Simultaneous analysis of signals and spectra from multiple sensors using data fusion

Spiegelberg, J.[1], Muto, S.[2], Yamamoto, Y.[3], Ohtsuka, M.[2] and Rusz, J.[1]

[1] Uppsala University, Sweden, [2] Nagoya University, Japan, [3] Sumika Chemical Analysis Service, Ltd., Japan

An electron microscope allows to analyze a broad range of material properties, not at last due to the versatile nature of operation modes and signals that derive from it. In a STEM measurement, for each image pixel one can obtain EEL, EDX or CL spectra, or also intensities of individual segments of a segmented ADF detector or pixelated camera. Further generalizing by introducing further measurement parameters, e.g., time in a time series, highlights the multimodal and multi-sensorial nature of the data structure in electron microscopy. From a data processing perspective, this wealth of information is both opportunity and challenge - a challenge typically not taken and an opportunity missed as most studies revert to analyze the acquired data sets one by one rather than to attempt to exploit the inter-set correlations for a better analysis result.

Blind source separation (BSS) methods can be used for an automated analysis of experimental data, e.g., by identifying spectral source signals in an EELS spectrum image. As of today, most BSS tools used in the microscopy community are restricted to matrix factorization techniques, such as non-negative matrix factorization, independent component analysis or vertex component analysis. Correlation between, e.g., EEL and EDX spectra, are thus left unused. In STEM, however, the data from all sensors can be considered to be coupled as they were measured on the same pixel. Considering BSS approaches, it is thus reasonable to assume that some (or all) of the spatial factors are shared between the data sets.

In this talk, we will introduce three different data fusion approaches, i.e., matrix concatenation, PARAFAC2 [1] and structured data fusion (SDF) [2] (see Fig. 1), as a framework to simultaneously analyze an arbitrary number of matrices (or tensors) stemming from different sensors in the microscope. This joint analysis scheme may improve the flexibility of the BSS model and offer better uniqueness properties. Thus, data fusion offers the possibility to quantitatively analyze the entire range of signals from the microscope beyond the capabilities of established BSS approaches.

By testing the algorithms' performance on simulated data sets, we identify SDF as most versatile tool. When applied to experimental a coupled EELS/EDX - HARECXS measurement of $Li_{0.2}Ni_{0.7}Mn_{1.6}O_{4-\delta}$ (see Fig. 2), we obtain a quantitative unmixing of the two distinct Mn species in the sample standing in line with predictions by simulation [3].

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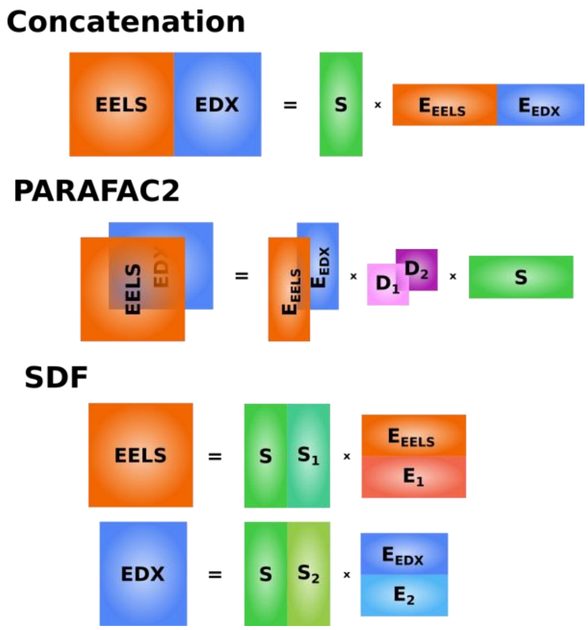

Fig. 1 Schematic representation of three data fusion approaches and the structure of the component matrices for a joined EELS/EDX measurement.

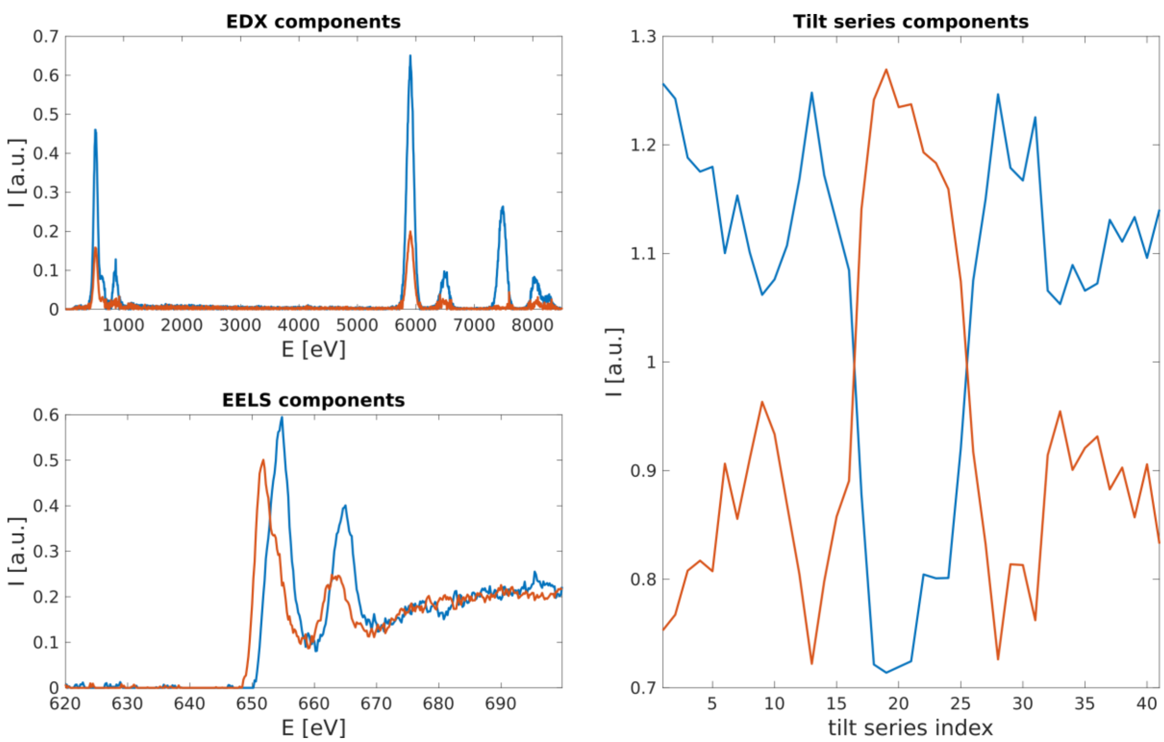

Fig. 2 Component spectra and tilt series weights obtained by a joined treatment using SDF on HARECXS data measured on $Li_{0.2}Ni_{0.7}Mn_{1.6}O_{4-\delta}$. The components corresponding to the two Mn species are well unmixed.