

X-ray Absorption Spectroscopy: materials inside – analysis tool

October 3 -8, 2017

Overview

Modern technology being advancing very rapidly demands new materials with improved properties in different field of our life from automotive or aerospace industries to electronics used in household and office appliances. The new materials have continued to be modified and improved at the expense of their composite construction. Composite elements or blocks have both own composition and structure (multilayer materials, nanoparticles with multi-element composition on different supports, glasses, ceramics and so on). To manage properties of the composite materials, first of all, scientists should know structure. However, commonly used method for structure determination – x-ray diffraction – could not be often applied because of absence of long-order atomic structure in the materials. In this case, X-ray Absorption spectroscopy comes to the aid providing information about electronic and local atomic structure around specified atoms: type of atoms, interatomic distance and atomic disorder as well as local geometry and oxidation state. That is why at the present X-ray absorption spectroscopy, also called as X-ray absorption fine structure (XAFS), is very popular and in great demand as analytical tool.

Topics to be covered

- ✦ X-ray absorption spectroscopy principle, Technical aspects of the XAFS experiments: X-ray source, Synchrotrons, Beamlines, Detection system, Analyzer crystals and Sample preparation.
- ✦ XAFS analysis by Athena: Energy calibration, Align scans, Deglitch, Self-absorption correction, Background removal, Forward Fourier transformation.
- ✦ Analysis of XANES and EXAFS spectra. Software: Athena, Artemis, Hephaestus, FEFF, WinXAFS, Viper and XANda.
- ✦ XAFS analysis by Athena: Linear combination fit, Peak fit, Difference spectra.
- ✦ Different XAFS techniques and its application: quick-XAFS, ED-XAFS (energy-dispersive XAFS), Surface-XAFS, HERFD-XANES (high energy-resolution fluorescence detection XANES).
- ✦ EXAFS analysis by Artemis: Feff calculation, Fitting parameters, Debye and Einstein models for fitting. The first independent fitting of EXAFS spectrum of metal, simultaneous fitting of several temperature-dependent EXAFS-spectra, EXAFS spectra at two different edges and combination of XAFS and XRD, XPS, HAXPES methods
- ✦ XAFS application: from compound/material characterization to investigation of processes (in operando/in situ) such as electrochemical charge/discharge, catalysis or thermally driven reactions, formation of bimetallic nanoparticles or nanoalloys etc.
- ✦ The charge transfer and multiplet calculations using CTM4XAS.

Course participants will learn these topics through lectures and hands-on practice in XAFS analysis. Also case studies and assignments will be shared to stimulate research motivation of participants.

Modules	A: Theory and Applications of XAFS : Oct 3– Oct 8, 2017 (lectures and tutorials) Number of participants for the course will be limited to fifty (50).
You Should Attend If...	<ul style="list-style-type: none">➤ Executives, engineers and researchers from manufacturing, service and government organizations including R&D laboratories.➤ Student at all levels (BTech/MSc/MTech/PhD) or Faculty from reputed academic institutions and technical institutions interested in learning about "<i>X-ray Absorption Spectroscopy analysis</i>".
Fees	The participation fees for taking the course is as follows: Participants from abroad : US \$300 Industry/ Research Organizations: INR 5000 Academic Institutions: INR 2500 Discounted price will be offered to Bachelor and Master Degree students. The above fee includes all instructional materials and assignments and 24 hr free internet facility. The participants will be provided with accommodation on payment basis.

The Faculty



Dr. Asanova Tatyana, Ph.D. in solid State Physics, Senior researcher scientist at Laboratory of Chemistry of Rare Platinum Metals, Institute of Inorganic Chemistry Siberian Branch of Russian Academy of Science, Novosibirsk, Russia. Being an expert in X-ray Absorption Spectroscopy. Her research objectives involve nanomaterials, battery materials, process of thermal decomposition of materials, formation of bimetallic nanoparticles.



Prof. Navdeep Goyal is a Professor of Panjab University, Chandigarh in Physics Department. His research interest is experimental solid-state physics: Dielectric properties of chalcogenide glasses, study of electronic structure of advanced functional materials, device applications of high T_c superconductors and magnetic properties of layered superconductors.



Dr. Sanjeev Gautam, faculty in Dr. S.S. Bhatnagar University Institute of Chemical Engineering and Technology, Panjab University Chandigarh. He is a specialist in X-ray Absorption Spectroscopy (XAS), X-ray magnetic circular dichroism (XMCD) and High-resolution X-ray diffraction (HRXRD) using synchrotron radiation. His research experience includes the synthesis and characterization of various inorganic compounds and study of electronic structure of advanced functional materials including carbon based nanomaterials.

Course Co-ordinators

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