometry, detector response, run, event, step management, visualization and user interfaces.

The user of Geant4 must build his own code by himself that cover [17] the geometry of the system, materials and particles involved, the generation of primary events and tracking through materials and electromagnetic fields and the governing physics processes, the response of sensitive detector components, the generation of event data and also, the analysis of simulation data at different levels of detail.

Fig. 2 provides the modeled experiment which is used in this work. The geometrical dimensions of the entire components of the detector are obtained from the manufacturer of a real one in the x-ray lab.

A beam of 25.2 keV photons is generated by the gun and passes through a narrow collimator with a rectangular slit of (4×1) mm dimension to form a pencil like beam then directed towards the sample. Another identical collimator is used in the way of the scattered beam in front of the Si(Li) detector located at a scattering angle of 90°.

Measurements were performed using some tissue - equivalent materials; Polyethylene, Cholesterol, Lucite, Water, White-matter, Muscle and Blood of cylindrical geometries of (12) mm radius and (15) mm length. The stored energy deposition data resulting from the simulation is analyzed to generate a histogram, so one can resolve the coherent and incoherent peaks from the total histogram, as shown in Fig. 3.



FIG. 2. Geometry of the setup as modeled in the simulation codes.



FIG. 3. The output spectrum obtained by the simulation.

Results and Discussion

The scattered spectrums were collected using an old model of Si(Li) detector. Its efficiencies at the incident and the scattered energies were obtained by simulation.

A million of photons were incident toward the detector first with the primary energy then with the scattered energy, and in every case we measured the number of photons in the full energy peak and divided it by one million. The relative efficiency \in_{inc}/\in_{coh} is:

$$\in_{inc}/\leq_{coh} = 1.0305$$
.

For each sample, differential coherent cross - sections and their corresponding form factors are given in Table 1 along with the atomic form factor obtained theoretically.

The results in the Table show that the differential coherent cross-section increases with increasing the atomic number of the sample. The form factors are in agreement with those obtained from previous theories. There is a better agreement with relativistic modified form factor (RMFF). Meanwhile, RFF predicts higher values.

A graphical representation of the results, shown in Fig. 4, shows the closer agreement of Geant4 results with the RMFF theory.

by simulation	1.					
		$d\sigma$	Atomic Form Factor $F(x,Z)$			
Sample	\overline{Z}	$(\overline{d\Omega})_{coh}$ (barn/atom.st)	Geant4	RMFF ^[18]	RFF ^[15]	NRFF ^[19]
PE	5.4439	0.0106 ± 0.0006	0.5173±0.0030	0.5489	0.5860	0.5794
Cholesterol	5.6483	0.0118 ± 0.0007	$0.5458 {\pm} 0.0030$	0.5721	0.5898	0.5956
Lucite	6.4673	0.0179 ± 0.0011	$0.6723 {\pm} 0.0051$	0.6662	0.6849	0.6612
Water	7.4167	0.0231 ± 0.0015	0.7631 ± 0.0068	0.7774	0.7952	0.7384
W-matter	7.4965	0.0243 ± 0.0016	0.7819 ± 0.0069	0.7869	0.8045	0.7449
Muscle	7.5269	0.0247 ± 0.0016	0.7889 ± 0.0070	0.7905	0.8080	0.7474
Blood	7.6132	0.0254 ± 0.0017	0.7997 ± 0.0077	0.8007	0.8181	0.7545
	0.9	, , , ,				

TABLE. 1. Differential coherent cross-sections and form factors for 25.2 keV at (90°) obtained by simulation.



FIG. 4. Atomic form factor as a function of atomic number.

The error in the cross-sections arises from statistical errors and at most reaches a percentage of 5.8%. Increasing the number of incident primaries will decrease this error, but the cost of this process will be the increase in the simulation run-time and thus the need to more powerful computers.

As the atomic number of the sample increases, the discrepancy about the RMFF theory values decreases, since the binding energy of the electrons participating in the scattering will decrease.

The literature reviewed showed other experiments which assure the superiority of RMFF theory for intermediate $(1 < x < 10A^{-1})$ and high momentum transfer $(x > 10A^{-1})$ [10, 14].

For heavier materials such as those used in [20], RFF gives higher values of the resulting form factor, but RMFF is still the most compliant.

Conclusions

The presented differential coherent crosssections and the atomic form factors for some low Z tissue-equivalent materials at intermediate momentum transfer 1.4344A⁻¹ are seen to be in good agreement with those obtained from the RMFF theory, which confirms its appropriateness in finding the coherent atomic form factor. The simulated results demonstrate the capability of using Geant4 to characterize tissue- equivalent materials of close low atomic numbers when the sample length is 15mm, which encourages using it in further radiation and medical physics applications.

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A further study on biological and industrial materials, using Geant4 toolkit at higher momentum transfer is being demonstrated.

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