L.14: Deepti, an application to visualize and analyze x-ray fluorescence spectra

A µ-XRF beamline (BL-16) has been setup on the Indus-2, with an experimental emphasis on atomic physics, fundamental parameters (FP) evaluation for quantitative x-ray fluorescence analysis, biomedical and material science applications involving heavy metal speciation and their localization. The beamline works in the x-ray energy range 4-20 keV. It provides both microfocused and collimated beams at the experimental station. BL-16 beamline offers a wide range of measurement capabilities which include microprobe XRF examination of a specimen for spatial distribution of elements, energy dispersive x-ray fluorescence (EDXRF) analysis and total reflection x-ray fluorescence (TXRF) characterization of materials at ppb (parts per billion) levels with a short spectrum acquisition time.

To assist BL-16 beamline users in XRF data analysis, an interactive, GUI based, user friendly application named *Deepti* (दीप्ति) is developed to visualize x-ray fluorescence spectra as well as to analyze fluorescence peak intensities of different elements using spectra unfolding. It is also possible to use Deepti on different Indus-2 beam lines for processing fluorescence spectra, hence it has been facilitated with an option to read, write and copy fluorescence spectrum data in various international used formats.

To eliminate spectral noise in the XRF spectrum, various noise removal techniques have implemented in the Deepti, such as programmable FFT filter. To remove fluorescence spectral background, a non-linear background subtraction method was developed and provided in the Deepti (Fig. L.14.1). The method allows users to define individual background points in the fluorescence spectrum and estimate full spectral background. Depending on the requirement of background smoothness, a polynomial of order from 3 to 11 can be used to fit. It is possible to select background points through a mouse click. Once selected, they appear as highlighted points in the fluorescence spectrum. The background subtracted spectrum can be superimposed on the raw spectrum for easy comparison. In addition, options are also provided to fit observed fluorescence peaks using Gaussian and Lorentzian curve fitting; it provides detailed fitting statistics in the tabular format. The standard statistical features such as net area determination, FWHM peak width, and standard deviation for a fluorescence peak can be obtained readily.

Apart from peak fitting features, Deepti also provides determination of the Gross and Net of a fluorescence peak without and with background subtraction respectively. The spectrum background is processed automatically using least square method. The region of interest (ROI) selection can be changed or moved easily over entire range of the spectrum channels. The area for a selected ROI populates in the table with detailed statistics and its file name. The processed data can be copied or exported to an Excel file.

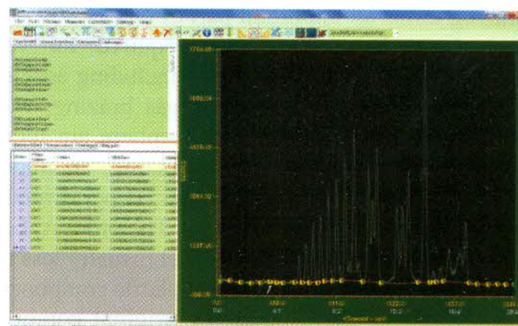

Fig. L.14.1: Non-linear background points marking and substraction

Quantitative estimation of the elements composition by spectroscopic techniques using X-ray fluorescence requires accurate data of x-ray interaction with matter. In the literature several empirical formulas have derived to obtain these fundamental parameters for x-ray interaction with matters and are available freely in the form of x-ray library functions. These x-ray libraries are mainly callable functions. In Deepti, x-ray library (xraylib) has been incorporated to use as x-ray calculator for many x-ray fundamental parameter constants.

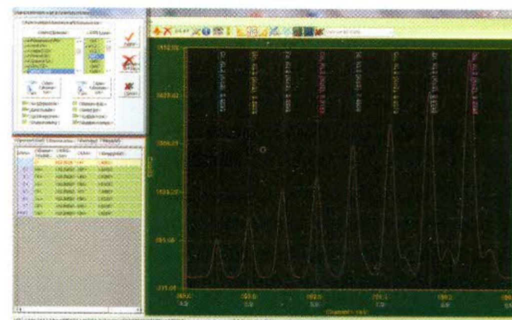

Fig. L.14.2: Tagging of emission energy lines on the XRF spectrum

Application also provides selection of any element of the periodic table, atomic shell and emission lines. The width of atomic shell, fluorescence yield, jump factor, Auger yield, edge energy, and electron configuration of any shell of any elements can be found easily. Further, emission line, denoted using IUPCA notation, can be selected; the energy of the emission line and its radiation rate can be obtained. Additionally facility is provided to tag (Fig. L.14.2) XRF spectra for multiple selected elements and their emission lines which are highlighted on the XRF spectrum in selected formats.

Reported by:
H.S. Vora (vora@rrcat.gov.in) and Rajiv Jain