

15.X-01 EXTENDED X-RAY ABSORPTION FINE STRUCTURE STUDIES OF BINARY METALLIC GLASSES. By J. Wong, General Electric Corporate Research and Development, Schenectady, New York, USA.

Extended X-ray absorption fine structure (EXAFS) is the oscillatory modulation of the absorption coefficient on the high energy side of an X-ray absorption edge of a constituent atom in a system. This mode of spectroscopy has been realized in recent years to be a very powerful tool for probing the local atomic environment at all states of matter, particularly since the advent of very intense synchrotron radiation in the X-ray region (Baer et al. IEEE Trans. NS-22 (1975) 22, 1794). In this paper the physical mechanism associated with the EXAFS phenomenon is described in light of the single scattering approximation (Sayers et al. Adv. X-ray Analysis (1970) 13, 248). The use of synchrotron radiation as a light source, experimental procedure, data analysis using a Fourier filtering technique (Sayers et al. Phys. Rev. Lett. (1971) 27, 1204) and the unique features of EXAFS as a structural tool are discussed. Recent EXAFS studies on selected binary metal-metalloid and metal-metal glasses will be presented (Wong, Topics in Applied Physics (1980) 46, Chapter 4). Information derived for the dynamic disorder and local structure of both metalloid and metal constituents in these glasses are described in some detail. Finally the strengths and limitations of EXAFS as a structural tool will be critically evaluated (Lee et al. Rev. Mod. Phys. (1981)).

15.X-02 ANOMALOUS DISPERSION. David H. Templeton, Materials and Molecular Research Division, Lawrence Berkeley Laboratory and Department of Chemistry, University of California, Berkeley, California 94720 USA

The intense continuous spectrum of synchrotron radiation permits anomalous scattering to be measured by several methods in great detail and with high resolution. This scattering varies significantly between elements and between different chemical states of the same element. The large changes in f' very near absorption edges are being used to resolve the effects of different elements in a variety of diffraction experiments with crystalline, partially ordered, or amorphous materials. Exceptionally large effects on both f' and f'' accompany the strong absorption lines at some absorption edges, for example of trivalent rare earth ions. These effects offer a powerful tool for solving the phase problem for macromolecular structures; data for one crystalline phase at several wavelengths can be analyzed much like data for a series of perfectly isomorphous derivatives. The highly polarized nature of synchrotron radiation has been used to observe X-ray dichroism (Acta Cryst. (1980) A36, 237) in crystals containing vanadyl, uranyl, or bromate ions. This dichroism adds a new dimension to anomalous scattering: a dependence on polarization and molecular orientation. Differences larger than 2 electrons/atom have been observed between parallel and perpendicular values of both f' and f'' in absorption and diffraction experiments with uranyl salts (unpublished work with L. Templeton). Some of this work used facilities of the Stanford Synchrotron Radiation Laboratory and was supported by the National Science Foundation (Grant CHE-7919532) in cooperation with the U.S. Department of Energy.

15.X-03 ON THE DIFFERENT APPLICATIONS OF SYNCHROTRON-X-RAYS IN CRYSTALLOGRAPHY. By Ruprecht M. Haensel, Institut für Experimentalphysik der Universität Kiel, D2300-Kiel 1, F.R.Germany

Besides the fields of "Anomalous Dispersion" and "EXAFS" to be covered in other parts of the conference, synchrotron radiation with its unique properties (high intensity, continuous spectral distribution, polarization and time structure) serves a number of other interesting applications in connection with problems in crystallography. Among those are X-ray energy-dispersive diffraction, absorption, emission and Raman spectroscopy, photoelectron emission, X-ray microscopy, lithography, topography, high sensitivity chemical analysis and the investigation of radiation induced centers. The high sensitivity and time structure of synchrotron radiation enable both static and dynamic measurements. The present state of affairs and future trends will be reviewed.

15.X-04 THE MOLECULAR ARCHITECTURE OF METAL ION ACTIVE SITES IN METALLOPROTEINS; STUDIES BY X-RAY ABSORPTION SPECTROSCOPY. By Keith Hodgson, Department of Chemistry, Stanford University, Stanford, CA 94305, U.S.A.

X-ray absorption spectroscopy (XAS) has proven useful on studying the environment of metal ions in biological molecules under non-crystalline conditions. Applications to elucidation of the structural features of active sites in hemocyanin, hemerythrin and cytochrome oxidase will be discussed. Recently, XAS studies of single crystals have shown that angular selective information can be obtained using the polarized property of synchrotron radiation. Advances in rapid data acquisition of XAS data (in the second range) by dispersive methods will also be discussed. Applications of these two recent advances to studies of metalloproteins will be considered.