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Molecular scattering function data of brain tissue

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Abstract

The interaction of photons with matter is of great importance for the study of energy transfer to the medium. The most sensitive studies on energy transfer are Monte Carlo simulation applications. In Monte Carlo modeling, the calculation of incoherent scattering is important. The incoherent scattering of a photon in a medium is decisive in terms of scattering angle and energy transfer to the medium. By incorporating the incoherent scattering coefficients into the Monte Carlo modeling program, it will be possible to determine the attenuation properties of photons of different energies interacting in the matter. In this study, incoherent scattering functions necessary for calculating molecular incoherent scattering coefficients were obtained by using atomic data according to the molecular content of white and gray brain matter. We believe that our results can be used and will be beneficial for researchers who make models and work experimentally.

***Keywords**: Brain tissue, photon interaction, incoherent, scattering function*

Beyin dokusunun moleküler saçılma fonksiyonu verileri

Öz

Fotonların madde ile etkileşimi, ortama enerji aktarımının incelenmesi açısından büyük önem taşır. Enerji aktarımı konusundaki en duyarlı çalışmalar Monte Carlo benzetişim uygulamalarıdır. Monte Carlo modellemede inkoherent saçılımın hesaplanması aşaması önem arzetmektedir. Fotonun bir ortamda inkoherent saçılma yapması, saçılma açısı ve ortama enerji aktarımı bakımından belirleyicidir. İnkoherent saçılma katsayılarının Monte Carlo modelleme programının içerisine katılmasıyla, maddede etkileşen farklı enerjili fotonların zayıflama özelliklerinin belirlenmesi mümkün olacaktır. Bu çalışmada, moleküler İnkoherent saçılma katsayılarının hesaplanması için gerekli olan inkoherent

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saçılma fonksiyonları, beyaz ve gri beyin maddesinin moleküler içeriğine göre atomik veriler kullanılarak elde edilmiştir. Sonuçlarımızın, deneysel çalışan ve modellemeler yapan araştırmacılar için yararlı olacağına ve kullanılabileceğine inanmaktayız.

***Anahtar kelimeler**: Beyin dokusu, foton etkileşimi, inkoherent, saçılma fonksiyonu*

1. Introduction

It is important to know the probability of interaction of photons with varying energy values in a medium, the type of interaction, the number of interactions and the energy transfer to the medium. By knowing this behavior of the photon in matter, the determining interaction properties between the photon and matter are revealed. Knowledge of which interactions the incoming photon makes, at what energy value, and how much energy is transferred to the medium as a result of these interactions, will provide valuable information about the characteristics of the matter.

Photon interaction cross-sections for molecular substances are necessary in the field of radiation technology [1-3]. Knowledge of the scattered radiation and an accurate description of the scattering process allows a complete understanding of the imaging system. The technique is based on differences in the distribution of photons scattered in an incoherent (Compton) manner from different molecular structures. Incoherent scattering distributions must be known in detail to simulate the radiological image. Radiographic techniques are based on differences in attenuation coefficients [4]. Accurate knowledge of attenuation coefficients has a great impact on industrial and safety applications, agriculture, biological and medical studies, where directly defining the material composition has become a priority [5]. Accurate values of interaction coefficients are necessary to establish regions where the theory is valid [4, 6]. Studies on attenuation coefficients have been reported by some researchers [6-16].

Photon interaction coefficients are used to determine changes in the structural properties of tissues. Determination of incoherent (Compton) scattering, one of the most important scattering mechanisms, is important and necessary. For this, the molecular incoherent scattering function must be calculated for tissues. The molecular incoherent scattering function must be obtained as a function of the momentum transfer variable (x) for all possible x values in the range of $0 \leq x \leq 10^3$ nm^{-1}.

In this study, incoherent scattering functions, which are an important multiplier in determining the characteristic incoherent interactions of the photon, were calculated according to the elemental composition in the molecular structure that constitutes the brain tissue. For this, it is necessary to know the atomic scattering function values for each element that makes up the white and gray brain tissue. Molecular incoherent scattering functions were calculated using atomic incoherent scattering functions and were presented in Table 1. Our results are intended to be used by researchers working on photon transfer modeling.

2. Method

Incoherent x-ray scattering of photons from free electrons was described by Klein-Nishina (KN) [17] with the differential scattering cross-section for unpolarized x-rays.

