

Numerical Aspects of Valence Electron Energy Loss Spectrometry

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The excellent energy resolution that can be achieved with field emission sources and monochromators makes valence electron energy-loss spectroscopy (VEELS) in the electron microscope a versatile tool for the study of the electronic structure of solids on a nanometer scale. Spectra in the energy range up to 50 eV show the longitudinal eigenmodes of the medium, caused by excitations from valence to conduction bands. The complex dielectric function $\varepsilon(E)$ showing transverse eigenmodes can be obtained from the loss-function $Im[-1/\varepsilon(E)]$ by Kramers-Kronig analysis (KKA). Additionally, the energy dependent refractive index, absorption coefficient and reactivity can be calculated. The results of this procedure are very sensitive to details of data treatment, such as how the zero-loss peak (ZLP) and multiple scattering (MS) effects are removed, presence of the Cerenkov losses (CL) [1], and the extrapolation of the high energy tail of the spectrum. The VEELS measurements are aided with the *ab initio* electronic structure calculations using a WIEN2k code [2].

The single scattering cross-section $S(E)$ and so the intensity of the VEELS spectrum is proportional to the loss-function:

$$S(E) = \left[\frac{e^2}{\pi \hbar v} \right]^2 \cdot D \cdot \Im \left[\frac{-1}{\varepsilon(E)} \right] \cdot \ln \left[1 + \left(\frac{\beta}{\theta_E} \right)^2 \right]$$

D is the thickness of the specimen in units of the mean free path, β is a collection angle and $\theta_E = E/(\gamma m_0 v^2)$ is a characteristic scattering angle for an energy loss E . During the KKA process a few very important steps must be performed in order to retrieve the loss function from an experimental spectrum [3]:

1. The deconvolution and a removal of the ZLP. The ZLP usually covers a considerable region of low energy losses, sometimes up to 5 eV. Fourier-Log Deconvolution (FLD) method is used to remove the ZLP and to turn the multiple-scattering distribution (MSD) into the SSD.
2. Normalization. Afterwards the obtained SSD is divided by the angular correction and then the loss-function is normalized. The normalization can be done using a known value of the refractive index n or using the plasmon energy E_p and a sum rule.
3. Kramers-Kronig relations. From the loss-function $Im[-1/\varepsilon(E)]$ one can calculate $Re[1/\varepsilon(E)]$ using Kramers-Kronig relations and then calculate the complex dielectric function, refractive index, absorption coefficient and reactivity.

We investigate the influence of the treatment procedure of the experimental spectrum on the data quality and reliability on a number of semiconductors. Our results are in good agreement with *ab initio* calculations with the WIEN2k code.

References:

- [1] M. St ger-Pollach et al., Cerenkov losses: a limit for bandgap determination and Kramers-Kronig Analysis, Micron, in print
- [2] K. Schwarz, P. Blaha, Computational Material Science 28 (2003) 259-273
- [3] R. F. Egerton, Electron Energy Loss Spectroscopy in the Electron Microscope (Plenum Press) 1986

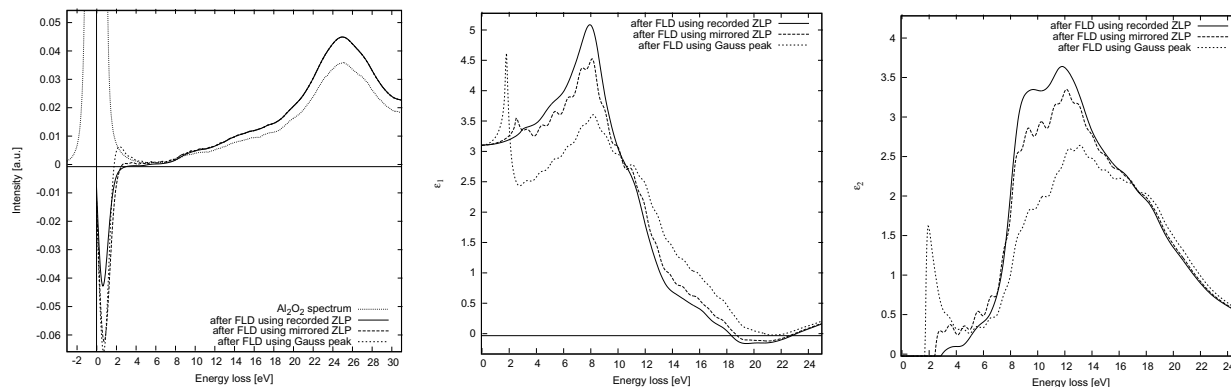


Figure 1: The left figure shows how a removal of the ZLP introduces artifacts. For the removal three different ZLPs were used: a separately recorded, one with a left side mirrored to the right and one is a fitted Gaussian. Removing these artifacts and extrapolation at lower energies is a crucial step especially in case of a semiconductor specimens. The middle and right figures present the dielectric functions $\epsilon_1(E)$ and $\epsilon_2(E)$. There are severe differences in $\epsilon_1(E)$ and $\epsilon_2(E)$ according to which ZLP was used.

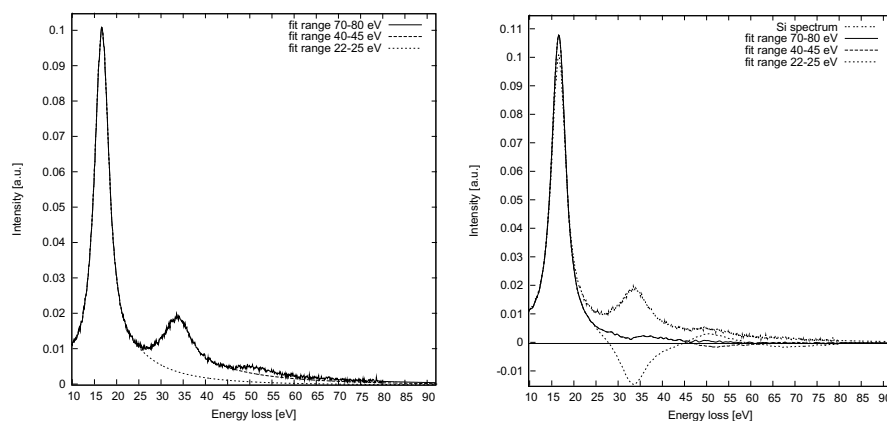


Figure 2: Left figure is a Si spectrum extrapolated at three different energies before the deconvolution and the right figure shows the same spectra after the deconvolution procedure. We can see how the extrapolation of the high energy tail influences the results.