Measuring Pixel Classification Accuracy Using Synthetic Spectrum Images

NIST researchers used a novel Monte Carlo simulation program, NISTMonte, that generates an electron-transport and X-ray generation Monte Carlo simulation for complex 3D geometries. NIST used "phantoms" or artificial data sets to generate X-ray spectrum images. The resulting data cubes are perfectly suited for measuring the accuracy of various pixel classification algorithms currently applied to microanalysis problems.

J.H.J. Scott, N. Ritchie (Div. 837)

The proliferation of commercial microanalysis equipment capable of acquiring electron-excited X-ray spectrum image data in the scanning electron microscope (SEM) has been a boon to researchers and industrial users who rely on X-ray microanalysis to characterize the spatial distribution of elements in solid microstructures. Frequently such systems come with software to classify the pixels in the acquired data cubes into distinct classes or categories. This is a difficult problem because of the physics of the interaction of the electron beam with the sample, differential absorption of the emitted X-rays, and susceptibility of the algorithms to noise. Metrics for measuring the fidelity of these classifiers are non-existent in the microanalysis community, mainly due to the lack of certified reference samples with known spatial phase distributions. Using techniques from the medical imaging community, classification accuracy metrics can be based on synthetic "phantoms", or artificial datasets with known properties. The availability of such phantoms enables the robust evaluation of classification schemes.

Using NISTMonte, an electron-transport and X-ray generation Monte Carlo simulation for complex 3D geometries, full electron-excited X-ray spectrum images were generated for multiphase phantoms.

Data cubes were generated by inputting synthetic datasets with known properties into the NISTMonte simulation package. This methodology is perfectly suited for measuring the accuracy of various pixel classification algorithms currently applied to microanalysis problems.

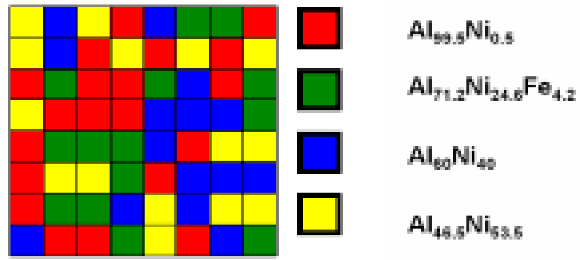

Figure 1: *in silico* phantom used to generate synthetic spectrum image data, the legend shows color codes for chemical phases in phantom.

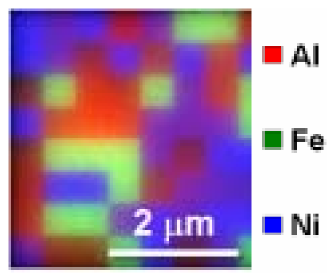

Figure 2: RGB false color X-ray intensity map derived from simulated spectrum image, the legend shows the map (red, green, blue) = (Al, Fe, Ni) X-rays respectively.

Future Plans: Additional spectrum image data cubes will be generated to develop a suite of benchmark problems with known solutions for classification methods. Current and future developers of classifiers can test their code's performance against their peers and against absolute metrics of interest to end users of the classifiers such as microanalysts

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