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Energy Dispersive X-ray Spectrum Simulation with NIST DTSA-II: Comparing Simulated and Measured Electron-Excited Spectra

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NIST DTSA-II is an open-source, comprehensive software platform for the analysis and simulation of electron-excited energy dispersive X-ray spectra (EDS) [1, 2]. The EDS spectrum simulation tool is based upon a Monte Carlo electron trajectory calculation that incorporates reference data for electron scattering and energy loss as well as characteristic X-ray generation parameters such as ionization energy, ionization cross section, and weights-of-lines as well as X-ray continuum (bremsstrahlung) generation. The user interface provides several target geometries, including a flat bulk target, a thin film on a flat bulk target, an embedded particle in a bulk matrix, and free-standing particles of various shapes (sphere, cube, cylinder, pyramid) on a substrate. For each electron trajectory segment, the generation of characteristic and continuum X-rays and their subsequent propagation and absorption within the target in the direction of the EDS are determined, including absorption by the detector window and surface electrode, as well as loss due to transmission through the EDS detector. The overall X-ray intensity is scaled by the solid angle which can be estimated to within approximately ±5% [3] and further refined by adjusting the sample-to-detector distance. The detector resolution function (i.e., peak broadening) is then applied to the intensity in each energy channel. The DTSA-II simulation calculates the absolute intensity for the user-specified dose (beam current × detector live-time), detector solid angle (active area, distance, and window transmission fraction), and detector elevation angle, enabling appropriate counting statistics to be applied to each channel intensity to create the final “noisy” spectrum. This simulated spectrum can then be directly compared with the measured spectrum. An example is shown in Figure 1 of measured and simulated spectra of FeS_2 at a beam energy of 15 keV. Several specific numerical comparisons are shown as the ratio of the X-ray peak intensity (background corrected using the DTSA-II P-B function) of the Monte Carlo (“MC”) simulation to the measured (“EXP”) intensity: Fe K-L3 (MC/EXP = 1.03); S K-family (1.14); Fe L-family (0.89); and for the X-ray continuum region 3 keV–3.5 keV (1.02). Deviations in the intensities between the simulated and measured spectra occur because of uncertainties in the measured spectrum (e.g., the probe current measurement) and due to uncertainties in cross-sections and other physical data for the simulation. Comparison of the spectra also reveals artifacts that occur in the measured spectrum, including the combined coincidence of the S K-family peak and Fe K-L3 silicon escape peak that produces the slight increase in the measured spectrum around 4.6 keV, which are not included in the simulated spectrum, as well as low intensity peaks for C, likely due to contamination, Al from polishing alumina, and Si, a trace constituent. Figure 2 shows a similar comparison for 60Au-40Cu (NIST SRM 482, Gold-Copper Alloys) at E_0 = 20 keV. Points of comparison include Cu K-L3 (1.06); Cu L-family (0.75); Au L3-M5 (1.10); Au M-family (1.49); and the X-ray continuum from 6 keV–6.5 keV (0.99). Extensive studies of pure elements and binary stoichiometric compounds excited at E_0 = 20 keV reveal that for the K-shell and L-shell X-rays in the energy range from 1 keV to 12 keV, the simulated and measured spectra generally agree within ±25%, whereas for M-shell X-rays, the simulated intensity exceeds the measured intensity by 25% to 100%. For the X-ray continuum in the 1 keV to 12 keV range, the agreement is generally within ±10%.

