

XAFS - X-ray absorption fine structure spectroscopy

This spectroscopic method uses the x-ray photoelectric effect to provide precise local structural information like distances, numbers of atoms, types, disorder. There are no spectroscopically silent atoms for XAFS, so it allows the analysis of all elements. One can measure amorphous materials, liquids, molecular gases, polycrystalline and crystalline materials.

Photoelectric effect

In this process an X-ray photon is absorbed by an electron of an atom. The electron may be removed from its quantum level, when the binding energy of it is less than that of the x-ray. The rest of the energy (energy of x-ray minus binding energy electron) is given to a photoelectron that is ejected from the atom. The excited state of the atom will rapidly decay in two possible mechanisms: X-ray fluorescence and Auger effect.

Experimental aspects

Because of the different mechanisms for the decay of the excited atom, there are different operations modes: Transmission, fluorescence, electron yield.

The quantity of interest is the absorption coefficient μ , which is linked over the following equation:

$$\frac{I}{I_0} = e^{-\mu(E)x}$$

μ depends to the initial and final intensity as well as to the thickness x of the sample.

Synchrotron radiation

Electrons are emitted by an electron gun and accelerated in a linear accelerator (linac). Then they are transmitted to a circular accelerator (booster synchrotron), where they reach an energy of 6 GeV. When they have enough energy they are injected into a large storage ring where they circulate in vacuum environment at constant energy. The electrons pass several magnets (bending magnets, undulators) this causes them to emit synchrotron radiation. The radiation may range over the whole electromagnetic spectrum and has the advantage that it is tunable.

Data analysis

- Pre-edge: Information about unoccupied states
- XANES (X-ray absorption near edge structure): information about local structure
- EXAFS (extended x-ray absorption fine structure): Information about the geometry of the local structure

References

- www.xafs.org
- www.esrf.eu
- G. Bunker, Introduction to XAFS, Cambridge University Press 2010

