Model based determination of the dielectric properties of nanomaterials from STEM valence loss EELS

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Dielectric properties of materials are crucial in describing the optical and electromagnetic response of materials as used in e.g. gate oxides, fiber optics, photonic crystals, semiconductor devices, etc. Since devices are becoming considerably smaller as the optical wavelength, the conventional measuring methods based on optical response are limited by their spatial resolution. Valence electron energy loss spectroscopy (VEELS) performed in as canning transmission microscope (STEM) is a good alternative to obtain the dielectric properties with excellent spatial resolution.

Formally, the dielectric function of a material is related to the single scattering distribution (SSD) for electron energy loss of fast electrons travelling through a thin object. The VEELS spectra however contain many other contributions like multiple scattering, retardation effects, surface plasmons etc. Especially retardation effects can be important to take into account as the speed of fast electrons in a microscope can be comparable with the speed of light in the dielectric medium. In that case, retardation effects such as guided light modes and Cerenkov losses will introduce energy losses and should be considered[1]. Retrieving the dielectric function is very sensitive to these signals especially in the band gap region. In view of the large convergence angles used in STEM VEELS it is almost impossible to remove these effects by angular selection in the experimental setup as it is possible for plane wave illumination in TEM[2].

Here a model based method is proposed that aims at modeling the experimentally observed energy loss taking into account relativistic effects. The model is based on a piecewise linear function describing Im(-1/ε) which can be analytically Kramers-Krönig transformed into the complex dielectric function ε_1, ε_2 (fig. 1). The model loss function is then calculated taking into account relativistic effects by calculating a relativistically corrected loss function and this model is then fitted to the experimental loss function. This method has the advantage of having parameters which are approximately local in terms of the loss function which tremendously improves the fitting procedure over eg. Drude-like models which model the dielectric function. This method has been implemented in the EELSMODEL program[3, 4]. The first results of this approach are shown for diamond films (fig. 2) and a qualitative agreement with bulk optical data is obtained although a considerable blue-shift occurs which is most likely due to surface effects. It is important to note here that the response of thin films or nanoparticles is expected to deviate from the bulk response exactly because of the appearance of surface effects and therefore we believe that surface effects should be measured rather than taken into account in the model.