References:
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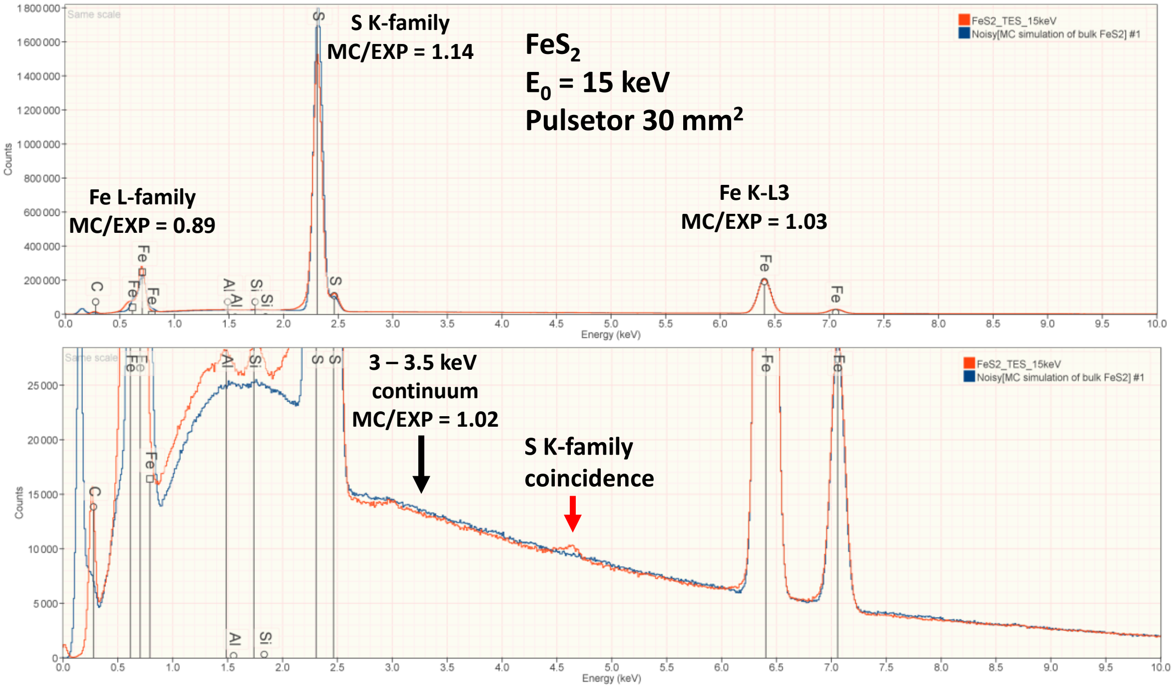

Figure 1. Comparison of measured (red) and simulated (blue) EDS spectra of FeS_2 at E_0 = 15 keV.

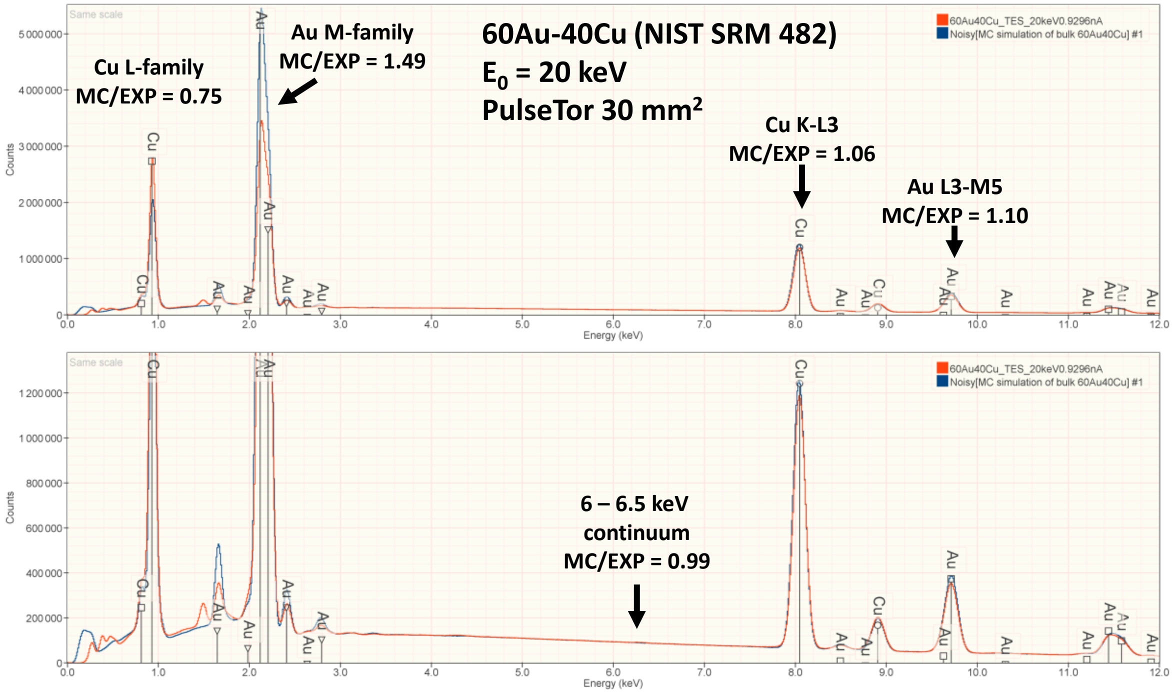

Figure 2. Comparison of measured (red) and simulated (blue) EDS spectra of 60Au-40Cu (SRM 482) at E_0 = 20 keV.