15. USE OF SYNCHROTRON RADIATION


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 categories, 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. Rebe, Institut Physique, Universite Kiel, D-2300 Kiel, FRG.

The evaluation of structural parameters from the extended X-ray absorption fine structure (EXAFS) data 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 simple scattering formalism of EXAFS the atomic background has to be removed. Generally this background is assumed to be monotonous with photon energy. Several experiments have shown however that an atomic extended fine structure which is caused by multi-electron 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 electron 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 simple scattering formalism and leads to a loss of information about long range order. A way out of this dilemma is to resort to multiple scattering calculations or to use the EXAFS spectra with X-ray scattering data in the photon energy range of anomalous dispersion.

15.X-6  ANOMALOUS SCATTERING STUDIES OF AVERAGE DISTRIBUTION PARAMETERS IN SIGMA AND TAU PHASES. By B. L. Yakel, Chemicals and Engineering Physics, Cornell University, Ithaca, New York.

If synchrotron radiation (SR) with energy near an atomic absorption edge is used to measure Bragg or diffuse diffractions, 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. Present results of long-range site-occupation parameter estimations, derived from single-crystal diffraction experiments with SR and conventional Mo Kα radiation, for sigma (σ) and MgCu₂ τ phases compared to theoretical elements are near-neighbors in the periodic table. Present results of long-range site-occupation parameter estimations, derived from single-crystal diffraction experiments with SR and conventional Mo Kα radiation, for sigma (σ) and MgCu₂ τ phases compared to theoretical.

15.X-7  APPLICATIONS OF X-RAY STANDING WAVES FOR BULK AND SURFACE STUDIES. By G. Materlik, Hamburger Synchrotronstrahlungs laboratorium HASYLAB, Hamburg, Germany.

Recent progress in studies with X-ray standing waves which has been realized by using synchrotron X-ray radiation is described in this paper. Most of the measurements were carried out by using the DRIVO instrument installed at the storage ring DORIS in Hamburg (A. Krolz, 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 damping or structural disorder. 2. Chemsorb-bed (Br on Si and Ge), M. Bedzyk and G. Materlik, and electrodeposited (Cd and Ti on Cu), G. Materlik, J. Zegenhagen and W. Uelhoff, sub-monolayer coverage of adorbate 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 W. Kivelchuk, 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).


The dependence of EXAFS on the energy range of anomalous dispersion in the absorption spectrum, only recently have synchrotron radiation experiments been performed at synchrotron radiation sources. The evaluation of structural parameters from the extended X-ray absorption fine structure (EXAFS) data 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 simple scattering formalism of EXAFS the atomic background has to be removed. Generally this background is assumed to be monotonous with photon energy. Several experiments have shown however that an atomic extended fine structure which is caused by multi-electron 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 electron 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 simple scattering formalism and leads to a loss of information about long range order. A way out of this dilemma is to resort to multiple scattering calculations or to use the EXAFS spectra with X-ray scattering data in the photon energy range of anomalous dispersion.

15.X-9  APPLICATIONS OF X-RAY STANDING WAVES FOR BULK AND SURFACE STUDIES. By G. Materlik, Hamburger Synchrotronstrahlungs laboratorium HASYLAB, Hamburg, Germany.

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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 damping or structural disorder. 2. Chemsorb-bed (Br on Si and Ge), M. Bedzyk and G. Materlik, and electrodeposited (Cd and Ti on Cu), G. Materlik, J. Zegenhagen and W. Uelhoff, sub-monolayer coverage of adorbate 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 W. Kivelchuk, 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).