Microsc. Microanal. 8 (Suppl. 2), 2002
DOI 10.1017.S1431927602102352

Spectral image analysis: Getting the most from all that data

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How do you comprehensively analyze the chemistry of a microstructure? One might do a series of point analyses or perhaps acquire a series of x-ray maps. Both of these have the potential to miss important features of the microchemistry. An alternative method would be to combine the best of both point analyses and mapping by acquiring complete x-ray spectra for a 2D array of points, otherwise known as spectral images. The challenge then becomes analyzing the large amount of resulting data.

Spectral images consist of a two-dimensional array of complete spectra comprising a three-dimensional data cube (two real space dimensions that are typically orthogonal and one spectral dimension such as for example x-ray energy). While the entire cube is difficult to view in its entirety, selected portions can be viewed with success. For example, in an x-ray spectral image, both the individual spectrum and collections of spectra covering selected areas can be extracted from the data cube providing a way to see the summed x-ray spectrum for a region. In addition, in the real-space dimensions, both individual slices and ranges of slices corresponding to the positions of x-ray lines (e.g., maps) can be extracted to show the real-space distribution of an element. One variation of these two types of manual spectral-image analysis includes background subtraction on a pixel-by-pixel basis. This method relies on either selective choice of background windows or enough statistics in individual spectra to identify the peaks and fit an appropriate background shape. Significant error can arise for example by assuming the intensity in a map arises from an x-ray peak from the expected element and not from bremsstrahlung or an unanticipated element with a peak in the same position. Another variation of the above methods utilizes x-ray maps and appropriate thresholds to reconstruct x-ray spectra from selected regions of a microstructure [1]. The subjective nature of manual analyses, such as those described above, is a potential source of error–either missing minor phases or chemical variations or misidentifying elements.

In order to make spectral image analysis more objective, robust and automated analysis techniques are required [2]. Firstly, the entire data set should be statistically interrogated. As an initial step in this an orthogonal factorization, such as principal components analysis (PCA), is typically performed [3,4]. This results, after suitable normalization of the raw data, in a series of abstract chemical components, the majority of which are due to noise and can be manually [4] or automatically [2] discarded. Secondly, the results should be physically meaningful. Principal components (images and spectra) have both negative and positive values due to the orthogonality constraint. In order to transform from these abstract principal components to physically realistic 'pure' (i.e., unmixed) components, orthogonality must be relaxed with the appropriate constraints applied [2]. Figure 1 is a schematic of the decomposition of a raw spectral image data set (D) with three chemical components (chemical phases in this case). It is assumed that any raw spectrum for a given pixel can be reconstructed by summing the products of pure-component image intensities (C) and pure-components spectra (S) for that pixel. Figure 2 is an automated x-ray spectral image (from the JEOL 5900LV, W-filament, 15kV) analysis of Hf(2wt%)Cu-Ag/Alumina braze joint illustrating the identification of Hf at the braze interface as well as correct identification of the other chemical phases and their distribution in the microstructure.

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[3] P. Trebbia and N Bonnet, *Ultramicroscopy* 34 (1990) 165.
[4] I.M. Anderson *Microsc. Microanal. 4 (Suppl 2:Proceedings*) (1998) 272.
[5] Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United Stated Department of Energy (DOE) under contract DE-AC04-94AL85000.

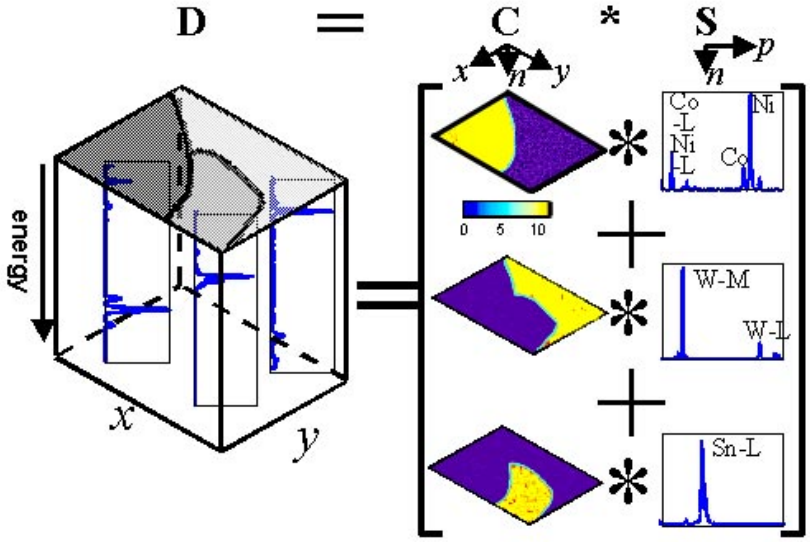

FIG. 1. Schematic of the transformation of a large raw spectral image data cube to a much more compact and still physically meaningful solution with automated x-ray spectral image analysis.

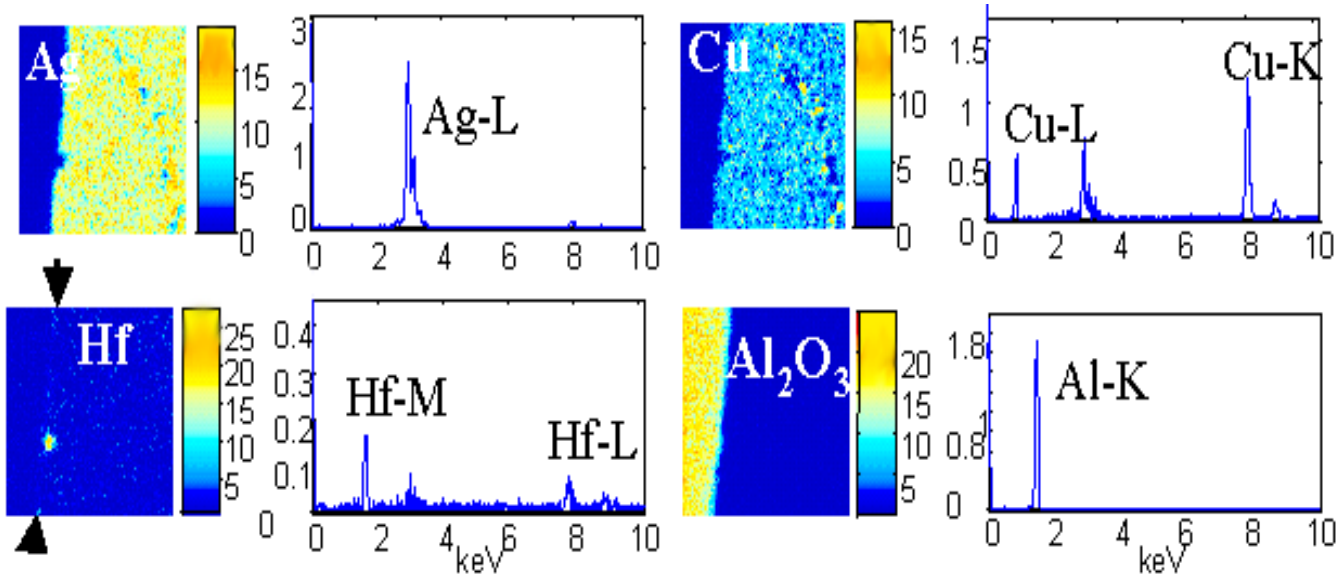

FIG. 2. Example of automated x-ray spectral image analysis of a Hf-containing braze joint. Arrows on Hf image correspond to interface position.

https://doi.org/10.1017/S1431927602102352 Published online by Cambridge University Press