the system mechanically, takes still or oscillation frames, the other processes the frames to obtain a set of reflection data. The orientation matrix of the crystal is determined by Higashi's auto indexing algorism. The processing of oscillation images is based on Wonacott's strategy for the oscillation-film method and estimates integrated intensity by Rossmann's five quadrant profile fitting algorism. Scale and temperature factors are refined by the method of Fox and Holmes. The quality of diffraction data was evaluated as follows; R-merge values being 0.04 ~ 0.05 range and data reproducibility better than that of a four-circle diffractometer, isomorphous and anomalous difference Patterson maps showing significant peaks corresponding to heavy-atom vectors, electron density maps being of high quality enough to asign amino-acids unambiguously, data collection rate being fast enough to collect a full set of diffraction data from one protein crystal.

PS-01.03.11 THE FIRST EXPERIMENTS WITH A HIGH POWER WIGGLER AT THE THIRD GENERATION EUROPEAN SYNCHROTRON RADIATION FACILITY
Å. Kvick, European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex, France

Twelve European countries have jointly built a 6 GeV third generation synchrotron radiation facility in Grenoble, France. The storage ring was successfully commissioned during 1992 and is now running routinely with 100 mA of electrons stored with lifetimes well in excess of 10 hours. The emittance is in close agreement with the predictions.

The installation of the first three beamlines was started in June 1992, and first beams in the experimental hutches were obtained in November 1992. This presentation will concentrate on beamline 2 also referred to as "The Materials Science" beamline, which is based on a 1.24 T multipole wiggler with 12 periods of 125 mm length. This wiggler is the highest power and highest flux insertion device presently planned at the ESRF. The total generated power is 5.6 kW and the characteristic energy at a 20 mm gap is E_c=30 keV (0.4 Å). The wiggler thus gives total integrated fluxes of close to 10^{15} photons/sec/0.1% over a wide energy range (10^{14} for instance at 80 keV).

The beamline was commissioned to full power operation during the brief November and December operational periods, and early experiments both with white beam and monochromatic beam have been performed since December 1992. To date experiments including high temperature (over 1900° C) phase transitions of perovskites, high pressure (180 kbars) phase transitions of Ge, complete data collections from proteins at short wavelengths (0.45 Å) using both imaging plates and imaging intensifier detectors, powder diffraction patterns of molecular sieves using imaging plates have been performed, and extensive further test are planned for the spring and summer periods. The presentation will concentrate on the results from the crystallographic experiments performed with this new source of synchrotron radiation.

PS-01.03.12 INEXPENSIVE UPGRADE OF A NICOLET P3M DIFFRACTOMETER. C. Svensson and B. Sommarin*, Inorganic Chemistry 2, Chemical Center, University of Lund, PO Box 124, S-221 00 LUND, Sweden.

The Data General Nova control computer of our Nicolet P3m single-crystal four-circle diffractometer has been out of order for some time. Because the motor controllers and drivers are integrated with the computer, the whole drive chain had to be renewed. We have connected the goniostat to a PC containing a commercial ISA-bus motion controller board and added an external unit with power supply and four servo amplifiers. To minimize the amount of work on the goniostat itself, the original DC motors have been retained, but the angle resolvers have been replaced by optical encoders using the original resolver mounts. Limit and zero point sensors have been added. The step size is 0.001° for all axes with a positioning precision of a quarter of a step. The setup of the servo system is facilitated by the tuning software supplied by the motion controller manufacturer.

The comprehensive crystallographic control software that is used for the upgraded instrument is the same as was developed for our Huber four-circle diffractometer (Svensson and Ståhl, J. Appl. Crystallogr., 1993). Only minor software modifications were necessary for the modified P3m. A new set of routines was written for the microprocessor-based motion controller board. These are downloaded as needed. Once the controller has received a command it is self sufficient and will run independent from the CPU and memory of the PC until completion. Several options on the general purpose board enhance the performance of the diffractometer, eg. the electronic gearing, the automatic S-curve profiling during acceleration and deceleration, the high speed position capture, and the extensive error handling. The controller also has analog-to-digital converter inputs that can, for example, be used for logging the temperature during a low-temperature experiment.

PS-01.03.13 A LABORATORY DISPERSIVE EXAFS SPECTROMETER. By J. Galy, P. Baules, J. Jaud, P. Lecante, A. Mosset,* CEMES-LOE / CNRS, 29 Rue J. Marvig, BP 4347, F31055 Toulouse Cedex, France.

