

MCLLS Approach to EDXRF Analysis on XOS Devices

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ABSTRACT

The Monte Carlo – Library Least-Squares (MCLLS) approach has been developed and implemented to model the complete spectral response of energy-dispersive X-ray fluorescence (EDXRF) spectrometers and perform an inverse elemental analysis by an iterative linear Library Least-Squares method for sample composition when an initial guess is provided. The approach contains three advanced technologies developed by CEAR researchers since 1970: a comprehensive and accurate Monte Carlo forward simulation code – **CEARXRF5**, Differential Operators for elemental libraries, and Detector Response Functions. From benchmark experiments with standard reference materials (stainless steels from NIST and aluminum alloys from Alcoa), this approach has been demonstrated to be very accurate. It is also very fast when Monte Carlo pre-calculations can be made for anticipated classes of samples. An integrated visualization system (Graphical User Interface) has been designed for analysts to easily use this approach.

The approach has been implemented on trace elemental analysis instruments from X-Ray Optical Systems, Inc. (XOS) developed for medical and industrial applications. XOS uses their doubly curved crystal (DCC) beam optics to provide a mono-energetic source and focus it to a very small spot. This instrument technology is called high definition XRF, or HD XRF. HD XRF also uses a digital pulse processor on the detection side, which is not required for MCLLS. Since the counting rates are generally high in real-time applications and there exist pulse pile up problems in the measurement spectra, the authors have also developed an exact method to correct for any spectral distortion due to pulse pile up. The authors have also developed an accurate detector response function for XOS specific devices. Benchmark experiments on standardized materials using the XOS systems are presented and illustrate that the entire sample spectra from samples can be generated and used. The CEAR and XOS teams compared the MCLLS results to the fundamental parameters (FP) approach as well. Some of those results are discussed here.

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