NEXAFS data normalization procedure: A case study at the C K-edge*

In this example we shall demonstrate the procedure to normalize the C K-edge NEXAFS spectrum obtained from drain current measurements on an as-coated polyacrylamide (PAM) thin film.

The incident photon flux has energy dependence arising due to the non-uniform absorption (irregular ups and downs) by the beamline optics (monochromator, grating, mirror etc.). Therefore data $I_{\text{sample}}(\hbar\omega)$ should be divided by incident flux to remove the "optics" effects.

To measure this incident flux a gold mesh (gold is very good candidate as it has no absorption in the C, N K-edge regions and a very small absorption in O K-edge region) is placed before the sample to enable simultaneous measurement of sample data and incident flux. Let us call this mesh current $I_{\text{mesh}}(\hbar\omega)$.

Then NEXAFS normalized data can be represented as

$$R(\hbar\omega) = \frac{I_{\text{sample}}(\hbar\omega)}{I_{\text{mesh}}(\hbar\omega)}$$

Unfortunately, the mesh is normally contaminated by adventitious carbon. Also it is not possible to clean/replace the mesh for every experiment. Therefore a properly clean gold/copper is used as a sample along with the same gold mesh used for the actual sample (Henceforth we shall take the clean sample to be gold. It may be kept in mind that copper can be used as well).

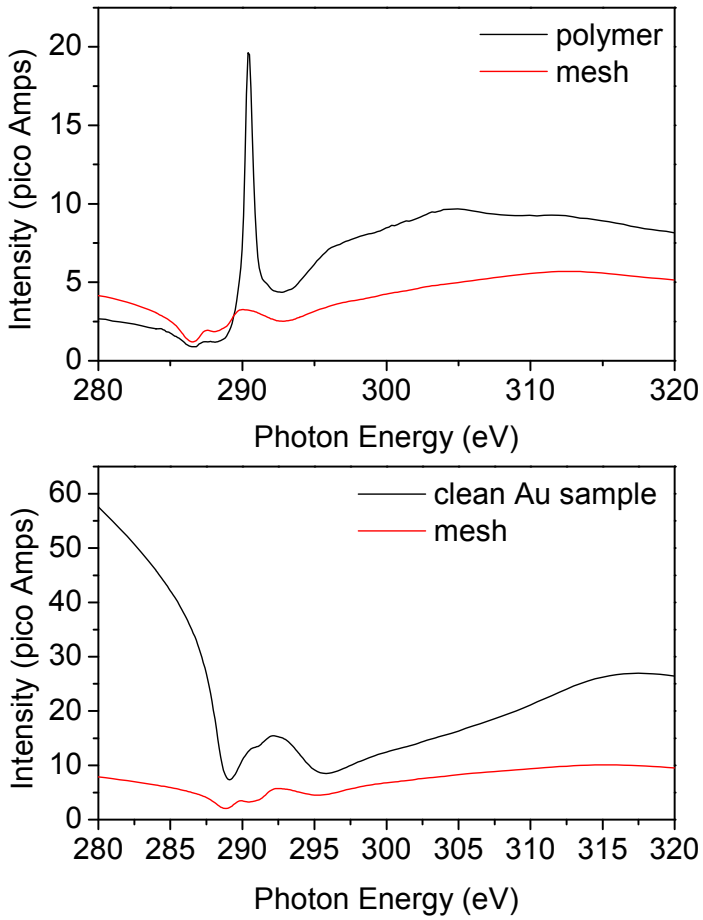

Fig. 1: The sample and gold data along with corresponding mesh data.

