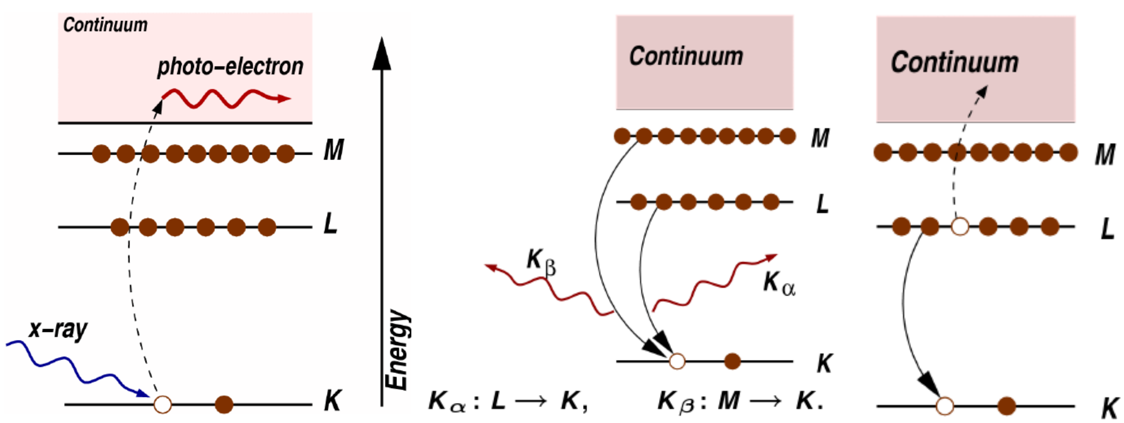
What kind of information your synchrotron technique may provide?

X-ray Absorption Spectroscopy (XAS) is an element-specific probe of local atomic and electronic structure. A monochromator is used to scan the incident X-ray beam through energies around the photoionization energy of a deep-core electron of a particular atomic species. The data are interpreted for quantitative information about partial pair distribution functions – including the number and species of and distance to surrounding atoms – and about partial electron densities of state. Because the time scale of the physical interaction is limited by the mean free path of the photoelectron, XAS is inherently a local probe and is sensitive specifically to local atomic correlations. Because neither the interpretation of the measurement nor the theory used to describe it are dependent upon assumptions of symmetry or periodicity, XAS is equally applicable to condensed matter in all forms, such as crystals, liquids, and soft condensed matter as well as amorphous and glassy materials.

What is the basic principle of your technique?

XAS measures the probability that a deep core electron will be promoted by an incident X-ray into an unoccupied bound or continuum state. An incident photon of sufficient energy will promote a deep-core electron. This creates a core-hole and a photoelectron whose kinetic energy is equal to the excess energy of the incident photon above the binding energy of that deep-core electron. This photoelectron propagates out from the position of the absorbing atom and scatters from neighboring atoms. The resulting interference results in an oscillatory fine structure on top of the step-like dispersion observed in the photo-absorption of an isolated atom.



The figure on the left shows a schematic of the photo-absorption process. The core-hole is eventually refilled by a higher-lying electron, resulting in the emission of a secondary photon (middle) or of an Auger electron (right).

What are the limitations of your technique?

(1) XAS is inherently a local probe and is insensitive to correlations on length scales above about 1 nm and so it views condensed matter through a different "lens" than X-ray scattering or vibrational spectroscopy. (2) Although most of the periodic table is accessible to XAS measurements, the lower energy edges (notably the K edges of the first row elements and the

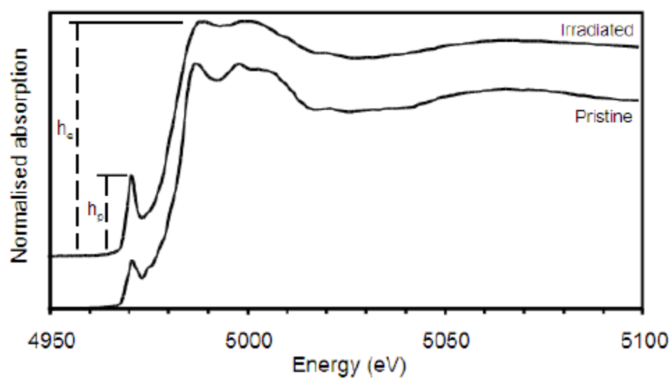
transition metal L edges) require UHV conditions. (3) A full interpretation of the XAS data may require substantial training.

What kind of sample does one need - i.e. minimum/maximum sample dimensions/shapes?

One of the great advantages of XAS is that sample preparation is often relatively simple, particularly for hard X-ray edge energies (above 5 keV or so). It is common to measure XAS on a wide variety of sample types and in a wide variety of environmental conditions (e.g. inside a furnace, cryostat, high pressure cell, or chemical reactor). With focusing optics, it is possible to measure sample heterogeneity on length scales of 10s of microns or less.

Examples of results, preferably, but not necessarily on a glass

Shown here are Ti K edge data on zirconolite as part of an effort to explore the effect of cumulative α-recoil damage on material structure and Pu retention. By depth profiling a polished, irradiated disk of zirconolite, we can explore the local structural changes in the amorphized surface layer.



From the increase in the *3d* peak just above 4970 eV and the damping of higher energy oscillations, we obtain quantitative data on these local structural changes.

A brief bibliography of relevant review articles.

- http://xafs.org/ : XAFS.ORG a community site for x-ray absorption fine-structure (XAFS) and related spectroscopies. The *Tutorials* and *Workshops* sections are particularly useful for the beginner.
- *X-ray Absorption: Principles, Applications, Techniques of EXAFS, SEXAFS, and XANES* in **Chemical Analysis vol. 92** edited by D.C. Koningsberger and R.Prins, John Wiley & Sons, 1988
- *Basic Principles and Applications of EXAFS*, Chapter 10 of **Handbook of Synchrotron Radiation**, pp 995--1014. E. A. Stern and S. M. Heald, edited by E. E. Koch, North-Holland, 1983.
- Theoretical approaches to x-ray absorption fine structure J. J. Rehr and R. C. Albers, **Reviews of Modern Physics Vol 72**, pp. 621-892 (2000).
- **Analysis of Soils and Minerals Using X-ray Absorption Spectroscopy** Kelly, S.D., Hesterberg, D., and Ravel, B., in *Methods of Soil Analysis, Part 5 -Mineralogical Methods*, (A.L. Ulery and L.R. Drees, Eds.) p. 367. Soil Science Society of America, Madison, WI, USA, 2008.