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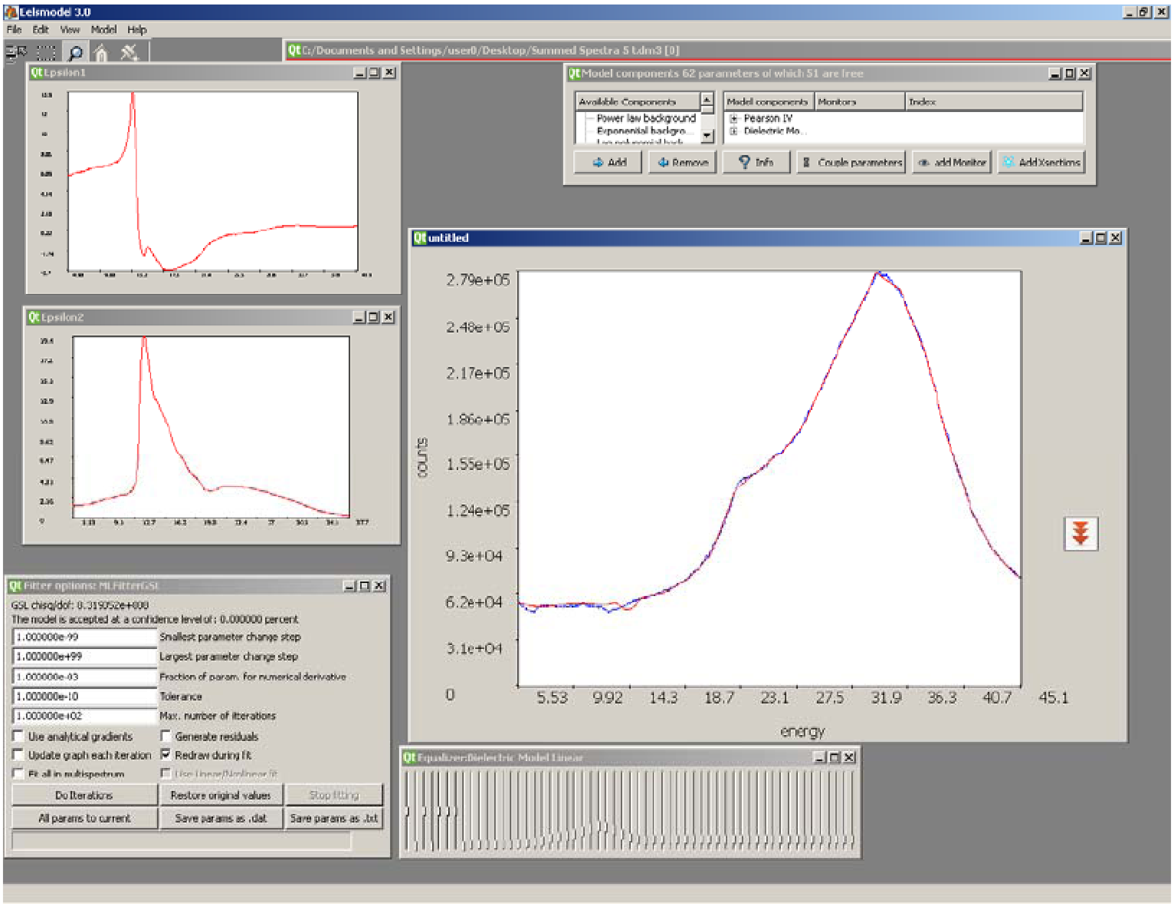

GSL chisq/dof: 0.319052e+000
The model is accepted at a confidence level of: 0.000000 percent

1.000000e-99 Smallest parameter change step
1.000000e+99 Largest parameter change step
1.000000e-03 Fraction of param. for numerical derivative
1.000000e-10 Tolerance
1.000000e+02 Max. number of iterations

☐ Use analytical gradients ☐ Generate residuals
☐ Update graph each iteration ☑ Redraw during fit
☐ Fit all in multispectrum ☐ Use Linear/Nonlinear fit

Figure 1. Screen shot of the implementation in EELSMODEL, showing a fit to an experimental diamond spectrum.

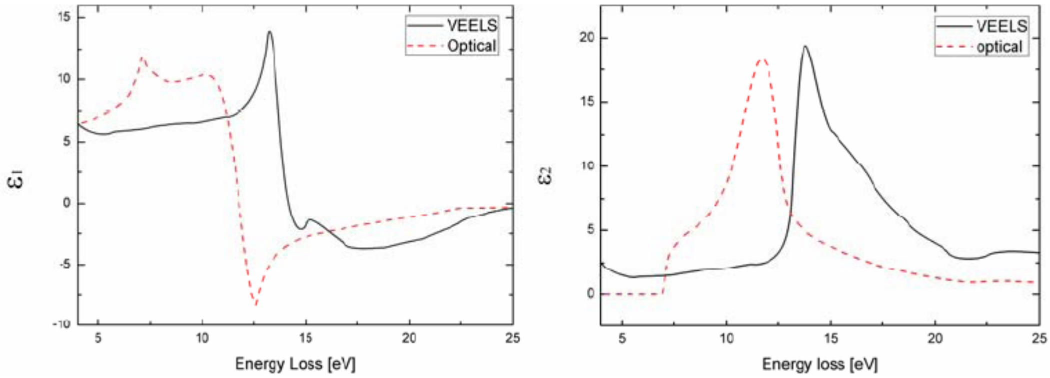

Figure 2. The dielectric function obtained from VEELS (solid line) with the reference bulk optical data (dashed line) for diamond.

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