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Study of the response of energy dispersive X-ray spectrometers using Monte Carlo simulations

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Abstract. *Energy Dispersive X-ray Fluorescence Spectrometry (EDXRF) is a popular non-destructive technique that is used for qualitative and quantitative identification of elements. Because of the speed of the analysis and its non-destructiveness this technique has been very often used for archaeological studies. In this work we used the XRF spectrometer from Amptek®, with a gold anode and a SDD detector to characterize samples of gold and we performed a quantitative analysis using the XRS-FP software. We also successfully employed the XMI-MSIM software to simulate the response of the Amptek® detector.*

Keywords: *XMI-MSIM, EDXRF spectrometry, Monte Carlo Simulation, XRS-FP*

1. INTRODUCTION

One widely used technique for elemental analysis and identification is Energy Dispersive X-ray Fluorescence Spectrometry (EDXRF). The basis for the analysis using this technique is to measure and identify characteristic X-rays that are originated when electronic transitions are triggered by interactions of the atoms with high energy, short wavelength radiation. When the energy of the radiation is appropriate such interactions tend to occur, and an inner orbital electron can be removed which leaves the said atom unstable, making an outer electron take the place of the ejected electron.

Additionally to the elemental identification mentioned before XRF can be used to quantitavely identify the composition of samples. In our laboratory we use the XRS-FP program to perform the quantitative evaluation of the spectra obtained with the XRF equipement. This program heavily depends on the existence of paterns with elemental and quantity concentration similar to the one of the samples under scrutiny to provide the most accurate results. This difficulty makes the posibility of using simulation codes to theoretically reproduce the spectral response of ED-XRF helping to estimate the composition of the sample very appealing (Laszlo et al. (1993)).

The program XMI-MSIM is a code designed for predicting the response of energy dispersive X-ray spectrometers using MC simulations (Schoonjans et al. (2012)). It is an open source tool, that can be run on GNU/Linux as well as Windows and Mac systems.

In this work we analysed the elemental composition of gold pieces present in the Laboratory of Physical Tests of the Polytechnic Institute at UERJ using EDXRF and subsecuently ran the simulations with the program XMI-MSIM in order to reproduce the response from the experimental setup.

1.1 Methodology

X-Ray Fluorescence (XRF) can be described as an atomic emission technique, based on the photoelectric effect. When an atom is exposed to short wavelenth X-rays or gamma rays the ionization of it may occur. If the atom is exposed to and energy greater than it's ionization energy and electron from the one of the inner shells may be expelled and one of the remaining ones in an outer shell may occupy the place of the expelled electron in a process the atom goes throu in order to return to a less energetic state. During the transition process a characteristics energy photon is liberated (Fig. 1). These energies of the characteristic X-rays emitted by the elements constituting the sample are measured. To measure them it is necessary to separate them by their wavelength or by their energy. In this work, the ED-XRF (Energy Dispersive X-Ray Fluorescence) technique is used, which analyzes the characteristic X-rays through the identification and measurement of their energies. This technique also provides a qualitative analysis because the emitted radiation intensity is directly proportional to the species concentration(Nascimento Filho (1999)).

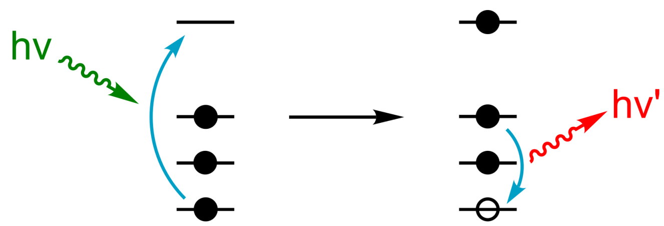

Figure 1- Esquematic representation of X-ray flourescence.

Briefly, an X-ray fluorescence analysis system is composed of three devices: an X-ray source, responsible for sample excitation, a detector that identifies and separates the characteristic X-rays and a multichannel plate that records the obtained spectrum and another electronic for signal feeding and amplification of signals from the detector (Parreira, 2007).

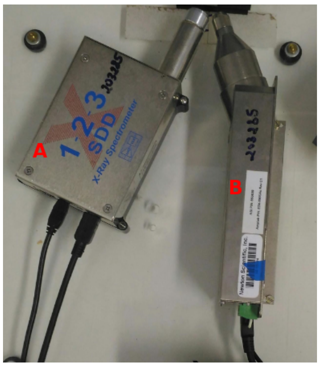

Figure 2- Representation of the equipement used.

The equipment used during this work is composed by a 123SDD detector (highlighted as A in Fig. 2), an X-ray tube with gold (Au) anode (highlighted as B in Fig. 2), electric source with voltage control and amperage, and a microcomputer where the analysis software is installed. For the experiment was used a monoenergetic X-ray beam with energy of 20 keV and 20μA and 600s adquisition time.

1.2 Qualitative analysis

At this stage we identify the chemical elements that make up the sample through its energy peaks. Samples are identified quickly without causing damage or sample destruction. The composition of the elements analyzed in this work is mainly Au and Cu.

1.3 Obtaining the spectrum

For a X-ray flourescence to be performed on a certain sample first we have to acquire the spectrum. The sample is excited using the X-ray source and once the relaxation process is completed the resulting X-rays are meassured on the detector. This detector has channels that discretize the received energy based on a scale previously set by a calibratioin process. The spectra is recorded in the computer for further analysis.

