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A STUDY ON DETERMINATION OF MASS ATTENUATION COEFFICIENT, EFFECTIVE ATOMIC NUMBER AND ELECTRON DENSITY OF SOME MATERIALS USING MONTE CARLO METHOD

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ABSTRACT

This work aims to calculate the effective atomic number and electron density by Monte Carlo method. In previous studies, the most widely used solution is to use the transmission method with the narrow gamma-ray beam. In the approach of this work, the gamma-ray beam after going through material is uncollimated to recording by NaI(Tl) detector. To do this, the inner diameter of detector collimator was enlarged with the aim of decreasing the strengthen of radioactive source. The obtained results were compared with NIST data and the experimental values which yield the maximum deviation of 9.05% and 3.43%, respectively. These results show the promising approach in determining the features of material.

Keywords: electron density, atomic number, Monte Carlo, MCNP.

TÓM TẮT

Nghiên cứu xác định hệ số suy giảm khối, nguyên tử số hiệu dụng và mật độ electron của một số loại vật liệu bằng phương pháp Monte Carlo

Nghiên cứu nhằm xác định các đặc trưng của vật liệu bao gồm hệ số suy giảm khối, nguyên tử số hiệu dụng và mật độ electron. Phương pháp được sử dụng phổ biến nhất trong các nghiên cứu trước đây là phương pháp truyền qua kết hợp với chùm photon được chuẩn trực trước và sau khi đi ra khỏi vật liệu. Trong cách tiếp cận của nghiên cứu này, chùm tia ra khỏi vật liệu không cần phải chuẩn trực nhằm mục đích đảm bảo tính thống kê mà không cần phải sử dụng nguồn mạnh. Kết quả nghiên cứu được so sánh với dữ liệu NIST và dữ liệu thực nghiệm cho thấy sự phù hợp tốt với độ lệch tương đối lớn nhất lần lượt là 9,05% và 3,43%. Kết quả này cho thấy đây là phương pháp hứa hẹn trong việc xác định các đặc trưng của vật liệu.

Từ khóa: mật độ electron, nguyên tử số, Monte Carlo, MCNP.

1. Introduction

Mass attenuation coefficient, effective atomic number and electron density are the important parameters of evaluation of material features when they were used as shielding materials against nuclear radiation [1, 2], tissue equivalent materials in medical field [3], aerospace applications [4]. The above parameters were usually determined by the

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transmission method. In this method, the collimated gamma-ray beam is necessary for getting the high accuracy.

In the present work, a new approach was applied to determine the mass attenuation coefficient, effective number and electron density in which the collimated gamma-ray beam is not mandatory. This aims to simplify the experimental set-up and also decrease the strengthen of source. For this one, the inner diameter of detector collimator needs to be enlarged. This led to the contribution of secondary photons which reduce the accuracy of the obtained results. To overcome this, an advanced gamma spectrum processing technique [5] was applied to separate the primary photons from the obtained spectrum. The accuracy of spectrum processing technique was evaluated by the calculated results of effective atomic number and electron density.

MCNP5 code [6] is widely used in nuclear physics with the aim of simulating the interaction of particles with material. In this work, the pulse height spectrum is generated by MCNP5. From the simulated spectra, the mass attenuation coefficient, effective atomic number and electron density was calculated and compared with NIST data [7] and experimental values [4].

2. Theory

For the narrow gamma-ray beam, the mass attenuation coefficient, $\mu(E)/\rho$, was calculated in the following equation:

$$\frac{\mu(E)}{\rho} = \frac{1}{d\rho}\ln\left(\frac{I_0}{I}\right) \quad (1)$$

where d is thickness of measured material; I_0 and I are the incident and transmitted fluxes, respectively.

The total molecular cross-section was defined as follows [4]:

$$\sigma_m(E) = \left(\frac{1}{N_A}\right)\left(\frac{\mu(E)}{\rho}\right)_c \sum_i n_i A_i \quad (mb) \quad (2)$$

where n_i is denoted as number of atoms of i^{th} element, N_A is Avogadro's number and A_i is atomic weight of i^{th} element.

