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PIXE real-time quantitative image projection applied to synchrotron XRF imaging using the X-ray Fluorescence Microprobe

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Energy dispersive spectra from proton induced X-ray emission (PIXE) analysis of minerals can display severe multi-element overlap that can hamper imaging approaches that rely on regions of interest. A method called *Dynamic Analysis* (DA), developed at the CSIRO, builds a matrix transform to unfold the contributions of overlapping elements, rapidly performing the effect of a linear least squares fit to each pixel spectrum [1]. Projection of companion variance images aid in tracking uncertainty contributions. Once constructed, the transform can be applied in real-time to image elemental distribution in other sample areas with similar elemental components.

PIXE and synchrotron X-ray fluorescence (SXRF) display many similarities, such as non-destructive trace element analysis, deep penetration and similar X-ray spectra. These similarities have enabled the adaptation of the DA method to generate real-time elemental images using the X-ray Fluorescence Microprobe (XFM). DA for SXRF has been implemented in the GeoPIXE software [2] using the recent compilations of sub-shell absorption cross-sections of Ebel [3], the Coster-Kronig rates, fluorescence yields and branching ratios of Elam [4] and an empirical treatment of scatter peaks.

The DA transform successfully deconvolutes overlapping elemental components (Fig. 1). However, it assumes a uniform matrix composition, which needs to be corrected. The correction uses projection of the elemental concentration images onto images of end-member component proportion. Fundamental parameter yields calculated for these components are then combined to estimate improved concentration images. This procedure is repeated to converge on self-consistent elemental concentrations for each pixel; initial concentration errors of >50% can be reduced to <3% in ~3 iterations (as compared with electron microprobe point analyses; [1]).

Quantitative images provide a platform for further refinement. Contrasts in sample composition between pixels can cause edge artefacts if X-rays generated sub-surface pass through minerals of different X-ray absorption on their way to the detector. This too can be successfully corrected in an iterative procedure, despite implicit assumptions about grain boundary angle (Fig. 3) [5]. Pile-up induced effects reflect the product of major element line intensities. This effect can be modelled using image products to construct corrections to remove pile-up artefacts in images [6].

The method was tested using 16.1 keV photons from the 2-ID-E XFM at the APS. Fig. 1 shows successful DA projection of elemental images of a test sample, consisting of metal pieces on a glass slide (Fig. 1a), despite severe spectral overlaps (Fig. 2). Fig. 4 shows images of a gold-bearing pyrite imaged under similar conditions [7].

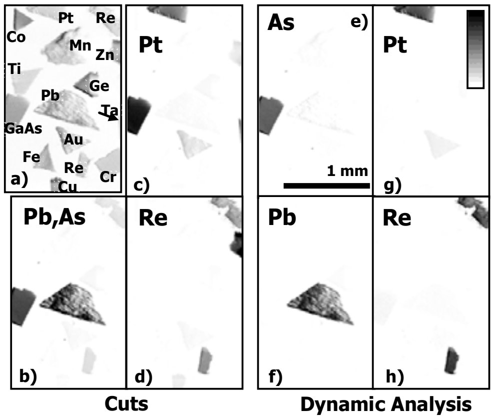

Fig. 1 Test sample (a) imaged using SXRF and projected using energy Cuts or the DA method (scan area 1.4 x 2.4 mm^2, 141 x 241 pixels).

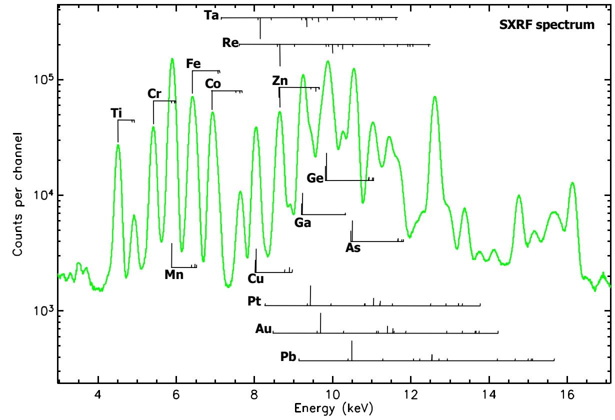

Fig. 2 Total SXRF spectrum over sample in Fig. 1a using 16.1 keV photons. Note the degree of overlap between constituent elements.

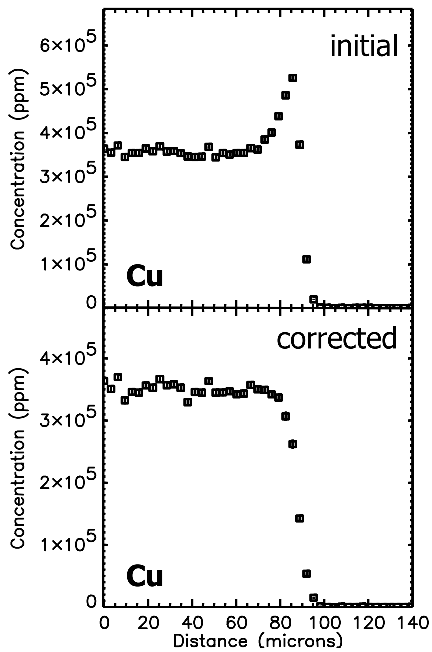

Fig. 3 Traverse across the edge of chalcopyrite ($CuFeS_2$; on left) bordering quartz showing concentrations before (top) and after (bottom) iterative differential absorption correction assuming all boundaries normal to sample surface.

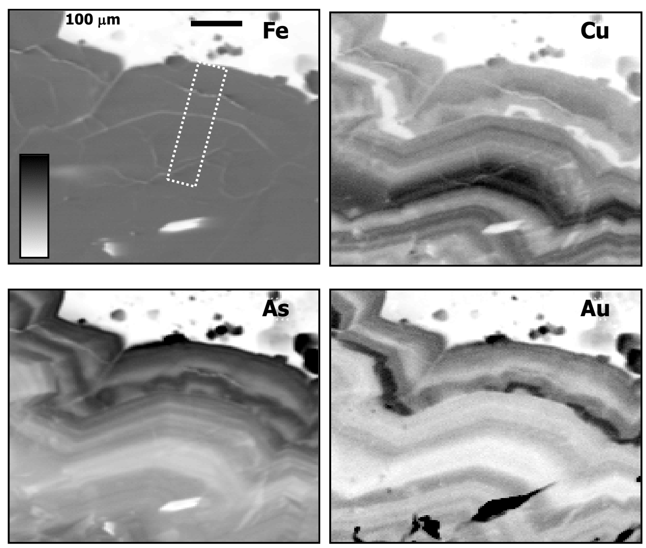

Fig. 4 DA images of pyrite in mineralized quartz from the Emperor gold mine, Fiji, analyzed using 16.1 keV photons (scan area = 600 x 600 μm^2, 160 x 160 pixels, APS 2-ID-E XFM).

References

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