

DTSA-II: A New Tool for Simulating and Quantifying EDS Spectra – Application to Difficult Overlaps

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DTSA-II [1] is a reinvention of the popular NIST-NIH Desktop Spectrum Analyzer [2] simulation and analysis product. DTSA-II is a from-the-ground-up reimplement of the basic standards-based spectrum analysis tools and provides spectrum simulation through the NISTMonte [3] Monte Carlo simulation package. DTSA-II has been designed to be both easy-to-use for the novice microanalyst and powerful for the expert. These conflicting goals are met by a series of *wizard-like* interfaces for performing common operations plus a Python-based command line for sophisticated operations. DTSA-II is available for many popular operating systems.

Using DTSA-II's wizard interfaces, it is possible to readily simulate spectra from a handful of geometries on user specified detector configurations including lithium-drifted silicon (Si(Li)), silicon drift detectors (SDD) and microcalorimeter detectors. These simulated spectra may be analyzed exactly as you might analyze a measured spectrum using a standards-based quantitative analysis wizard. Together, they form a powerful yet easy-to-use tool for interpreting experimental measurements.

We applied DTSA-II to study certain notoriously difficult peak overlaps. This application demonstrates how DTSA-II's spectrum simulation and standards-based spectrum analysis tools may be combined through a Python script to perform an otherwise tedious numerical experiment. Traditionally, (Th-M & Ag-L), (Fe-L & F-K), (Pb-L & S-K) and (Al-K & Br-L) are considered practically impossible to differentiate using EDS. By eye, it is easy to mistake one for the other. Despite its popularity the eye is not the best tool for deconvolving EDS spectra – fitting standards can do a much better job. We demonstrate this by considering spectra consisting of mixtures of each of these pairs of elements for various different count statistics. Using a Python script, we generated spectra for a range of compositions between pure one element and pure the other for a nominal total number of x-ray events of 10^3 , 10^4 , 10^5 and 10^6 counts. For each combination of composition and counts, 10^3 spectra were generated and fit using a high quality (10^6 count) reference spectra. The fit values were compared to the known values. The experiments were repeated for a nominally 135 eV and a nominally 175 eV resolution Si(Li) detector. Modern Si(Li) detectors at close-to-best resolution (5 kcps OCR) are capable of collecting this number of counts in 0.2, 2, 20 and 200 seconds and a state-of-the-art SDD (500 kcps OCR) can collect the same number in < 0.002, 0.02, 0.2 or 2.0 seconds. While these times might seem short, they are the types of acquisition times appropriate for x-ray mapping and for high speed particle analysis. All spectra (both unknown and reference) were simulated with Poisson count statistics using NISTMonte. The unknowns were created by mixing noise-free spectra according to the desired k-ratios and then applying Poisson statistics. The noisy unknowns were fit with the noisy references and the fitted k-ratios tabulated for comparison with the known k-ratios. The results are discussed in the figures.

The results demonstrate that even for difficult overlaps and for relatively poor count statistics, it is feasible to make confident statements and attach credible uncertainty estimates to fitted k-ratios. Our results also demonstrate that while there is no doubt that detector resolution helps, there is no replacement for x-ray counts. In fact, in many circumstances, it may be better to

compromise resolution for count rate as can be done on a Si(Li) detector by increasing probe current and decreasing the pulse process time.

[1] DTSA-II, Nicholas W. M. Ritchie (2008); public domain software available from the National Institute of Standards and Technology website:

<http://www.cstl.nist.gov/div837/837.02/epq/dtsa2/index.html>

[2] Desktop Spectrum Analyzer, C. Fiori, C. Swyt, and R. Myklebust (1991); public domain software available from the National Institute of Standards and Technology website:

<http://www.cstl.nist.gov/div837/Division/outputs/DTSA/DTSA.htm>

[3] Nicholas W. M. Ritchie, Surf. Interface Anal. 2005; 37: 1006–1011

[4] F. H. Schamber in “X-ray Fluorescence Analysis of Environmental Samples”, Thomas Dzubay, Editor, Ann Arbor Science Publishers (1977)

