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16.01 - NMR/EXAFS/XANES

MS-16.01.01 New Insights into the Structure and Reactivity of Biological Molecules Using X-ray Absorption Spectroscopy

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Structure and function in biological (as well as other) materials is often determined by an "active site" which commonly involves transition metals in a single site or in clusters. Accurate electronic and geometric structural information of such a site can provide the means to understand in detail how the material carries out a reaction. X-ray absorption edge and extended fine structure (EXAFS) provides a very sensitive way to probe a selected "active site" and obtain accurate metrical details under physiologically-relevant and non-crystalline conditions.

This talk will review the basic principles underlying the use of X-ray absorption edge and EXAFS to obtain such information and compare these results with those that can be obtained from crystallography. New approaches to the quantitative analysis of EXAFS data will be described. The use of these methods to investigate several biological and non-biological systems will also be given. Included will be recent results on the nitrogenase enzyme system which illustrate the ability of EXAFS to probe longer-range order. Other examples will include Cu and Fe-containing proteins and non-biological materials.

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MS-16.01.02 DIFFRACTION ANOMALOUS FINE STRUCTURE (DAFS): UNIFYING THE SENSITIVITIES OF DIFFRACTION AND XAFS INTO A SINGLE NEW CRYSTALLOGRAPHIC TECHNIQUE. by Larry B. Sorensen, Department of Physics, University of Washington, Seattle, Washington 98195-USA

The simple theory and potential applications of a new x-ray structural technique, Diffraction Anomalous Fine Structure (DAFS) which combines the short-range order sensitivity of x-ray diffraction with the short-range order sensitivity of x-ray absorption, will be presented. Because of its combined long-range and short range sensitivities, DAFS is potentially a powerful adjunct and extension of conventional diffraction and XAFS methods for polyatomic and spatially modulated structures. For these systems, DAFS provides: (1) Spatial, or components, selectivity whenever different spatial regions, or components, of the sample produce diffraction peaks at separate locations in reciprocal space. Then the local atomic structure of each region, or component, can be measured using one of its characteristic diffraction peaks. (2) Site selectivity from DAFS crystallographic intensity measurements for inequivalent Bragg reflections. Since the DAFS sigal from each Bragg peak is a linear combination of the DAFS contributions from the individual sites, the sites can be separated by resolving the individual contributions. Experimental demonstrations of each sensitivity will be presented.

MS-16.01.03 ON THE COMPLEMENTARITY BETWEEN MAGNETIC CIRCULAR X-RAYS DICHROISM AND MAGNETIC RESONANT SCATTERING By G. Schütz, Experimentalphysik II, Universität Augsburg, Germany, S. Stähler, Fak. für Physik, E12, Technische Universität München

The availabitity of intense synchrotron light with well defined polarization characteristics led in the last decade to the development of powerful new methods to study the magnetic aspects of the electronic structure of solids using x-rays.

Two of these methods, the measurement of magnetic circular x-ray dichroism (MCXD) at inner-shell absorption edges and the study of magnetic resonant scattering with linearly polarized x-rays, are based on the same physical phenomenon namely the difference in the absorptive part of the scattering amplitude for right and left circularly polarized photons in magnetic matter.

The origin of this effect is explained in simplified pictures to demonstrate that the experimental data contain new symmetry- and element-selective information on the local spin and orbital moment and on the magnetic structures.

The principles, potentials and limits of the experimental techniques of these methods are outlined and typical results are discussed in terms of the complementarity of magnetic circular x-ray dichroism and magnetic resonant scattering studies to address a manifold of ferro(i)- and antiferromagnetic materials e.g. single crystals, polycrystalline (powder)-samples, (diluted) alloys, surfaces and thin layers.

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Structure Determination of Materials Using Non-Crystallographic Techniques

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The appropriate method for the structural determination of real materials is dependant on the degree of long range order present within the sample. If such long range order is absent, conventional single crystal or powder diffraction techniques are no longer applicable and X-ray Absorption Fine Structure (XAFS) spectroscopies offer some of the most versatile methods of probing the fundamental local chemical structure. They have been used, for instance, in conjunction with Magic Angle Spinning NMR (MASNMR), to probe the environments of alkalis and exchanged ion-exchanged cations in oxide glasses. Such direct determinations of local atomic structure point to specific microstructures supporting the particular ion transport characteristics of these materials. In metal oxides like $LiNbO_3$, XAFS measurements pinpoint the environments of particular impurities like Fe^{3+} and Co2+, thereby helping to explain the non-linear optical properties of these materials. There is considerable scope for extending these techniques to follow the development of order from the disordered state. We describe the recent work in which glancing angle fluorescence XAFS has been employed to chart the local structures of ion-implanted dopants in amorphised silicon during subsequent epitaxial regrowth. Fluorescence XAFS has also been used to

