Modelling of Amptek's Experimenter's XRF Kit for X-ray Fluorescence Analysis Using MCNPX Code

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Abstract. In this study, we present the modeling of the Amptek Experimenter's XRF Kit using the MCNPX Monte Carlo code to simulate and analyze X-ray fluorescence (XRF) spectra of Fe-Cr binary alloys with varying chromium content ranging from 1 to 50 at%. The model includes detailed geometrical and material descriptions of the spectrometer setup, X-ray source, and detector. By applying the F2 and F8 tallies along with Gaussian energy broadening, the MCNPX simulations allow for accurate prediction of spectral features, including peak shapes and relative intensities. The results were compared with experimentally measured spectra, showing a good agreement in both peak positions and relative intensities after correcting for known energy offsets. Particular attention was paid to matrix effects, which were found to significantly influence the net peak areas in alloys of studied compositions. A quantitative correlation between simulated and measured data was established, and polynomial fitting functions were derived to model the dependence of photopeak intensities on elemental composition. The study demonstrates the reliability and potential of Monte Carlo simulation as a powerful tool for quantitative XRF analysis, especially in complex systems affected by matrix effects.