Calculation of mass attenuation coefficients for x-ray fluorescence analysis using Rayleigh to Compton scattering ratio

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This report presents a study to determine the mass attenuation coefficient (MAC) by means of a Rayleigh to Compton (R/C) scattering ratio using the MCNP6 code [1]. A great difficult on the analysis of unknown materials composition is to account for self-absorption of the fluorescence photons that must be considered in the elemental concentration calculation. The number of characteristic X-rays emitted is counted by a detector and the elemental composition can be calculated. The self-absorption prevents a percentage of the emitted X-ray from reaching the detector leading to a lower calculated elemental concentration than the real one, which will depend on the material itself. Therefore, the self-absorption needs to be accounted for and proper correction in the elemental concentration calculation. The MAC is a way to account for the effect of each type of interaction and their probability. This work used Monte Carlo simulations to calculate the R/C for chemical elements up to atomic number 20 in a given energy. The experimental setup consists of an (22.16 keV due to the Kα) line X-ray tube (silver anode, 40 kV, 100 μA), a sample holder and a SiPin detector. Measurements of reference materials were performed at the scattering angle of 90^o. The experimental setup is shown in Figure 1. The powders materials were powder pressed into a thin cylindrical shape of 25.4 mm diameter and 1.0 mm thick; Lucite, Teflon and Aluminum were plates.

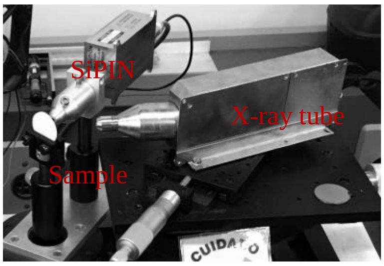

Figure 1. Experimental setup for X-ray.

Discussion

The simulations of an X-ray fluorescence analysis of also simulated material's disks by the MCNP6 code enabled the calculation of the R/C scattering ratios; the corresponding MAC were calculated with the XCOM program. The obtained data was plotted and fitted to a sixth power polynomial function in order to calculate the MAC for unknown materials, see Figure 2.

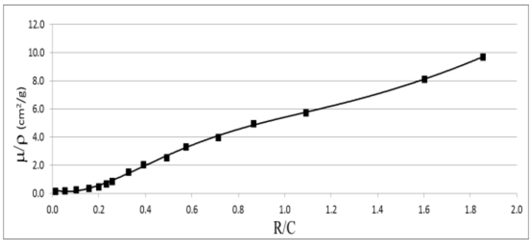

Figure 2. Data and the adjusted curve.

A great advantage of this methodology is that, by measuring the R/C scattering ratio for a single energy, the MAC of unknown materials can be calculated for others energies, sufficing for this, the determination of a R/C scattering ratio versus MAC curve for the energy of interest by Monte Carlo calculations. The correlation between the R/C scattering ratio to the MAC has proved to follow a single polynomial function for the first twenty elements of the periodical table with a correlation factor higher than of 0.998 for the sixth order function. The results presented here has proven to be of great asset to X-ray fluorescence measurements in order to correct for the self-attenuation, which is a difficulty encountered for quantitative analysis of unknown material. A great advantage of this methodology is that, by measuring the Rayleigh to Compton scattering ratio for one energy, the MAC of unknown materials can be calculated for others energies.

References

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