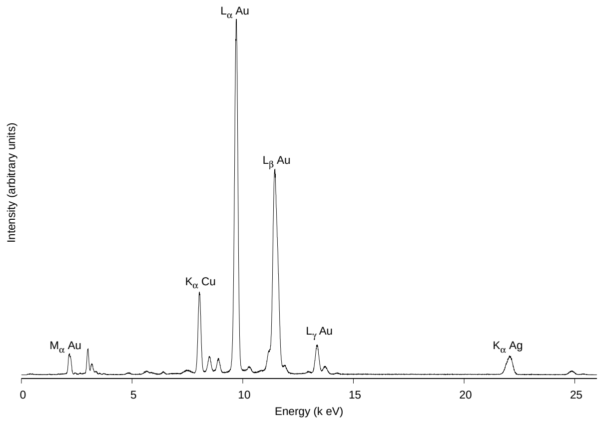

Figure 3- Example of X-ray flourescence spectrum. Main features for Au, Cu and Ag have been signaled.

2. RESULTS

We examined the samples labeled $1Au16$ and $1Au18$. Examples of EDXRF spectra and the simulated response are presented in Fig. 4 and Fig. 5.

	Quantification XRS-FP		Simulation XMI-MSIM	
	$1Au16$	$1Au18$	$1Au16$	$1Au18$
Cu	42.79%	17.19%	41.80%	15.00%
Au	57.21%	82.81%	57.60%	85.00%

Table 1- Resultados XRS-FP, XMI-MSIM

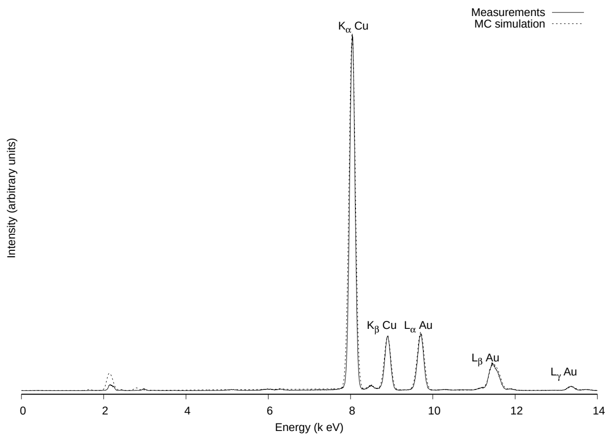

Figure 4- EDXRF and Monte Carlo simulation spectra for sample 1Au16

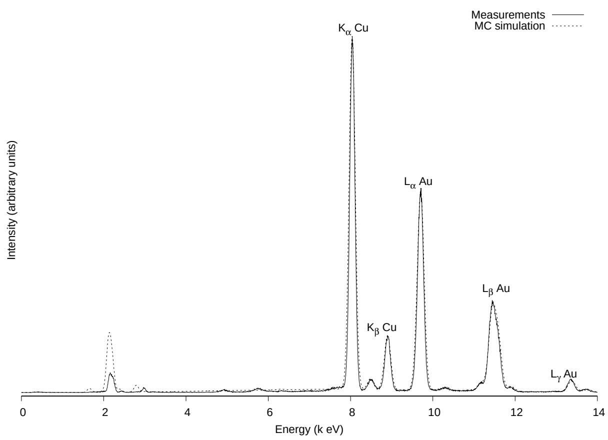

Figure 5- EDXRF and Monte Carlo simulation spectra for sample 1Au18

3. CONCLUSIONS

We have successfully used the software XMI-MSIM to simulate the response of XMI-MSIM software to simulate the response of the Amptek® XRF spectrometer.

Acknowledgements

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REFERENCES

A General Monte-Carlo Simulation of Energy-Dispersive X-ray-Fluorescence Spectrometers Part 1. Unpolarized Radiation, Homogeneous Samples. Laszlo Vincze, Koen Janssens and Freddy Adams. Spectrochimica Acta Part B, 48(4), 553-573, 1993.

A General Monte-Carlo Simulation of Energy-Dispersive X-ray-Fluorescence Spectrometers Part 2. Polarized monochromatic radiation, homegeneous samples. Laszlo Vincze, Koen Janssens, Fred Adams, M.L. Rivers and K.W. Jones. Spectrochimica Acta Part B, 50(2), 127-147, 1995.

A General Monte-Carlo Simulation of Energy-Dispersive X-ray-Fluorescence Spectrometers Part 3. Polarized polychromatic radiation, homogeneous samples. Laszlo Vincze, Koen Janssens, Fred Adams and K.W. Jones. Spectrochimica Acta Part B, 50(12), 1481-1500, 1995.

A General Monte-Carlo Simulation of Energy-Dispersive X-ray-Fluorescence Spectrometers Part 4. Photon scattering at high X-ray energies. Laszlo Vincze, Koen Janssens, Bart Vekemans and Fred Adams. Spectrochimica Acta Part B, 54(12), 1711-1722, 1999.

T. Schoonjans, L. Vincze, V. , A. Solé, M. Sanchez del Rio, Ph. Brondeel, G. Silversmit, K. Appel, C. Ferrero, A general Monte Carlo simulation of energy dispersive X-ray fluorescence spectrometers - Part 5, Polarized radiation, stratified samples, cascade effects, M-lines, Spectrochim. Acta B. 70, (2012) 10–23.

Nascimento Filho, V.F. Técnicas analíticas nucleares de fluorescência de raios X por dispersão de energia (EDXRF) e por reflexão total (TXRF). *Piracicaba: Escola Superior de Agricultura Luiz de Queiroz*, 1999.

Parreira, P.S. Metodologia de ED-XRF e aplicações com um sistema portátil. *vol 1, N. 02*, 2007. Publicação Técnica