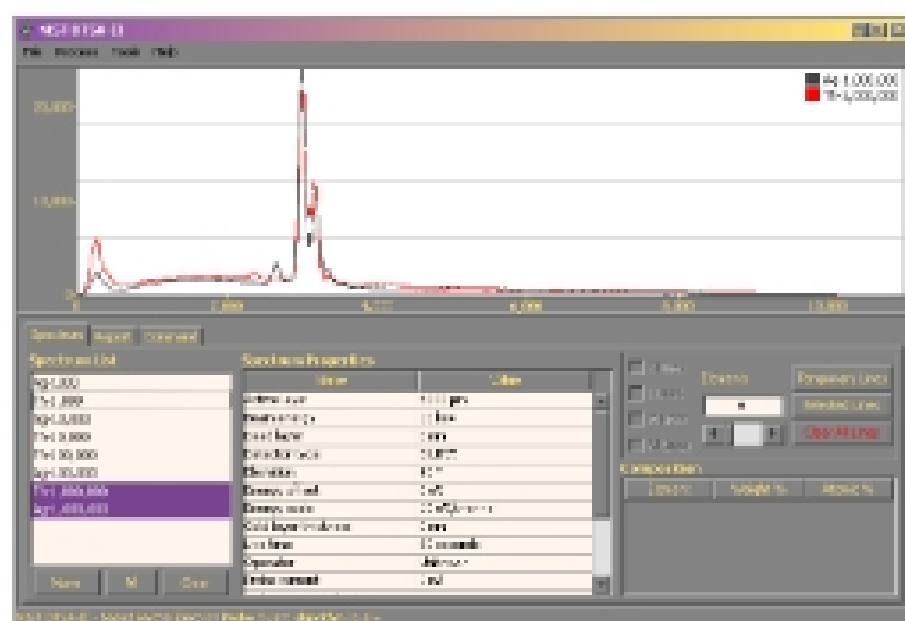


FIG 1: The main screen for the DTSA-II software showing Monte Carlo simulated 10^6 count Ag and Th spectra. ($E_0=10$ keV)

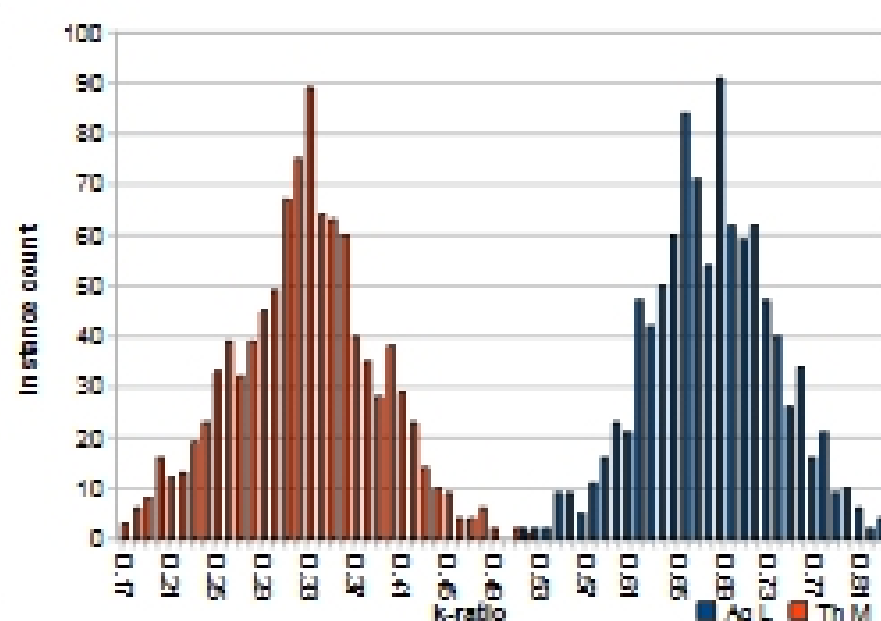


Fig 2: Histograms of 10^3 simulated 10^4 count simulated measurements of 0.32 Ag and 0.68 Th. The standard deviations of these two distributions are represented by the circled points in Fig. 2

