

**15.X-05** EXAFS STUDIES IN MATERIAL SCIENCE-RECENT DEVELOPMENTS. E.D. Crozier, Physics Department, Simon Fraser University, Burnaby, B.C., Canada.

The EXAFS technique permits specification of the local structure around an X-ray absorbing atom. It has been applied, with notable success, to a wide range of problems involving ordered and disordered systems of interest in materials science. This paper will first review the status of structural determinations. The accuracy of determining radial distances to, and number and identity of, coordinating species will be examined. Methods of analyzing systems in which the distribution of atoms is asymmetrical will be discussed. Theoretical progress in including multielectron and inelastic effects in the EXAFS formalism will be summarized.

Near edge spectroscopy, which is concerned with the structure within 30 to 40 eV of the absorption edge, contains information complementary to that contained in the extended fine structure. Recent advances in deducing the coordination geometry of an X-ray absorbing atom from the near edge structure will be reviewed.

The problems and possibilities offered by EXAFS studies of materials at high pressures will be reviewed.

One of the first applications of the EXAFS technique was to problems in catalysis and surface science. Two recent developments in the detection of the surface EXAFS signal, measurement of electron yield and measurement of photon-stimulated desorption ion yield as a function of X-ray excitation energy will be described and their merits illustrated by recent results in surface crystallography.

**15.1-01** X-RAY POWDER DIFFRACTION STUDIES USING SYNCHROTRON AND CONVENTIONAL RADIATION SOURCES. By P. Thompson and A.M. Glazer, Clarendon Laboratory, Parks Road, Oxford OX1 3PU.

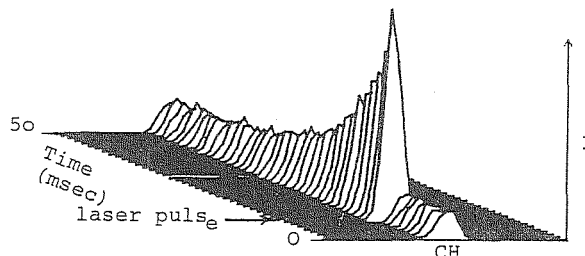
Pilot studies of X-ray powder diffraction experiments using synchrotron radiation will be described. These indicate that very high resolution can be achieved with relative ease, and in addition very rapid exposures are possible.

A general-purpose powder diffraction instrument currently under construction for use at the Daresbury synchrotron is discussed. This instrument will allow both conventional and energy-dispersive studies to be carried out, giving rapid determination of accurate structural parameters. The apparatus will be particularly suitable for the examination of materials in controlled environments such as high temperatures/high pressures etc.

Refinement techniques similar to those currently used in neutron diffraction applied to X-ray powder data sets will be discussed, and it is shown that these techniques, previously applied to energy-dispersive measurements (Glazer, Hidaka and Bordas, *J. Appl. Cryst.* (1978) **11**, 165) may also be used successfully with conventional Debye-Scherrer geometry.

**15.1-02** S.R. TIME-RESOLVED STUDY OF LATTICE CHANGES INDUCED BY LASER PULSE EXCITATION. By D. Pruss, G. Huber, H. G. Danielmeyer, Inst. Appl. Physics, Univ. Hamburg, Jungiusstrasse, Hamburg-36, and H. D. Bartunik, E.M.B.L. Outstation Hamburg, Notkestrasse 85, Hamburg-52, W-Germany.

The  $RE^{3+}$  ionic radius is expected to change by possibly 0.1 Å upon excitation of electronic 4f-5d transitions. Such changes might cause dynamical distortions of the lattice of monoclinic compounds containing  $RE^{3+}$ . The time-dependence in x-ray reflection spectra of  $Ce_{0.2}Tb_{0.8}P_5O_{14}$  and  $CeP_5O_{14}$  (monoclinic  $P2_1/c$ ) has been followed on a time scale of 100 μsec before and after excitation by a 10 ns laser pulse using synchrotron radiation from DORIS at the double-focusing instrument X11. Individual reflections were recorded with a position-sensitive linear gas detector (A. Gabriel). A timing circuitry was synchronizing an excimer laser ( $Xe^*Cl$ , 30 mJ per pulse focused onto the specimen,  $\lambda = 307$  nm) running at a repetition rate of 5 Hz. Data were accu-



culated over about 1000 repetitions.

In contrast to doped materials the unique feature of materials such as  $REPO_4$  for our experiments is that one expects plain  $\theta$ -shifts, not just a broadening of the X-ray reflexes: Excitation of all RE ions shifts the crystal into a new pure state with different equilibrium lattice parameters, resulting from the new ionic radii and a new temperature.

The figure shows a typical spectrum. The intensity profile is plotted versus time for every 2nd time frame. Upon laser excitation strong variation in the integrated intensity is observed with an exponential time behaviour corresponding to a lifetime of 7 msec. The intensity change is correlated with a small shift in the Bragg angle indicating a reversible maximum change in the d-spacing by  $\Delta d/d \approx 10^{-3}$ . Analysis of the results is in progress.

Even higher time resolution in the sub-μsec range is required for investigations of lattice effects due to excitation of 4f-5d transitions in  $CeP_5O_{14}$ . Such a time resolution may be obtained with S.R. using the pulsed time structure (at DORIS pulse width of 100 psec with a repetition rate of  $10^6$  sec<sup>-1</sup>) and by varying the time lag between the exciting laser pulse and the probing S.R. pulse. A first application of this technique is in progress.