15. 4–5 A PROGRAM SYSTEM FOR STRUCTURE DETERMINATION BY USING THE "LAMBDA TECHNIQUE". By W. Konz, J. Spilker, G. Schäfer and K. Fischer, Fachrichtung Kristallographie, Univ. des Saarlandes, D-6600 Saarbrücken, FRG.

A difference Patterson function from intensity differences measured at wavelengths around the absorption edge of an anomalous scatterer (e-atom), may have a real and imaginary part. Synchrotron radiation permits selection of wavelengths such that "symmetry conditions" on the f'_e and f''_e can be fulfilled for 2 or 3 wavelengths ("Lambda Technique", K. Fischer, Z. Naturforsch. 36a (1981) 1253).

The program FORSYN (Eichhorn, Kristallographie Saarbrücken, FRG (1982) unpublished, complete revision of FORDAP by Zalkin, LRL, Livermore/Cal., USA, 1962) was modified in order to compute the real ($L_c(u)$) and imaginary part ($L_s(u)$) of a difference Patterson map. FORMAP (Eichhorn, Kristallographie Saarbrücken, FRG (1983) unpublished) was changed appropriately being able now to search for all vectors between e-atoms and normal scatterers (n-atoms) on the basis of known positions of the e-atoms. Vectors from the first e-atom to all the other e-atoms are used as search vectors. The result is a density distribution approximating the electron density of all the n-atoms.

Test computations both on data from an acentric mineral structure (hemimorphite) and on simulated intensity data of other structures will be presented in order to investigate practical limitations of the Lambda Technique.

Thanks are due to the Deutsche Forschungsgemeinschaft for financial support.

15. 4–6 PRACTICAL EXPERIENCES WITH THE "LAMBDA TECHNIQUE" ON THE STRUCTURE OF $KNbO_3$. By H. Schenk-Strauß, K. Fischer and A. H. Millhouse, Fachrichtung Kristallographie, Univ. des Saarlandes, D-6600 Saarbrücken, FRG.

Synchrotron X-rays from the storage ring DORIS in Hamburg were used to test the applicability of the Lambda Technique (K. Fischer, Z. Naturforschung 36a (1981) 1253) in structure determination. For this study $KNbO_3$ was used at room temperature where it has a pseudosymmetric crystal structure and is ferroelectric.

3 different wavelengths were selected near the Nb K-edge to satisfy the symmetry constraints on the anomalous scattering terms. The energy-dependent fine structure of f' and f'' was determined by measuring an absorption spectrum and using the Kramers-Kronig transformation. The measurements were done on the two-axis-diffractometer (U. Bonse, K. Fischer, Nuclear Instr. and Meth. 190 (1981) 593) supplied with a Ge (111) double crystal monochromator (Bonse, K. Fischer et al., Z. Kristallogr. 162 (1983) 31). The structure determination experiment and the absorption measurement were performed in exactly the same configuration to ensure that the energy resolution was identical for both. During the measurement of Bragg intensities, the state of polarization of the monochromatic beam was simultaneously determined using a Compton-Polarimeter (Smend, Schaupp, Cerwinski, Millhouse, to be published, 1984), which was found to be crucial for precise data reduction. The experimental setup, method of data analysis, and results will be presented.

Thanks to the BMFT for financial support.

15. 4–7 ANOMALOUS SMALL ANGLE SCATTERING OF GUINIER-PRESTON ZONES IN AL-ZN ALLOYS. By P. Goudeau+, A. Naudon+ A. Fontaine++ and C. Williams+++. LURE, Université de Paris-Sud, 91405 Orsay, France.

+ Métallurgie Physique, 86022 Potiers, France
++ Physique du Solide, Bat. 510, Orsay, France
+++ Physique de la Matière Condensée, Collège de France, 75005 Paris.

We present here a new method of determining the concentration of an element in the Guinier-Preston zones which occur after quench in aluminum based alloys, by anomalous small-angle X-ray scattering (SAXS).
For dilute Al-Zn alloys, one have only the Laue scattering $I_L = C_A (1 - C_A) (f_A - f_B)^2$.
For more concentrated Al-Zn alloys, the SAXS intensities due to G.P. zones, having a concentration of zinc atoms C_1 much higher than in the remaining matrix where it is C_2, are proportional to $(C_1-C_2)^2 (f_A-f_B)^2$; ant the integrated SAXS intensities Q_o in the particle model are given by $Q_o = (C_1-C_A) (C_A-C_2) (f_A-f_B)^2$ Va, where Va is the mean atomic volume of the alloy.
The SAXS intensities have been compared far from the Zn absorption edge (scattering factor f_o) and near the absorption edge (λ = 1.2834 Å, scattering factor $f = f_o + if'(\lambda) + if''(\lambda)$). The results obtained at different wave-lengths were normalized with an Al-Ag alloy, giving a response of similar shape and intensity but where no anomalous effects should be observed. Furthermore, for each wavelength, the absorption of the sample was determined by the diffraction of an amorphous carbon. So the scattered SAXS intensities are obtained on an absolute scale and quantitative values can be deduced concerning the f' factors and both zinc concentrations of G.P. zones in binary and ternary Al-Zn and Al-Zn-Mg alloys.

15. 4–8 LAMBDA TECHNIQUE AND OTHER SYMMETRY CONDITIONS ON ANOMALOUS SCATTERING COEFFICIENTS FOR STRUCTURE DETERMINATION USING SYNCHROTRON RADIATION. By K. Fischer and W. Konz, Fachrichtung Kristallographie, Universität des Saarlandes, D-6600 Saarbrücken, Federal Republic of Germany.

