USE OF MONTE CARLO SIMULATION METHODS TO IMPROVE X-RAY DETECTOR RESPONSE FUNCTION

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An accurate X-ray detector response function is needed for many applications involving X-ray spectroscopy and elemental analysis. Previously, a semi-empirical detector response function using Gaussian peak models and exponential tails was used to characterize detector response functions. The limitation of such an approach is that it is only valid for photon energies less than about 60 keV. The use of Monte Carlo methods to simulate detector response functions has been developed to expand the valid energy range. In addition to improved accuracy, other benefits are: it can be used to predict spectral shape characteristics and detection efficiency of the X-ray detector spectral response for any specified incident energy; and it is a powerful variance-reduction technique. The detector response functions are convolved with the incident X-ray photon detector surface flux spectrum to generate pulse-height spectra that can be compared with experimental spectral data.

The Monte Carlo-based detector response function model incorporates complete X-ray interaction physics including coherent interaction, incoherent interaction (with Doppler effects), photoelectric absorption and X-ray fluorescence, and pair production and bremsstrahlung for incident energy higher than 1.022 MeV. Furthermore, a semi-empirical electron transport model is used with tuning parameters to accurately describe the flat continua of the spectra.

Benchmark experiments of the Monte Carlo detector response function on the Si X-ray detectors were performed on the elements Al, Si, Ti, V, Cr, Mn, Co, Ni, Cu, Zn, and Pb, excited by 17.5 keV mono-energetic X rays on a micro-focused X-ray spectroscopy analyzer. The parameters of the semi-empirical electron model are optimized by weighted least-squares regression of the pulse-height spectra from pure-element samples. Comparisons with experimental spectra are presented and indicate good agreement, demonstrating that the Monte Carlo Simulation Method can be an alternative accurate approach to generate detector response functions. As the detector response functions are pre-calculated with high statistical precision, they can be used as an excellent variance-reduction approach to speed up the convolution process.