15. X—4   TIME-RESOLVED X-RAY DIFFRACTION AND SPECTROSCOPY. By D. M. Mills, Cornell High Energy Synchrotron Source (CHESS), and School of Applied and Engineering Physics, Cornell University, Ithaca, New York.

Although the pulsed nature of the radiation emitted from storage rings has for some time been exploited for studies in the vacuum ultra-violet region of the spectrum, only recently have synchrotron radiation users begun to perform time-resolved diffraction and spectroscopy at x-ray energies. Time-resolved x-ray experiments performed at synchrotron radiation sources fall naturally into two catagories, those which do not depend on the actual time-structure of the emitted radiation but rather rely on the high flux and those which take explicit advantage of the modulated or pulsed nature of the x-ray beam. It is with these experiments that this presentation is concerned.

A survey of recently performed time-resolved x-ray experiments will be given with emphasis on the techniques used. Future directions for this field will also be discussed.

15. X—5   GENERAL PROBLEMS IN THE STRUCTURAL ANALYSIS BY EXAFS. By P. Rabe, Institut für Experimentalphysik, Universität Kiel, D-2300 Kiel, FRG

The evaluation of structural parameters from the extended X-ray absorption fine structure follows several steps each of which may introduce uncertainties in bond lengths and coordination numbers:
1. Recording the spectra: Absorption spectra are subject to statistical noise. An increasing noise is directly related to an increasing uncertainty in the bond lengths, coordination numbers, and Debye-Waller factors determined in the subsequent steps of the data analysis.
2. Normalization procedure: To convert the experimental spectra to a form which can be compared with the single scattering formalism of EXAFS the atomic background has to be removed. Generally this background is assumed to behave monotonous with photon energy. Several experiments have shown however that an atomic extended fine structure which is caused by multielectron excitation is underlying the EXAFS. This low frequency fine structure may interfere with the EXAFS especially in cases where the amplitudes are small due to thermal damping or structural disorder.
3. Fourier transform or curve fitting: The finite range over which the EXAFS can be observed leads to a substantial broadening of peaks in the Fourier transform. As a result close lying coordination shells cannot be resolved unambiguously. Moreover the electron-atom scattering phases and amplitudes have to be known. In fortunate cases reference samples with electronic and structural properties comparable to those of the sample under investigation are available from which these parameters can be extracted. In other cases a combination of experimental and calculated phase shifts lead to reliable bond lengths. Finally at photon energies close to the absorption edge the spectra are dominated by multiple electron scattering. This range is permanently lost for an interpretation with the single scattering formalism and leads to a loss of information about a long range order. A way out of this dilemma is to resort to multiple scattering calculations or to complete the EXAFS spectra with X-ray scattering data in the photon energy range of anomalous dispersion.

15. X—6   APPLICATIONS OF X-RAY STANDING WAVES FOR BULK AND SURFACE STUDIES. By G. Materlik, Hamburger Synchrotronstrahlungslabor HASYLAB, Hamburg, Germany, INVITED PAPER at the Microsymposium organized by C.J. Sparks.

Recent progress in studies with x-ray standing waves which has been realized by using synchrotron x-radiation is described in this paper. Most of the measurements were carried out by using the ROEMO instrument installed at the storage ring DORIS in Hamburg (A. Krolzig, G. Materlik and J. Zegenhagen, Nucl. Instr. & Meth. 208, 613 (1983)).
The movement of the x-ray interference field across the crystal net-planes, generated by passing a Bragg reflection, was used in following studies: 1. Position distribution, lattice relaxation and limits for vibrational amplitudes were determined by higher order measurement on shallow layers of implanted bulk impurities (G. Materlik and J. Zegenhagen, Phys. Lett. subm.) 2. Chemisorbed (Br on Si & Ge, M. Bedzyk and G. Materlik, subm.) and electrodeposited (Cd and Tl on Cu, G. Materlik, J. Zegenhagen and W. Uelhoff, subm.) sub-monolayer coverages of adsorbates were studied to characterize the adsorbate structure perpendicular to the diffraction planes which were oriented parallel to the surface. 3. The position of 1/4 monolayer of Br on Si was measured with a Si x-ray interferometer parallel to the (111) surface plane of the analyzer crystal (G. Materlik, A. Frahm and M.J. Bedzyk, Phys. Rev. Lett. 52, 441 (1984)). 4. The electron emission yield was measured to determine the crystal perfection layer-by-layer perpendicular to the surface using the electron energy loss process (M.J. Bedzyk, G. Materlik and M. Kovalchuk, subm.) and 5. The electron emission yield of a non-centrosymmetric GaAs crystal was measured and reveals the shift of the diffraction planes relative to the atomic planes as a function of photon energy E as described by $f'(E)$ and $f''(E)$.

15. X—7   ANOMALOUS SCATTERING STUDIES OF AVERAGE DISTRIBUTION PARAMETERS IN SIGMA AND TAU PHASES. By H. L. Yakel, Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830, U.S.A.

If synchrotron radiation (SR) with energy near an atomic absorption edge is used to measure Bragg or diffuse diffracted intensities, anomalous dispersion can change scattering cross sections enough to reveal long- or short-range structural features in materials whose constituent elements are near-neighbors in the periodic table. We present results of long-range site-occupation parameter estimations, derived from single-crystal diffraction experiments with SR and conventional Mo Kα x radiation, for sigma (σ) and $M_{23}C_6$ tau (τ) phases composed of such elements.

The σ crystals examined with conventional radiation were selected from phases containing Cr and Fe; Cr, Fe, Ni, Mo and Mn; Cr and Mn; and W and Re. SR diffraction data were obtained from a Cr-Fe crystal and from the polynary σ crystal. Tau crystals chosen from $(Cr_{23-x}Fe_x)C_6$ phases with $x = 7.3_6$, 4.1_3, 1.7_0 and 0.7_4, and from a $(Cr_{15.73}Mn_{4.18}Fe_{3.09})C_6$ phase, were studied with conventional radiation; intensities of Bragg reflections from the binary crystal with $x = 0.7_4$ were also measured with SR tuned near Cr and Fe K edges.

Analyses of these data sets show that usefully accurate, moderately precise long-range site-occupation parameters can be derived from extensive, precisely measured Mo Kα Bragg reflection intensities for all the binary Cr-Fe σ and τ phase crystals examined. However, site-occupation parameters could not be recovered by analyses of conventional data from crystals of the Cr-Mn and W-Re σ phases and the Cr-Mn-Fe τ phase. Distribution parameters of Mo atoms on the 5 sites of the σ structure could be derived from conventional data for the polynary σ crystal, but