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Determination of the mass attenuation coefficients for X-ray fluorescence measurements correction by the Rayleigh to Compton scattering ratio

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ABSTRACT

X-ray fluorescence technique plays an important role in nondestructive analysis nowadays. The development of equipment, including portable ones, enables a wide assortment of possibilities for analysis of stable elements, even in trace concentrations. Nevertheless, despite of the advantages, one important drawback is radiation self-attenuation in the sample being measured, which needs to be considered in the calculation for the proper determination of elemental concentration. The mass attenuation coefficient can be determined by transmission measurement, but, in this case, the sample must be in slab shape geometry and demands two different setups and measurements. The Rayleigh to Compton scattering ratio, determined from the X-ray fluorescence spectrum, provides a link to the mass attenuation coefficient by means of a polynomial type equation. This work presents a way to construct a Rayleigh to Compton scattering ratio versus mass attenuation coefficient curve by using the MCNP5 Monte Carlo computer code. The comparison between the calculated and literature values of the mass attenuation coefficient for some known samples showed to be within 15%. This calculation procedure is available on-line at www.macx.net.br.

1. Introduction

Electromagnetic radiation in the X-ray energy range interacts with matter by three main processes: (a) photoelectric effect; (b) Compton scattering and; (c) Rayleigh scattering. In the first case the photon transfer all of its energy to a well bound electron; in the second case the photon transfers only part of its energy to a loose electron and is deviated from its trajectory, the amount of energy transferred will depend on the scattering angle; in the third and last case, the photon is deviated from its trajectory but no energy is transferred [13].

The photoelectric interactions displace electrons from the material atoms and, by electronic rearrangement, leads to characteristic X-rays which energy is peculiar to each atom and the electronic level of the transition. Therefore, qualitative analysis may be conducted by measuring the energy of the characteristic X-rays and subsequent identification of the chemical element.

Nevertheless, not only the incident photon flux on the sample interacts within it, but also the emitted characteristic X-ray may undergo one of the processes described before, leading to a loss of information which, in turn, presents a difficulty when quantitative analysis is being performed.

The intensity of each type of interaction depends on the photon energy, chemical composition and density of the material. Therefore, the response function of the measuring system, including the X-ray tube and the incident and reflected beam, is very complex.

The attenuation coefficient provides a measure of the interaction probability of incident photons in matter per unit mass or unit area [14]. Several studies in the literature seek accurate measurements of the mass attenuation coefficient of building materials [2,18], metal alloys, mineral samples [9,6], and biological samples such as bone, muscle and fat [1].

The mass attenuation coefficient is dependent on the photon energy and the material, and is a combination of each individual interaction effect. Therefore, the knowledge of mass attenuation coefficient is of great importance for proper determination of the

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concentration of each element in the sample being assayed by X-ray fluorescence.

One way to determine the mass attenuation coefficient of unknown materials is by transmission measurements [18], which requires adequate measuring setup, sources, material thickness and shape. For fluorescence measurements it can be a drawback because of the very low energies involved, from few keV to about a 100 keV, for precise transmission measurement, especially because it does not require thin samples, in addition to the fact that not necessarily there will be sources available for every energy of interest.

The measurement of the Rayleigh to Compton scattering ratio (*R*/*C*) is an alternative to the transmission method. Some works in the literature use this technique for scattering tomography [8,4] and the determination of effective atomic number [10,11,16,17].

The main idea of the paper was to present an alternative proposal for the works presented by Duvauchelle [7] and Pereira [16]. These works present the determination of the effective atomic number for mixtures and compounds by using Rayleigh to Compton scattering ratio (*R*/*C*) for the calculation of the mass attenuation coefficient of these materials. Here, Monte Carlo simulations have been used for the determination of the *R*/*C* for several materials in a given energy and subsequently calculating the mass attenuation coefficient for samples. This new method requires only the knowledge of the *R*/*C* of a sample, which is experimentally determined. This is especially important when using the X-ray fluorescence technique at low energies.

The methodology presented in this work is based on a direct relationship between Rayleigh to Compton scattering ratio determined at a given irradiation energy and the mass attenuation coefficient for the range of energy of interest. The K-edge energy imposes a limitation in which, bellow this energy, the relationship is lost. The Rayleigh to Compton scattering ratio and the sample analysis is performed in a single measurement.