The so-called "Lambda Technique" (K. Fischer, Z. Naturforsch., 36a (1981) 1253) demands selection of 3 wavelengths such that the following "symmetry conditions" on the real (a_e) and imaginary (b_e) part of the scattering factor of an anomalous scatterer (e-atom) are met:

$$\lambda_1 < \lambda_2 < \lambda_3$$
$$a_1 = a_2 \mp a_3$$
$$b_1 > b_2 \approx b_3$$

This leads to the approximate determination of the electron density distribution $\Sigma\rho(r)$ of all normal scatterers (n-atoms) without "knowing" reflection phases.

Three more symmetry conditions were set up which permit

1) eliminating the vectors between 2 different anomalous scatterers (K. Fischer, Ehses, Schäfer, Schenk-Strauß and Spilker, Fortschr. Mineralogie, 60 (1982) 71)

2) suppressing (e-e)-vectors and providing directly the (approximate) electron density distribution of the normal scatterers in the correct space group (not Patterson group) including enantiomer and/or polarity, from 2 wavelengths only.

3) Providing (e-e)-Patterson vectors and (e-n)-vectors (without (n-n)-vectors as in a normal Patterson function) in correct space group symmetry from 2 wavelengths, both vector sets being added together.

A study of the practicability of these symmetry constraints and their limitations by experimental errors will be presented. It is based on test computations using the program described in the abstract by Konz, Spilker, Schäfer and K. Fischer (Abstract, XIII IUCr Congress, 1984).

Thanks are due to the Deutsche Forschungsgemeinschaft for financial support.

15.4–9 STRUCTURAL STUDIES OF AMORPHOUS MATERIALS USING SYNCHROTRON RADIATION AND ANOMALOUS SCATTERING*. By A. Bienenstock, A. Fischer-Colbrie, J. Kortright, R. Lorentz, K. Ludwig, W. Warburton, L. Wilson, Stanford Synchrotron Radiation Laboratory, Stanford University, SLAC Bin 69, P.O. Box 4349, Stanford, CA, 94305, USA and P. Fuoss, AT&T Bell Laboratories, Holmdel, NJ 07733 USA.

In this talk, applications of synchrotron radiation and anomalous x-ray scattering to the determination of short-range atomic coordinations in polyatomic amorphous materials will be discussed. The advantages and limitations of differential anomalous scattering (DAS) techniques will be reviewed. It will be shown that the DAS technique provides information which is not obtainable in any other way and vastly increases our ability to determine the coordinations of specific elements in amorphous materials, particularly when combined with EXAFS analysis. The degree of success we have achieved in obtaining valid partial distribution functions will be described.

*Supported in part by the NSF through the Stanford University Center for Materials Research and by the DoE through the Stanford Synchrotron Radiation Laboratory.

15.5–1 CRYSTALLIZATION OF METALLIC GLASSES STUDIED BY SYNCHROTRON X-RAY RADIATION. By W.Minor, University of Warsaw, Poland, B. Schönfeld, Hamburger Synchrotronstrahlungslabor, DESY, F.R.G, B.Lebech, Risø National Laboratory, Denmark, B.Buras, University of Copenhagen, Denmark and W.Dmowski, Technical University, Warsaw, Poland.

Metallic glasses containing Fe are soft magnetic materials with potential technological applications. When crystallizing they become brittle and lose their magnetic properties. Therefore studies of the crystallization process in metallic glasses are of both scientific and technological interest. Studies of the crystallization process have been made by us by means of x-ray synchrotron radiation and the energy dispersive method, which enable the recording of a full diffraction pattern in a relatively short time. The amorphous to crystalline transition were investigated in $Fe_xSi_{90}B_{10}$ ($69<x<83$). We used the white spectrum of the synchrotron radiation at DORIS (Hasylab) in the energy range up to 50 keV which for the scattering angle 21 corresponds to 11 $Å^{-1}$. The crystallization was followed either by heating the sample stepwise from 20 °C to 1000 °C or by repeatedly recording the diffraction patterns obtained from a sample while annealing at a fixed temperature close to the crystallization temperature. Several time series of isothermal patterns have been obtained and used to study the kinetics of the crystallization. The crystallization of α-Fe in $Fe_{83}Si_7B_{10}$ at 350 °C is nearly complete after 700 minutes.

15.6–1 SMALL ANGLE SCATTERING ON SINGLE OSTEONS USING SYNCHROTRON RADIATION. By A. Ascenzi*, A. Bigi**, M.H.J. Koch ***, A. Ripamonti**, and N. Roveri**,
* Istituto di Anatomia Patologica, Policlinico Umberto I, Universita' di Roma,Italy. **Istituto Chimico "G.Ciamician", Universita' di Bologna, Italy. *** EMBL Outstation Hamburg, c/o Desy Hamburg.

Small angle X-ray diffraction patterns of single osteons have been recorded using synchrotron radiation at EMBL c/o Desy, Hamburg. The first six meridional reflections corresponding to the collagen axial periodicity have been measured, whereas using X-ray conventional sources the first three reflections could be recorded only for the most ordered samples.

The intensity distribution of the meridional reflections is in agreement with a model in which inorganic blocks at the level of the main band of collagen fibrils are arranged with the same axial periodicty of the collagen structure.

The intensity distribution of the meridional reflections is different from that of the native collagen fibers. However, the appearance of the strong first and third reflections indicates that the projected electron density is a step-function. The falling off of the intensity can be ascribed to the height of the step, representing the inorganic blocks at the level of the main band of collagen fibrils and much greater of any other possible density fluctuation.