Use cases for the XAS Data Interchange format

1 Conventional XAS

In a conventional XAS experiment, we measure a sample somewhere between 2 and 10,000 times, possibly requiring dead-time or other corrections. Some data processing is required to correct, calibrate, and/or align the data. Those scans are then merged into a single spectrum.

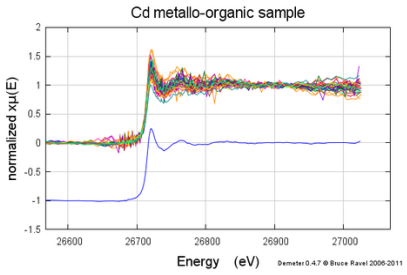

Figure 1: The merge of several dozen scans at the Cd K edge on a sample dilute in Cd.

XDI is about how we express the merged spectrum. In some case, *XDI* may also be a suitable format for the individual XAS measurements, as well.

2 XRF imaging experiments

In an imaging experiments the heterogeneity of our samples is measured. XAS can be measured on particular spots. In this example (Tappero et al, New Phytologist 175:4, 641-654, (2007) doi:10.1111/j.1469-8137.2007.02134.x), the Co and Ca distribution in leaf of a metal accumulating plant is shown. Co micro-XAS spectra are measured at two spots on the leaf.

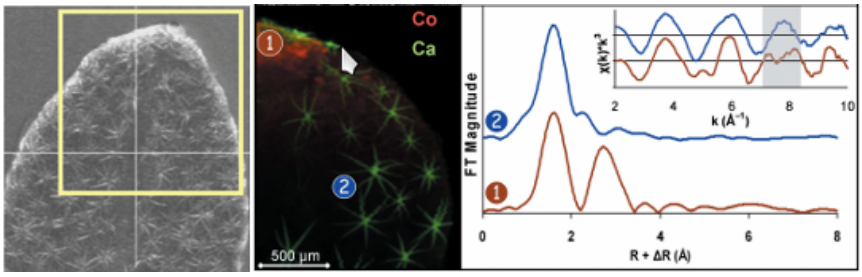

Figure 2: Co K edge micro-XAS measured at two spots on a leaf.

XDI is about how we express the micro-XAS spectrum extracted from the imaging experiment.

3 Difraction anomalous fine structure (DAFS)

An anomalous scattering experiments yields energy-dependent scattering intensities. Here we see DAFS data measured (Ravel et al. PRB 60, 778-785 (1999) doi:10.1103/PhysRevB.60.778) near

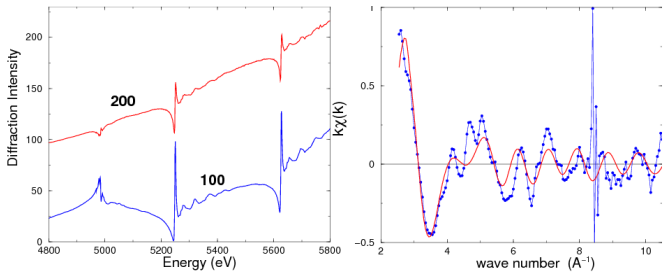

Figure 3: A DAFS measurement on BaTiO3 and the $\chi(k)$ spectrum extracted from it.

the Ti K and Ba L3 edges on BaTiO3. From these data, $\mu(E)$ or $\chi(k)$ spectra are extracted and interpreted as position-selective EXAFS.

XDI is about how we express the $\mu(E)$ or $\chi(k)$ spectrum extracted from the anomalous diffraction measurement.

4 Non-resonant inelastic scattering

A NIXS experiment can used to measure a XANES spectrum in an X-ray energy loss channel. Here we see a XANES-like spectrum for graphite in the X-ray Raman channel, superposed over the Comptopn scattering. (Bergmann, et al. Chem. Phys. Lett. 369 184 (2003) doi:10.1016/S0009-2614(02)02003-1)

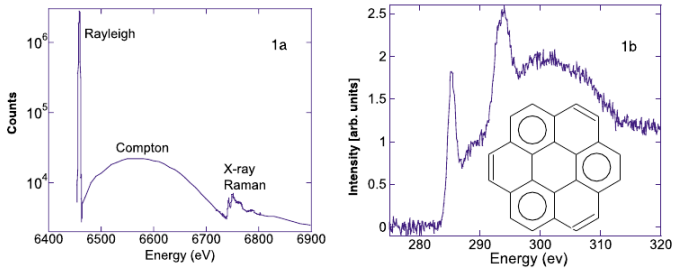

Figure 4: NIXS data measured on graphite and the XANES spectrum extracted from it.

XDI is about how we express the $\mu(E)$ spectrum extracted from the non-resonant inelastic scattering measurement.