Introduction
Since their inception during the Manhattan project, Monte-Carlo simulations have been used for a variety of applications in physics, mathematics, engineering, finance and more. When applied to X-ray fluorescence spectroscopy, it is well known that Monte-Carlo simulations are useful for predicting the spectral response of samples irradiated with an X-ray beam of given characteristics. This requires the development of a dedicated computer code that simulates the histories of a large number of individual photons, whose trajectories in the system are modeled as a number of straight steps. At the end of each step, an interaction occurs, leading to a change in direction, energy and polarization state. A photon’s trajectory is terminated when it leaves the system, or when the detector captures it. If detection occurs, one count is added to the appropriate channel of a virtual multichannel analyzer. The algorithm is greatly optimized through the introduction of variance reduction techniques.

XMI-MSIM
• Software package dedicated to the Monte-Carlo based simulation of ED-XRF spectrometers
• Useful for predicting the outcome of experiments, optimization and design of spectrometers in silico, detection limits estimation, quantification
• Based on the work of Vincze et al.
• Physical datasets (cross sections, line energies etc.) provided by xraylib
• Simulation of M-lines and cascade effects (radiative and non-radiative)
• Improved detector response function: pulse pile-up and fluorescence/Compton escape peaks. Custom detector response functions are callable through plug-ins.
• Highly accurate Compton peak scattering (optional) based on the work of Fernandez and Scot
• Support for multheadning (OpenMP) and multiprocessing (MPI)
• Graphical user interface: create input-files, launch simulations and visualize results
• Batch mode: vary one or two simulation parameters and investigate the influence on the intensity
• Import excitation spectra from ASCII files or use the X-ray sources window to produce an appropriate excitation spectrum based on Ebel’s X-ray tube model or radionuclides.
• Callable as a plugin from PyMca: quantification of XRF data
• Written in ANSI-C and Fortran 2003
• Based on GNU Scientific Library, libxml2, libxslt, HDF5, GTK+...
• Extensive documentation
• Distributed under the GNU General Public Licence: www.github.com/tschoonj/xmimsim

References

Experimental
Validation measurements were performed at beamline L of HASYLAB, Hamburg. The beam was unfocused and monochromatized using a multilayer monochromator at varying energies, depending on the sample. The intensity of the beam was reduced using exit slits and a 1mm Al absorber. The X-ray fluorescence and photons were collected using a Vortex Si drift detector.