pyEELSMODEL: python library for model-based EELS quantification

Daen Jannis[1,2], Mr. Jo Verbeeck[1,2]
[1]EMAT, Universiteit Antwerpen, Antwerpen, Belgium, [2]NANOlab, Universiteit Antwerpen, Antwerpen, Belgium

Electron energy loss spectroscopy is a powerful method used to investigate the elemental abundance and electronic structure of a material. Extracting this information from the experimental data is a complex process and multiple methods exist to get the results where each of them have their own advantages and disadvantages. Moreover, each method has free input parameters which influences the final results and can lead to experiments bias and reproducibility issues, especially in the common case where all parameters and the exact workflow is not shared.

In this work, an open-source python package (pyEELSMODEL) is presented which offers multiple alternative EELS quantification methodologies[1] . The library allows a transparent way to share a specific data processing workflow from raw data to a resulting plot that can appear in a paper. pyEELSMODEL expands upon the former EELSMODEL (c++) software which introduced the model-based philosophy in the EELS community [2]. This method attempts to describe the experimental data with a physical model and optimizes the parameters of this model via a minimization scheme such as least squares or maximum likelihood. The values of these optimized parameters can be used to estimate information on the material such as eg. elemental abundance. The new pyEELSMODEL package is written in python making it, in general, easier to integrate and extend as compared to the former c++ code. Multiple robust quantification workflows are available and can be easily used by the novice EELS user via eg. Jupyter notebooks.

This package is also particularly useful for testing and validating novel data processing methodologies since its results can easily be benchmarked against more common methodologies and could act as a test standard against which to make performance claims.

In this presentation, we will demonstrate the use of pyEELSMODEL on several experimental STEM-EELS maps showcasing the robustness and speed of the model-based quantification methodology for modern large size datasets. In Fig. 1, EELS quantification is used to get elemental maps on a mix of copper and silver nanoparticles on top of a carbon substrate. The lower plots show the resulting fitted model on silver (a) and copper (b).

Fig 1. Elemental maps of copper and silver nanoparticles on top of a carbon substrate. (a) Shows the fitted model on a silver nanoparticle whereas (b) shows a fit on the copper nanoparticle.

Keywords:

EELS, Quantification, Model-based

Reference:

[1] pyEELSMODEL repository: https://github.com/joverbee/pyEELSMODEL
[2] Verbeeck J. et al; Model based quantification of EELS spectra; Ultramicroscopy; 2004; doi:10.1016/j.ultramic.2006.05.006