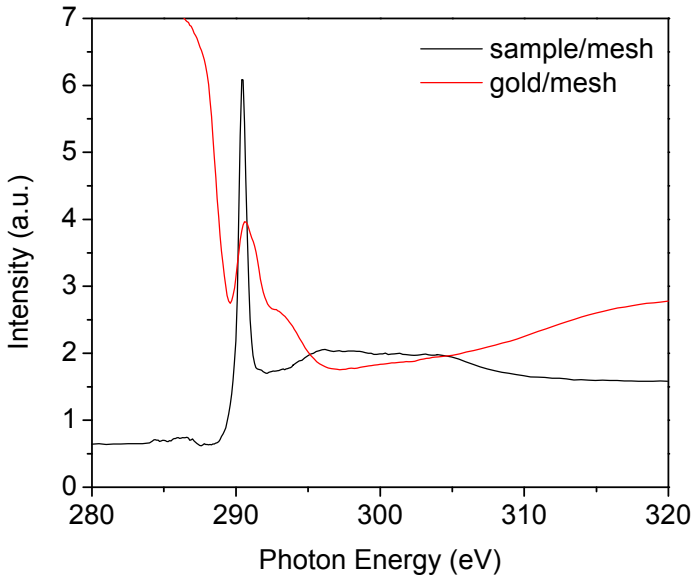

Fig: 2: Data obtained after dividing by corresponding mesh currents.

Now one can get rid of the effect of adventitious carbon as follows.

$$R(\hbar\omega) = \frac{\left(\frac{I_{\text{sample}}(\hbar\omega,t)}{I_{\text{mesh}}(\hbar\omega,t)}\right)}{\left(\frac{I_{\text{Au}}(\hbar\omega,t')}{I_{\text{mesh}}(\hbar\omega,t')}\right)} \quad (1)$$

As the two experiments (with sample and gold) are done at two different times (different synchrotron flux) the parameter t is shown, however, the effect of time cancels out. Note that if the X-axis of the two measurements (sample and gold) do not match interpolation is required.

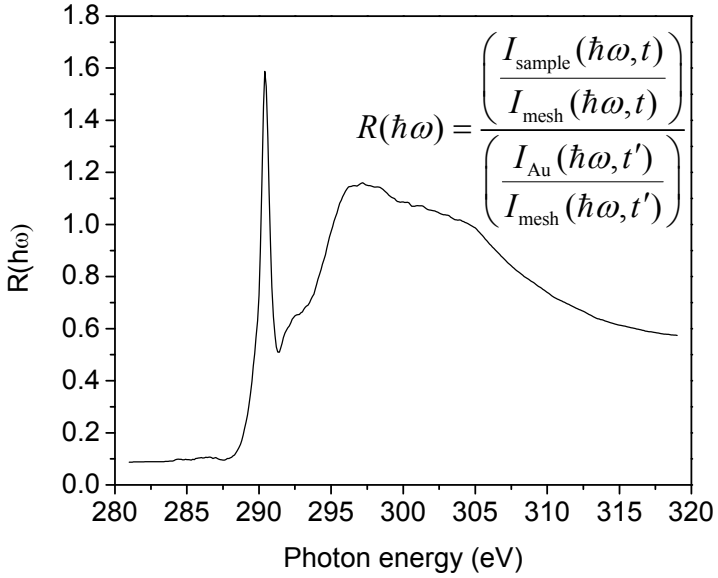

Fig 3: Corrected data

Data alignment

However, due to beam position shift as well as mechanical movements of beamline optical components the flux vs. energy behavior is not identical at different times. Therefore the data taken at two different times should be aligned before the above normalization procedure as described below.