At lower incident energies, the electron binding energy reduces the likelihood of incoherent scattering interactions. This fact leads to a modification of the KN [17] formula by multiplying the incoherent scattering function (hereafter referred to as ISF), which gives the binding effect of the electron at low momentum transfer values, by the correction factor $S(x,Z)$ [18-19]. By taking the ISF into account, the total incoherent scattering cross section per atom can be calculated for inelastic scattering.

Since there is no interference between the scattered waves and the effect of molecular bonding on $S(x,Z)$ is very small, the IAM approach can be applied to the ISF $S_m(x)$ of a molecule or mixture. Molecular ISF $S_m(x)$ can be calculated using the atomic ISF $S_i(x,Z_i)$ according to the elemental composition and density of the tissue, according to the formula below for all values of x.

$$\frac{S_m(x)}{W} = \sum_i \frac{w_i}{M_i} S_i(x, Z_i) \tag{1}$$

Here, M_i, w_i, and Z_i are the atomic mass, the mass fraction, and the atomic number of the ith element, respectively. W is the molecular weight. $S_i\,(x,Z_i)$ is the atomic incoherent scattering function of the ith element. $S_i\,(x,Z_i)$ data were obtained from the tables of Hubbell et al., [20].

3. Results and discussion

Elemental contents of brain tissue were researched. Elemental content data of white and gray brain tissue [12, 21-24], and whole brain tissue [24-30] were tested separately. Chou et al., [22] elemental content data were found to be most compatible with experimental data. Therefore, $S_m(x)$ values were calculated with the elemental data of Chou et al., [22] and are presented in Table 1. Theoretical molecular ISF values of the brain tissue listed in Table 1 were calculated in the range $0 \leq x \leq 1000$ nm^{-1} using the formula given in equation (1). ISF values obtained for brain tissues are the most important multiplier to calculate incoherent scattering coefficients. By incorporating the obtained coefficients into the Monte Carlo modeling program, the attenuation properties of photons at different energies interacting in the matter can be determined. In this regard, we believe that our results will fill an important gap in the literature.

Table 1**:** The theoretical molecular incoherent scattering functions ($Sm(x)$) presented for white and gray brain tissues

x(Å^{-1})	***$S_m(x)$* *White Brain***	***$S_m(x)$* *Gray Brain***
0	0	0
5.00 E-03	0.0995	0.0965
1.00 E-02	0.3741	0.3642
1.50 E-02	0.8496	0.8275
2.00 E-02	1.5006	1.4626
2.50 E-02	2.3346	2.2754
3.00 E-02	3.3439	3.2586

Table 1. (continued)

4.00 E-02	5.8503	5.7036
5.00 E-02	8.9601	8.7370
7.00 E-02	16.6969	16.3013
9.00 E-02	25.9014	25.3167
1.00 E-01	30.8547	30.1765
1.25 E-01	43.6842	42.7272
1.50 E-01	56.3254	55.2629
1.75 E-01	68.2821	67.0897
2.00 E-01	79.1764	77.9007
2.50 E-01	97.4558	96.1083
3.00 E-01	111.3777	110.0610
4.00 E-01	129.4131	128.2927
5.00 E-01	139.4719	138.5115
6.00 E-01	145.6375	144.7191
7.00 E-01	150.0117	149.0527
8.00 E-01	153.5596	152.5265
9.00 E-01	156.6452	155.5350
1.00 E+00	159.4508	158.2775
1.25 E+00	165.3195	164.0673
1.50 E+00	169.6858	168.4416
2.00 E+00	174.7855	173.6356
2.50 E+00	176.9862	175.9099
3.00 E+00	177.8991	176.8604
3.50 E+00	178.2815	177.2595
4.00 E+00	178.4509	177.4363
5.00 E+00	178.5677	177.5577
6.00 E+00	178.5987	177.5896
7.00 E+00	178.6094	177.6005
8.00 E+00	178.6137	177.6050
1.00 E+01	178.6147	177.6059
1.50 E+01	178.6151	177.6062
2.00 E+01	178.6151	177.6063
5.00 E+01	178.6151	177.6063
8.00 E+01	178.6151	177.6063
1.00 E+02	178.6151	177.6063
1.00 E+03	178.6151	177.6063
1.00 E+06	178.6151	177.6063
1.00 E+09	178.6151	177.6063

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