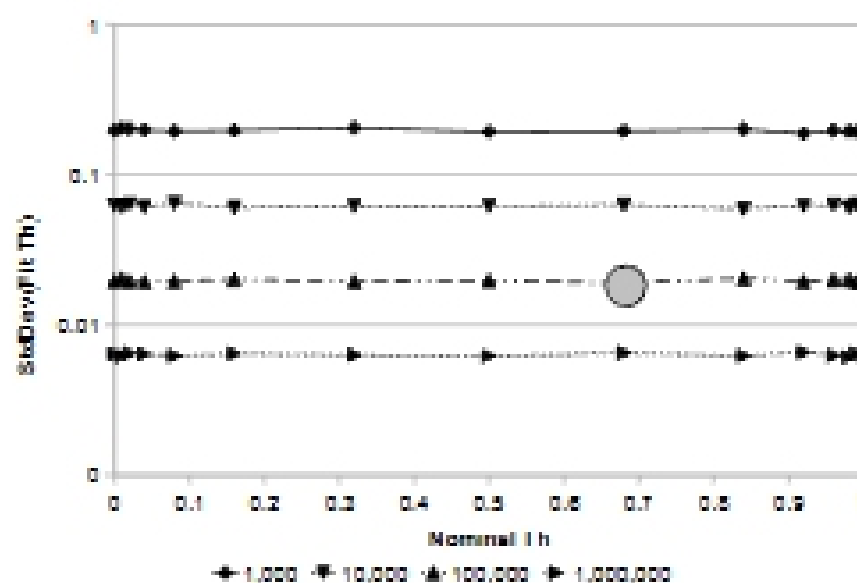
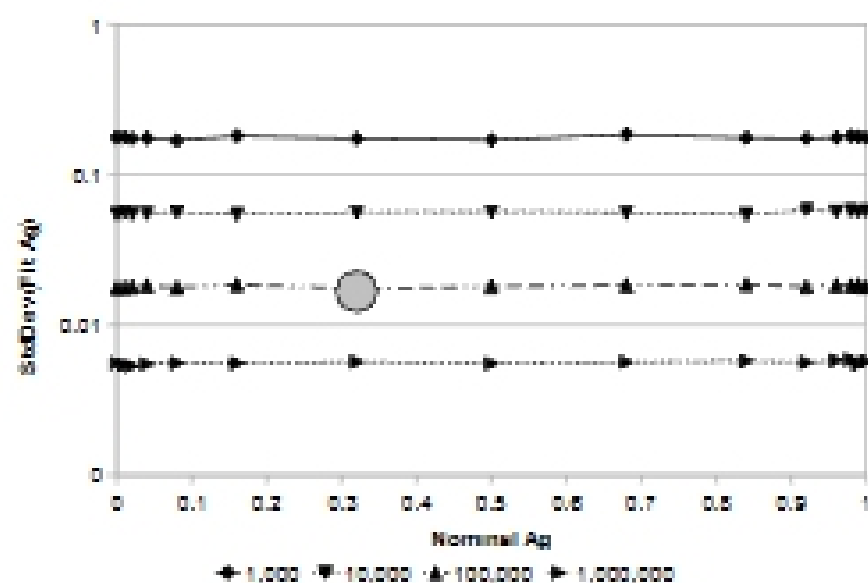


FIG 2: The standard deviation of the fits for the Ag-L / Th-M overlap. As the number of counts in the spectrum increases from 10^3 to 10^6 , the ability to reliably differentiate Ag-L from Th-M improved. For a 10^6 count spectrum, this data suggests that it is possible to quantify Ag and Th to better than 1% regardless of the presence of the other element. For comparison, the scaled filter-fit covariances [4] were 0.17, 0.05, 0.02 and 0.005 for Ag and 0.21, 0.07, 0.02 and 0.007 for Th suggesting that the filter-fit covariances are an excellent estimate of the fit uncertainty.