EELS of Si-nanocrystals by hyperspectral segmentation and multivariate factorization.

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This work is focused on advanced data analysis methods for the characterization of Si NCs by high angle annular dark field and electron energy loss spectroscopy (HAADF-EELS) in the aberration corrected and monochromated scanning transmission electron microscope (STEM). These Si-NCs are embedded in multilayer stacks wheres SiO_2, SiC and Si_3N_4 are used as dielectric barriers. We generate and analyse maps from measured properties on the spectrum images (SI), such as characterization of the plasmon peak and relative thickness.

Plasmon energy reveals the approximate spatial distribution of the Si-NCs and barrier dielectric material. It is not possible to get a direct measurement of the pure contribution of the Si-NC to the EELS spectrum, as all measured data present at least a mixture of nanoparticle and substrate plasmon. Fitting these two features may be reliable only when they are well separated in energy and exhibit significant differences in FWHM [1]. However, for other non-favorable situations, segmentation of the EELS-SI by mathematical morphology can be of help. Following this scheme, averages of the spectra in the particle and dielectric areas can be generated, along with slices of the EELS-SI. These slices are then analyzed using multivariate analysis algorithms for a factorization of the EELS data. Non-negative matrix factorization (NMF) and bayesian linear unmixing (BLU) were used. Moreover, the pure Si-NC plasmon is recovered using this approach. Finally, the possibility of extracting electro-optical properties by thickness-normalized Kramers-Kronig analysis of the spectra will be explored.

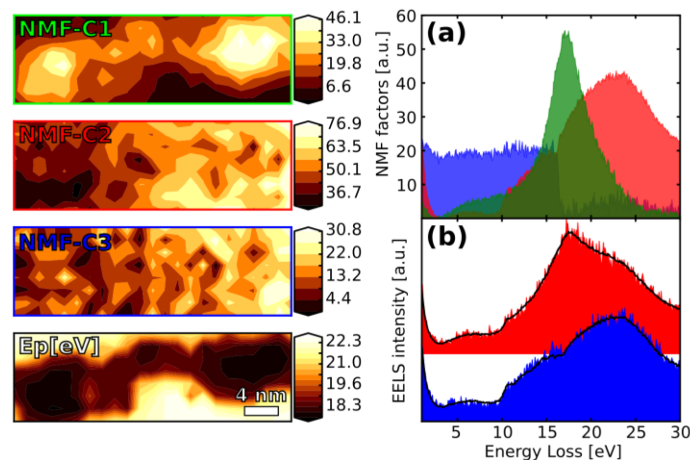

Fig. 1: The left panels show the factorization resulting maps from a Si-NC region with the plasmon energy map below. From the same factorization, the right panels show factors, (a), and the comparison of the model with raw EELS spectra from the region, (b).

Références

A. Eljarrat et al. (2013) *Nanoscale* **5**, 9963-9970
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