Spectral unmixing of electron energy-loss spectra using vertex component analysis applied to nanoscale systems

Martial Duchamp* and R. E. Dunin-Borkowski

Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ER-C) and Peter Grünberg Institute 5 (PGI-5), Forschungszentrum Jülich, D-52425 Jülich, Germany

*contact e-mail: martial.duchamp@gmail.com

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Abstract

Due to the sub-eV energy resolution, electron energy-loss spectroscopy (EELS) spectra not only provide a signal proportional to elemental concentration but also allows to map the state above Fermi level which determined the physical properties of materials like conduction or oxidation states [1]-[2]. Of particular interest, atomically resolved oxidation states have been shown but associated maps are mainly obtained by fitting or by integrating over a few eV range the peaks of interest which are not ideal for low signal-to-noise EELS dataset and not make full use of the spectral fine structure [3]. Principal component analysis [4] and independent component analysis [5] have previously been applied to EELS datasets to extract chemical maps with enhanced signal-to-noise. Recently, spectral unmixing techniques have been used to (i) improve signal-to-noise and (ii) extract chemical maps together with their associated spectral signatures. Several algorithms have been applied to EELS datasets, including non-negative matrix factorization [6], vertex component analysis (VCA) and Bayesian linear unmixing [7]. These algorithms are based on the idea of decomposing the original dataset in the form of a product of two matrices, with constraints applied during matrix decomposition (e.g., spectral signatures and abundance maps can be constrained to be positive quantities). We have applied VCA to obtain chemical maps and spectral signatures from large EELS datasets acquired in the scanning transmission electron microscope [8]. The materials that we have studied include InP/ZnS nanoparticles [9], while the spectral information has been obtained with atomic spatial resolution [10]. A detailed explanation of the VCA concept and algorithm will be presented and the use of a user-friendly script will be illustrated and offered for dissemination.

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