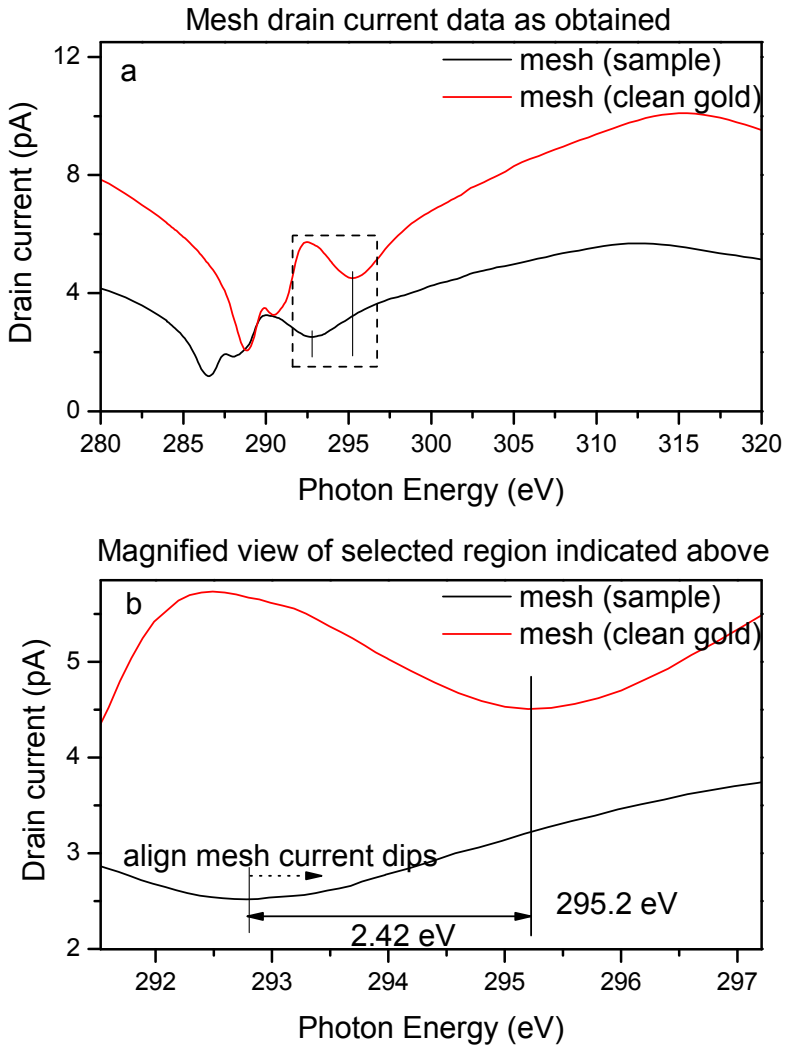

Fig. 1: Procedure for data alignment. (a) Drain currents from passivated gold mesh as obtained. Prominent features in spectra are to be aligned. For the C K-edge the best chosen feature is the 2nd major dip in the spectrum as indicated by vertical lines; (b) Magnified view of the region of the 2nd dip in the spectra as indicated by the dashed box in (a).

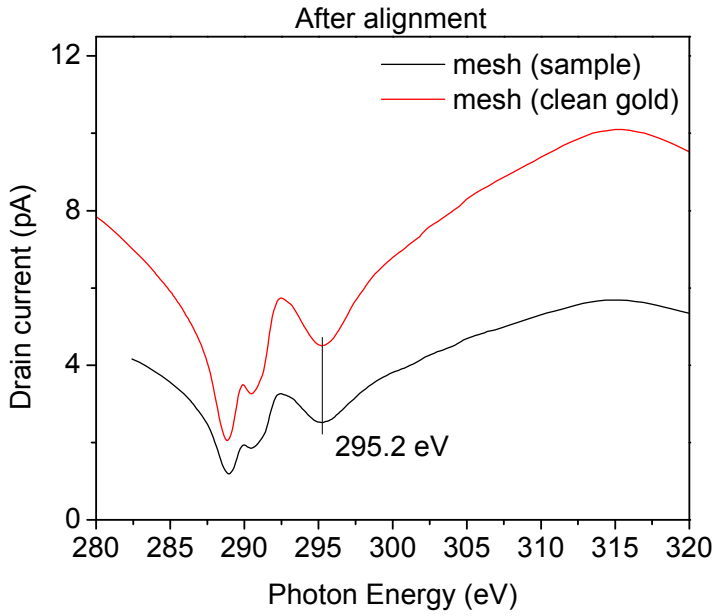

Fig. 2: After the dips have been aligned.