For one atom in the compound, the effective atomic cross-section was determined based on the total molecular cross-section as shown in the following equation:

$$\sigma_a = \frac{\sigma_m}{\sum_i n_i} \quad (mb) \quad (3)$$

Based on the mass attenuation coefficient, the effective electronic cross-section of i^{th} element was defined as follows [4]:

$$\sigma_e = \left(\frac{1}{N}\right)\sum_i\left(\left(\frac{f_i A_i}{Z_i}\right)\left(\frac{\mu}{\rho}\right)_i\right) = \frac{\sigma_a}{Z_{eff}} \quad (mb) \quad (4)$$

where f_i and Z_i are fractional abundance and atomic number of i^{th} element in the molecule, respectively. From Eq. (3) and Eq. (4), the effective atomic number was calculated in the following equation [4]:

$$Z_{eff} = \frac{\sigma_a}{\sigma_e} \tag{5}$$

And, the effective electron density, N_e, was determined as follows [4]:

$$N_e = \frac{N_A}{\sum_i n_i A_i} Z_{eff} \sum_i n_i \quad (\text{electron/g}) \tag{6}$$

3. Calculation of attenuation features of some materials by using Monte Carlo simulation

3.1. Monte Carlo simulation model

Currently, the Monte Carlo method is widely used in many fields, particularly in nuclear physics. The advantage of this method is to simulate easily the very complex interaction of particles with material. In some cases, it is a very useful solution such as simulation of the operation of nuclear reactor. MCNP code was built upon the Monte Carlo method. There are two main reasons why the MCNP is commonly used. First, the obtained result from MCNP code is highly significant and thus it is used to evaluate the experimental data. Second, it is very easy to change the value of simulation parameters in such a way that the obtained results are comparable to the experimental ones. This also helps us save time and money.

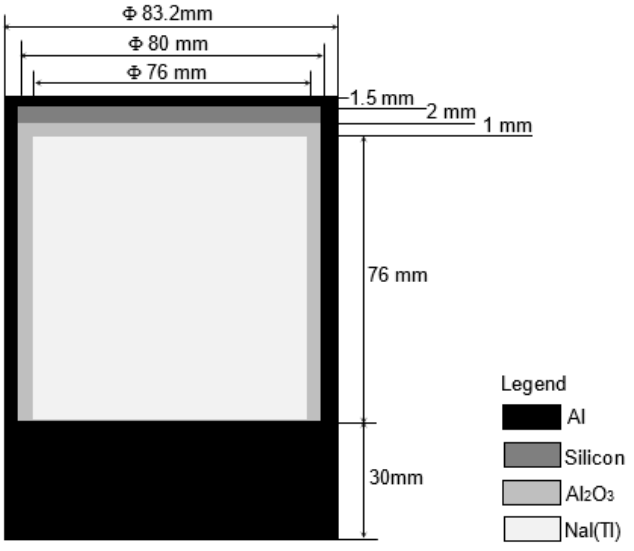


Fig. 1. *The geometrical description of NaI(Tl) detector used in Monte Carlo simulation*

In previous studies, the Monte Carlo simulation model of NaI(Tl) detector as shown in **Fig. 1** was validated [8, 9]. By comparing the simulated values of full-energy peak energy, peak to Compton ratio and energy resolution with the experimental data, the results

showed the good agreement. Thus, it can be concluded that the simulation model of NaI(Tl) detector used in this work is completely reliable.

The ^{137}Cs source used in simulation was seen as the point one. The source was placed at a distance of 10 cm from the material plate and 25 cm from the detector. The material plate is in rectangular form of dimensions 10 cm × 10 cm with thickness of 1 mm. The detector was surrounded by collimator with the inner diameter of 9.5 cm. Arrangement of source, material plate and detector was shown in **Fig.2b**.

