Interpreting Five Dimensional X-ray Images with Machine Learning

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The Color X-ray Camera (CXC) [1] is a unique imaging spectrometer capable of recording both the position and energy of each X-ray event on the detector. With a frame readout rate of 1000 Hz, the camera is able to produce data at a rate of approximately 140 MB/s. When combined with a micro focused X-ray source, the CXC can create X-ray maps of heterogeneous materials by addressing the beam to an array of points on the sample and saving a hyperspectral data cube at each point. With maps of large specimens running for as long as 40 hours, the amount of data that needs to be processed and interpreted can easily exceed 1 TB. Using both machine learning and "Big Data" techniques, these data can be compressed (typically as sparse matrices), compiled (by separating data based on isotropic or non-isotropic scattering) and interpreted to provide information about specific materials in the sample. Figure 1 shows an example of data analysis from a five dimensional image of a series of minerals in an epoxy mount. The goal was to identify and separate the materials based on both the compositional information (i.e., XRF) and crystallographic information (i.e., XRD). To achieve this, a self organizing map (SOM) [2] was used as an unsupervised classification method, first on the compositional data, then further refined using the crystallographic data.

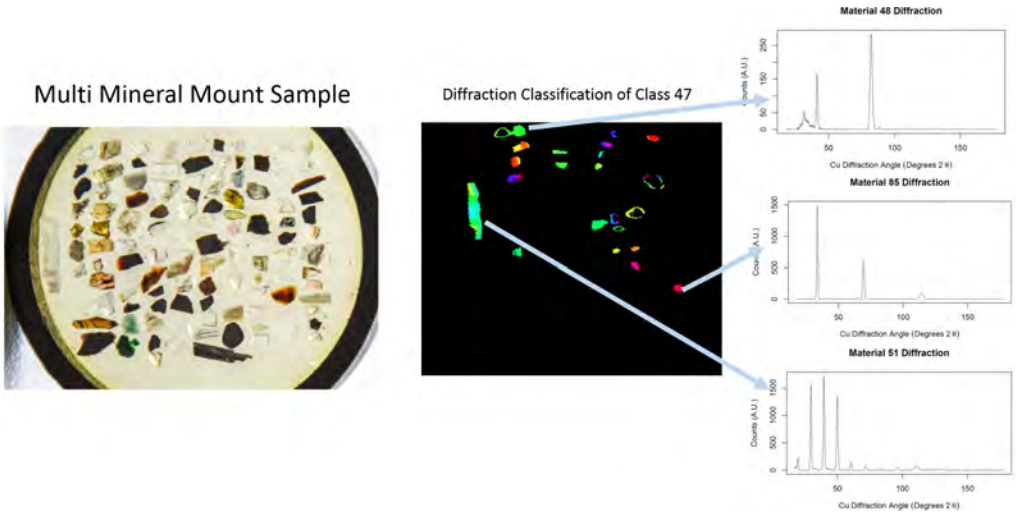

Figure 1: (Left) A photograph approximately 100 minerals in a flat polished epoxy mount. (Right) A mask of class 47, as identified using an SOM on the XRF data, then again on the XRD data to identify the materials present. The diffraction patterns from some of those materials are shown on the right.

References:
[1] Scharf, O., Ihle, S., Ordavo, I., *et al*, Compact pnCCD-based X-ray camera with high spatial and energy resolution: A color X-ray camera, Analytical Chemistry, **83** (2011), p. 2532:2538.
[2] Kohonen, T., Self organized formation of topologically correct feature maps, Biological Cybernetics, **43** (1982), p. 59:69.