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IT-5-P-1976 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 (HAADF) and electron energy loss spectroscopy (EELS) in the aberration corrected and monochromated scanning transmission electron microscope (STEM). These Si-NCs, of high interest for photovoltaic applications, are embedded in multilayer stacks where SiO_2, SiC and Si_3N_4 are used as dielectric barriers.

A comparison will be made between different techniques that exploit the information within low-loss EELS-spectrum images (SI). In this sense, the generation of maps from measured properties on the spectrum, such as characterization of the plasmon peak and relative thickness from the measured spectra was complemented with segmentation of the EELS-SI using mathematical morphology (MM) and a detailed exploration of spectral factorization using multivariate analysis (MVA).

Plasmon energies determined at the EELS-SI reveal the approximate spatial distribution of the Si-NCs and barrier dielectric material (SiO_2, SiC and Si_3N_4, depending on the case). This method is better suited than the examination of the HAADF images, because of the appearance of spurious features from the inhomogeneity of the sample, masking the Si-NC positions (see Fig. 1 and 2). Nevertheless, it was not possible to get a direct measurement of the pure contribution of the Si-NC to the spectra, as all measured data present at least a mixture of nanoparticle and substrate plasmon. Fitting these two peaks using a double plasmon model (DPM) is reliable only when they are well separated in energy and exhibit significant differences in FWHM, i.e. low energy narrow peak vs high energy wide peak (as in Si-NCs in a SiO_2 substrate) [1]. However, for other non-favorable situations, segmentation of the EELS-SI by MM 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 MVA algorithms (NMF and BLU) for a factorization of the EELS data (see Fig. 3).

The collection of computational tools enabling nanometric spatial resolution imaging of the Si-NCs using sub-eV energy resolution EELS will be presented. Maps of measured properties, such as mean free path to sample thickness ratio, will be plotted for the three studied systems with different dielectric barriers. Moreover, the extraction of particular features by segmentation and factorization of the EELS data will allow recovering the pure Si-NC plasmon in each sample. Finally, the possibility of extracting electro-optical properties by thickness-normalized Kramers-Kronig analysis of the spectra will be explored.