In order to obtain the simulated spectrum in which the full-energy peak exhibits Gaussian energy broadening, we use the FWHM (full-width at half maximum) function as follows:

$$FWHM = a + b\sqrt{E + cE^2} \quad (7)$$

where a = – 0.0137257 MeV; b = 0.0739501 MeV$^{1/2}$ and c = – 0.152982 MeV^{-1} [8]

3.2. Spectrum processing technique

To determine the linear attenuation coefficient, the experiment arrangement was required as presented in **Fig. 2a**. In this set-up, the narrow photon beam emitting from source was collimated before they reach the detector. Thus, the linear attenuation coefficient was calculated easily by using the Beer-Lambert law:

$$I_d = I_0 e^{-\frac{\mu(E)}{\rho}\rho d} \quad (8)$$

For the experiment arrangement as shown in **Fig. 2b**, the Beer-Lamber law was modified as follows:

$$I_d = BI_0 e^{-\frac{\mu(E)}{\rho}\rho d} \quad (9)$$

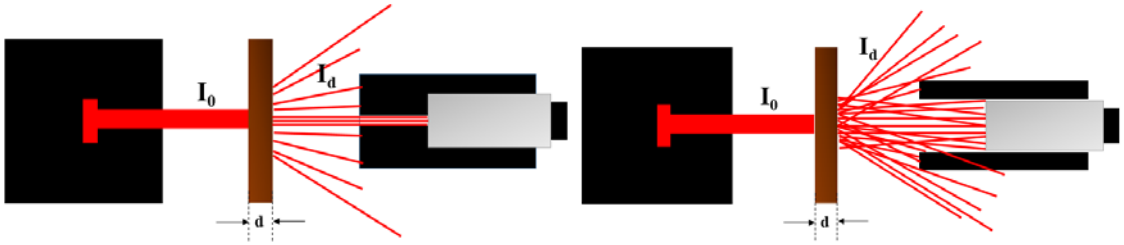
where B is the build-up factor which modified the contribution of secondary photons to transmission spectrum.

In present study, we used the experiment arrangement as shown in **Fig.2b**. The suitable spectrum processing technique is necessary to separate the secondary photons from the obtained transmission spectrum. In this spectrum processing technique, the Gaussian function was used to fitting the transmission peak. The area under Gaussian peak was used to calculate the mass attenuation coefficient using Eq.(1). From this, we can calculate the effective atomic number and the effective electron density using Eq.(5) and Eq.(6). The mathematical form of Gaussian function was defined by the following equation:

$$G(x) = \frac{A}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x - x_0)^2}{2\sigma^2} \right) \quad (10)$$

And, the contribution of secondary photon component in transmission spectrum was fitted by the fourth-order polynomial with the mathematical form as follows:

$$poly(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)^2 + a_3(x - x_0)^3 + a_4(x - x_0)^4 \quad (11)$$



a) b)

Fig. 2. *The experiment arrangement for transmission method in two cases of detector collimator of*
a) small inner diameter and b) very larger inner diameter

The transmission spectra were analyzed by using Colegram software [10]. The spectrum processing technique was validated based on the agreement of calculated results with theoretical data (NIST) as well as the previous experimental data.

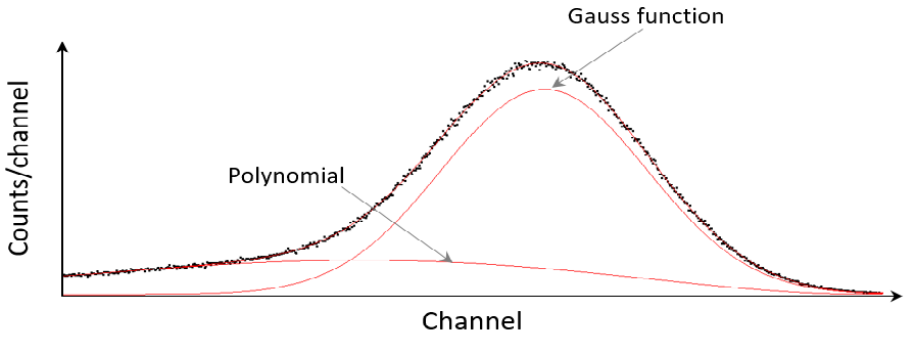


Fig. 3. *The spectrum processing technique applied to analyzing the transmission spectrum*

