

Modern methods in x-ray absorption spectroscopy: theory, experiment, data analysis

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I will present the summary of the experimental technique of the x-ray absorption spectroscopy (XAS) and physical principles of the XAS with emphasis on the condensed matter (from amorphous materials till monocrystals). I will cover x-ray absorption near edge structure (XANES) and extended x-ray absorption fine structure (EXAFS) spectra, how they are extracted from the XAS, and basic theory used in data analysis. Differences and similarities between data obtained from x-ray and neutron diffraction will be discussed.

Theoretical modelling of EXAFS will be covered, as well as how to obtain local atomic structure parameters from experimental data. I will explain different data analysis methods, including conventional fitting procedures, and advanced methods like radial distribution function reconstruction, atomic structure reconstruction using reverse Monte-Carlo, combination of molecular dynamics and EXAFS.

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