Absolute energy calibration

Absolute energy calibration is performed to determine the X-axis precisely and generally performed using gas-phase absorption (eg. Ne and/or N_2) or by photoemission of known sample.

From calibration data the position of the above mentioned feature used in relative energy calibration is determined. For the C K-edge the value was found to be 290.5 eV[1], i.e., both sample and clean gold spectra should be shifted by, $290.5 - 295.2 = -4.7\ \mathrm{eV}$.

[1] This particular value depends on the particular synchrotron beamline where the experiments are performed. In our case it was the BL 8.1 L BEAR beamline of the Elettra Synchrotron (Trieste, Italy).

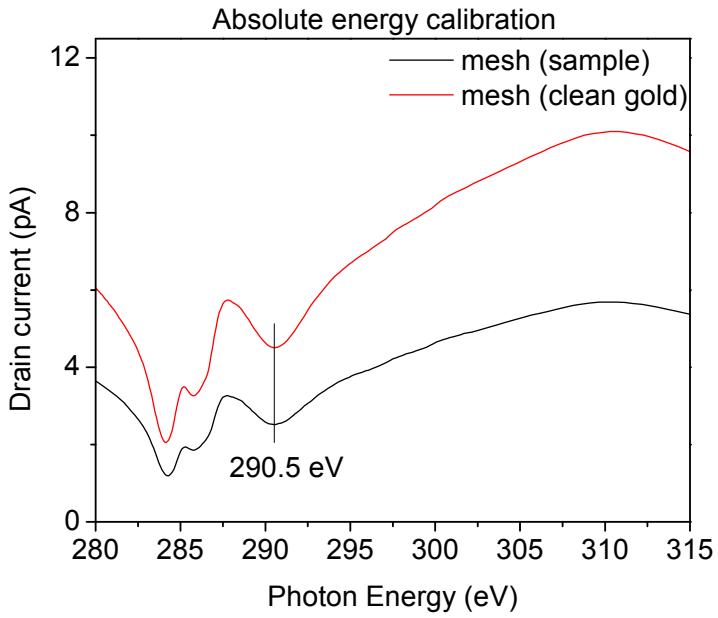

Fig. 3: After aligning the dips to the correct energy value obtained from gas phase measurements.

After alignment and absolute energy correction of all data (sample, mesh; gold, mesh) one can calculate $R(\hbar\omega)$ using eqn. (1).

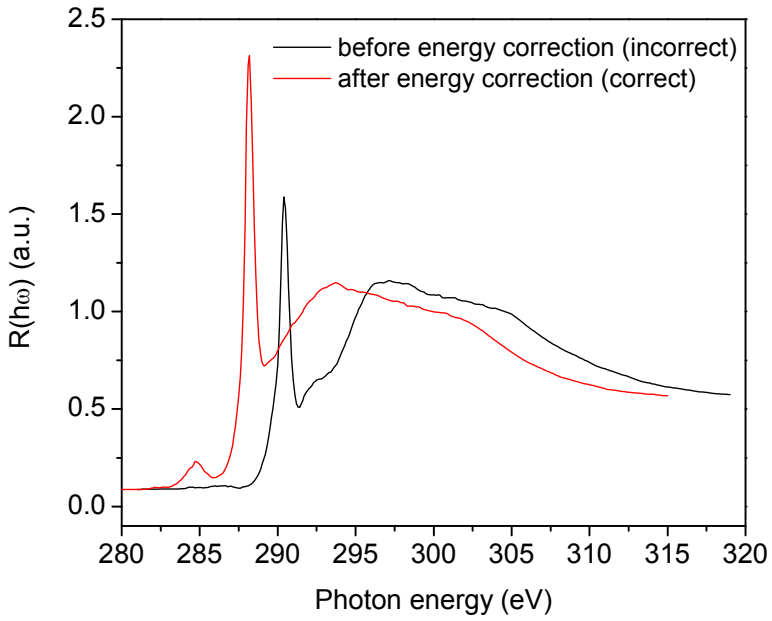

Fig. 4: Final energy corrected data.

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