4. Results and discussion

4.1. The calculated results of mass attenuation coefficient

The mass attenuation coefficient of some materials was determined and presented in **Table 1**. The simulated results were compared with theoretical ones which yield the maximum deviation of 5.95%. This value is even better which is below 2.06 % in comparison of the simulated results with experimental data for PMMA and Kapton materials. These results have confirmed that the Monte Carlo method can be used as the alternative solution in calculating the attenuation features. Besides, it is clear that the spectrum processing technique applied in this study is completely suitable.

Table 1. *Mass attenuation coefficient of some materials*

Material	Chemical components	μ/ ρ × 10^{-2} (cm^2g^{-1})				
		Our work (a)	Experiment [4] (b)	RD_b (%)	Theoretical value [7] (c)	RD_c (%)
PMMA	$(C_5O_2H_8)_n$	8.71	8.67	0.05	8.34	– 4.44
PET	$(C_{10}H_8O_4)_n$	8.19	--	--	8.03	– 1.99
PVC	$(C_2H_3Cl)_n$	8.37	--	--	7.90	– 5.95
Teflon	$(C_2F_4)_n$	7.45	--	--	7.40	– 0.68
PE	$(C_2H_2)_n$	9.20	--	--	8.80	– 4.55
PP	$(C_3H_6)_n$	9.22	--	--	8.80	– 4.77
PS	$(C_8H_8)_n$	8.63	--	--	8.30	– 3.98
Kapton	$(C_{22}H_{10}N_2O_4)_n$	8.07	8.24	2.06	7.91	– 2.02

$$RD_i(\%) = \frac{i-a}{i} \times 100\%, \; i = b, c.$$

4.2. The calculated results of the effective atomic number and electron density

The calculated results of the effective atomic number and electron density of Kapton and PMMA materials were presented in **Table 2**. These results were compared with theoretical and experimental data which yield the maximum deviation of 9.05% for theoretical values and 3.43% for experimental values. It is important to note that our calculated results are much better suited for experimental values than theoretical ones. For this reason, we think it was due to both experimental data and our obtained results are directly determined based on the transmission spectra whereas the theoretical values was obtained the interpolation method.

Table 2. *The calculated results of the effective atomic number and electron density*

Material	Our work (m)	Experiment [4] (n)	RD_n (%)	Theoretical [7] (p)	RD_p (%)
			Z_{eff}		
Kapton	5.044	5.223	3.43	5.026	–0.36
PMMA	3.664	3.745	2.16	3.360	–9.05
			$N_{eff} \times 10^{23}$ (electrons/g)		
Kapton	3.152	3.170	0.57	3.090	2.00
PMMA	3.309	3.324	0.45	3.294	-0.46

$$RD_i(\%) = \frac{i-m}{i} \times 100\%, \; i = n, p.$$

5. Conclusions

In this study, we applied successfully the new approach to determine mass attenuation coefficient and electron density. The obtained results are in agree with theoretical values (NIST) as well as experimental data which yield the maximum deviation of 9.05% and 3.43%, respectively. In addition, the obtained results strongly confirm that enlarging the inner diameter of detector collimator had no significant effect on the accuracy of calculated results. This resulted in decreasing the strengthen of radioactive source in experimental measurement. Although our results were compared and evaluated with theoretical data but limitation of this study is in experimental data. Indeed, the comparison of our results with experimental values is only applied for two materials, Kapton and PMMA However, the initial results show that the method used in this study is a promising approach to determining the mass attenuation coefficient, effective atomic number and electron density by simulation method.

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