The difficulty in constructing a Rayleigh to Compton scattering ratio versus mass attenuation coefficient curve is the availability of the necessary number of well-known materials with different chemical composition. A way to overcome this problem is the use of the Monte Carlo method.

The Monte Carlo method is broadly used for photons and particles transport [5,12,15,19]. It became a powerful tool, very flexible and enables the analysis of a wide energy range. When applied together with a spectrometry system, provides means to determine the detector's response function, optimizing both time and financial resources.

Among the available codes, the MCNP5 – Monte Carlo N-Particle Code, developed by the Los Alamos National Laboratory [21,22], has been widely used for all kinds of purposes involving radiation transport.

2. Materials and methods

2.1. Experimental setup

The experimental setup consists of an X-ray tube (silver anode, 40 kV, 100 μA), a sample holder and a SiPin detector at a scattering angle of 90°. A distance of 12 mm from the sample to the X-ray tube with a collimation of 15 mm length and 6 mm internal diameter; a distance of 35 mm from the sample to the detector with a collimation of 25 mm length and 4 mm internal diameter. The silver anode provides an X-ray photon flux of 22.16 keV due to the Kα line. The experimental setup is shown in Fig. 1.

2.2. Reference materials measurements

Experimental measurements of well-known materials were carried out in order to be used as reference for the simulation setup

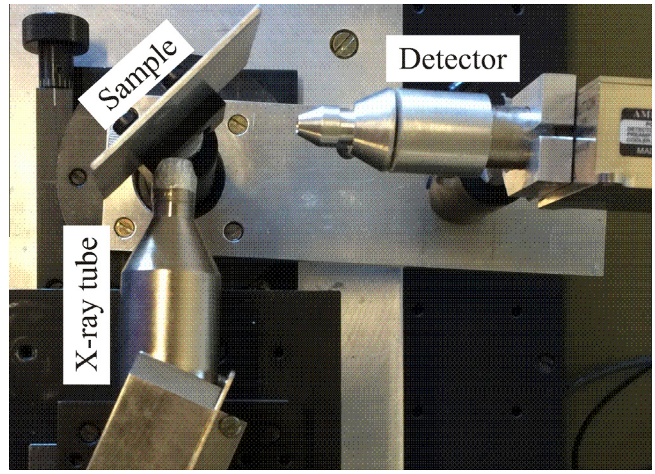

Fig. 1. Experimental setup for X-ray fluorescence measurement.

and verification of the results. The materials were powder pressed into a thin cylindrical shape of 25.4 mm diameter and 1.5 mm thick, with the exception of aluminum, which is metal. The materials used as reference are: Lucite, H_3BO_3, Na_2CO_3, $(NH_4)_2SO_4$, MgO, Aluminum, $CaSO_4(2H_2O)$ and KCl.

Because the energies for the Compton and Rayleigh peaks are close to each other, they might interfere with each other, leading to wrong Rayleigh to Compton scattering ratio values. In order to overcome this difficulty, only the left half of the Compton peak and the right half of the Rayleigh peak were considered, the continuum was subtracted taking as reference the lowest extreme of the peak.

2.3. Simulation of the measurement system

The simulation of the detector can be greatly simplified because only the ratio Rayleigh to Compton scattering areas of the spectrum will be used. Therefore, the knowledge of absolute detection efficiency is not necessary and, for this reason, the actual detector can be replaced, in the simulation, by simply counting the number of photons passing through a surface entrance window, discriminated by energy. The detection surface was defined by a sectional cut at the center of a sphere. Nevertheless, the experimental measurement must account for any difference in the efficiency detection between the Rayleigh and the Compton scattering areas of the spectrum.

The X-ray tube simulation was also simplified. It was considered as a pencil beam source of electromagnetic radiation of 22.16 keV, striking the sample right at its center. Because the knowledge of the peak areas absolute values is not necessary, but only the ratio Rayleigh to Compton scattering areas, there is no need to consider attenuation in the surrounding air, therefore, the measuring setup was simulated in vacuum. Both distances from the radiation source to the sample and the sample to the detector were 3 cm; the detector radius was 0.5 cm. Fig. 2 shows the simulation of the irradiation geometry of the X-ray fluorescence measuring system.

As the procedure is based in the ratio of areas of the same spectrum, not absolute values, the distance between sample and detector does not impose influence on the results, therefore, it is not critical to use the same distances used in the simulation for the experimental measurements.

2.4. Simulated material

For this approach, it was considered only the elements from Hydrogen to Calcium, excluding the noble gases, encompassing