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Toward a maximum information utilization approach in EDXRF analysis of soil samples

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We have recently presented a new approach in signal processing [1], where all events are accounted for, as opposed to other systems, where only the events satisfying the conditions of preset discriminations are collected. In our processors a minimum two spectra are collected, one for the accepted events, satisfying the discrimination conditions, and one for the rejected events, failing to meet the quality levels set by the discriminators. Such an approach is mandatory for proper spectroscopy, as it must be known whether the rejected events were rejected because they were degraded, noisy, event plus noise pile up or event plus event pile up. In the last case we have two lost events, while in the previous cases we have one lost event. It is also frequent when high input rates are used that multiple pile ups can occur, implying that the rejected event corresponds to multiple lost events. This development prepared the technological background to use the fundamental parameter method in Energy Dispersive X-Ray Fluorescence (EDXRF) analysis.

In our fundamental parameter approach the detector response function is parameterized, and a Voightian line shape is used for the model description of the characteristic x-ray peak in the spectrum. We will present the model description for the scattered peaks. The x-ray spectrum available for the analysis does not usually contain direct information on the presence and quantity of the low atomic number elements, as their characteristic x-ray lines are not visible in the EDRXF x-ray spectrum. Therefore, it is necessary to use all the possible sources of information to derive the bulk matrix composition.

The information available from the spectrum and can be used for the approximate determination of the bulk matrix composition are the x-ray lines of elements visible in the spectrum and the scattered peaks of the primary radiation. Further easily available information are the sample thickness and density.

This information is not sufficient to determine the bulk matrix composition unambiguously with the desired accuracy. To obtain further information for bulk matrix composition verification, sample arrangement techniques were investigated and the richness of the additional information will be reported.

Beyond these developments, our software package contains an equipment characterisation software in addition to the Fundamental Parameter XRF software. This is also a necessary tool, as the detector and excitation function may change in time, and re-calibrations of the detector and the primary excitation function is offered from a single measurement on a well-designed standard.

Reference

[1] T. Papp, A.T. Papp and J.A. Maxwell, Quality assurance challenges in x-ray emission based analyses, the advantage of digital signal processing; Analytical Sciences 21 (2005) 737-745