[1] A. Eljarrat et al. (2013) Nanoscale 5, 9963-9970

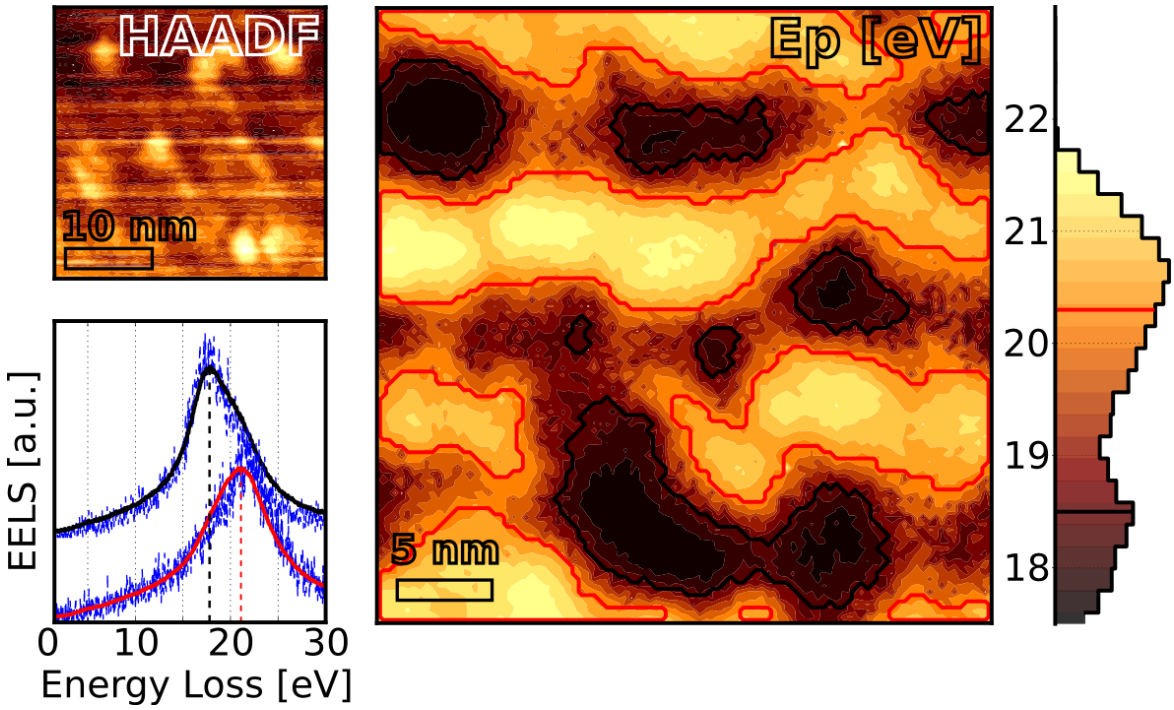

Fig. 1: HAADF (upper left panel) and EELS (blue dashed lines, lower left panel) simultaneously acquired of a SiC sample. The EELS is analyzed to form the plasmon energy map (central panel, with thresholded histogram at left). Si-NC and SiC regions are marked off in this map and the average EELS are overlayed to the raw EELS (black=Si-NC, red=SiC).

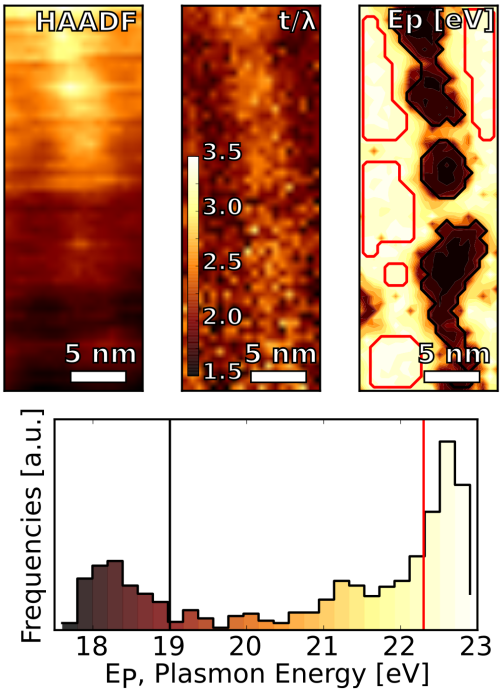

Fig. 2: Results from the SiO2 sample, showing the superior sensitivity of the plasmon energy map above the HAADF and relative thickness map. Si-NC and SiO_2 positions are marked off in the map and in the histogram (lower panel) as thresholds, using the same color code as Fig. 1.

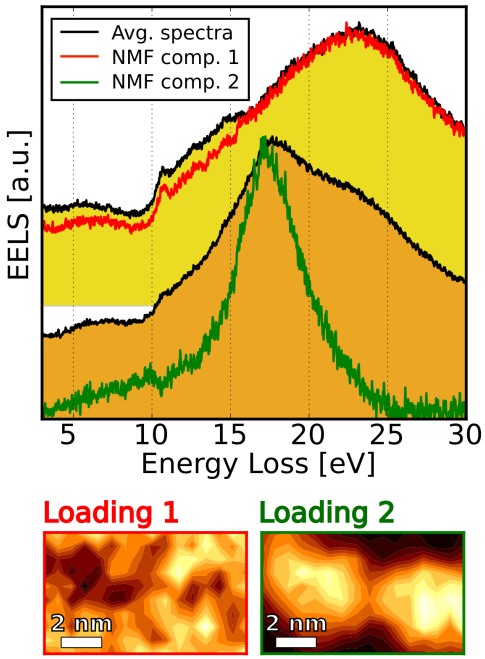

Fig. 3: MVA factorization results vs. average EELS from the same EELS-SI shown in Fig. 2. After segmentation of the upper Si-NCs region, factorization reveals two different nanoparticles, and their contribution to EELS (comp. 2) is separated from the background SiO_2 spectra (comp. 1).