The study of short range order in non-crystalline or poorly crystallized materials usually involves LAXS (Large Angle X-ray Scattering) and/or EXAFS (Extended X-ray Absorption Fine Structure) measurements. Synchrotron radiation emitted by large storage rings constitutes the best source currently available for EXAFS experiments. However, the practical interest of a laboratory facility promoted the development of various devices making use of the weak Bremstrahlung spectrum produced by sealed-off or rotating anode X-ray tubes. Most of existing in-lab spectrometers use Johanson or Johann type bent monochromators and work in sequential mode.

An alternative technique makes use of the divergent character of the beam produced by X-ray tubes. X-rays falling on a single crystal settled in transmission or reflection geometry with different incidence angles are diffracted for Bragg related different energies. All intensities can then be simultaneously recorded using a linear position sensitive detector. Mechanical motion suppression during data collection decreases measurement times and also reduces potential drift and background, allowing long exposures in the case of low intensity X-ray sources or diluted samples.

In this paper, we report the principle and the construction of a laboratory EXAFS spectrometer optimized for transmission dispersive mode. Factors determining energy range and resolution are detailed. An empirical energy calibration procedure is proposed. EXAFS spectra obtained for copper metal foil, molecular complex copper acetate, germanium oxide and zirconium oxychloride compare favourably with data obtained using conventionnal synchrotron facility.

PS-01.03.14 HX-1B FULLY MICROCOMPUTERIZED FOUR CIRCLES SINGLE CRYSTAL DIFFRACTOMETER CONTROL SYSTEM AND AUTOMATED CRYSTAL STRUCTURE ANALYSIS SYSTEM. By Shen Jinchuan*, Jin Xing, Yang Daihua and Liang Jun, Test Centre, China University of Geosciences, Wuhan 430074, P.R. China.

On the basis of an obsolete Picker Single Crystal Diffractometer

01-Instrumentation and Experimental Techniques (X-rays, Neutrons, Electrons)

System, a new fully microcomputerized single crystal diffractometer control system and crystal structure analysis system have been developed successfully. The system works on a powerful flexible and expandable microcomputer system (80286/80386 CPU). Some features of this system are as follows:

(1) Highly stable X-ray generator and electronic recording system;

(2) A PC-80286 based powerful, flexible and expandable diffractometer control system, including 48 instructions written in QUICK BASIC programming language, and it is easy to add instructions with new functions;

(3) Peak searching with profile show on the screen simultaneously, parameters for peak recognition are easy to change so as not to lose weaker peaks;

(4) Data collection can go according to the index both from a calculation of formula or an index data file prepared by the user;

(5) A PC-386 based Crystal Structure Analysis System is equipped with several advanced software packages like HX-MULTAN/ HX-SHELX/ HX-SAPI etc. in PC-286/ 386/ 486 versions with co-processor;

(6) It includes a high resolution color crystal structure and crystal form displaying and drawing system (1024×768×256 TVGA mode). This system has been proved to be quite reliable by the fact that it has run normally up to over 4000 hours already.

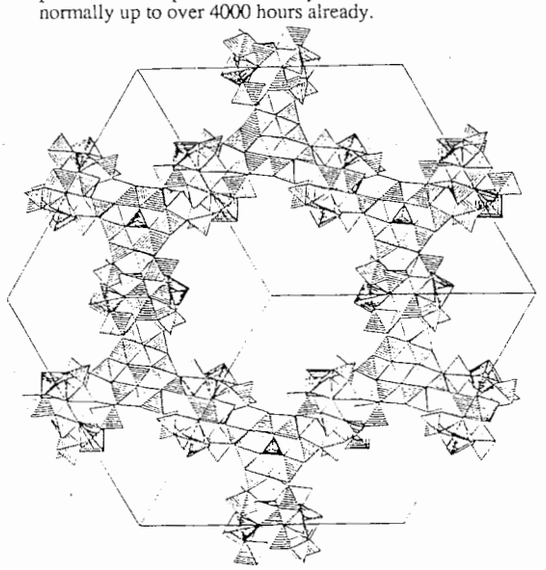

Figure 1 Cacoxenite crystal structure drawn by this system. $P6_3/m$,a = 2.7559nm; c = 1.055nm.

01.04 – Magnetic Scattering

MS-01.04.01 NEUTRONS AND X-RAYS FOR THE STUDY OF MAGNETISM. by M.Blume*, Deputy Director, Brookhaven National Laboratory, Upton New York, USA

While neutrons have long been the probe of choice in studying magnetism, the development of synchrotron sources has led to increasing use of x-ray in such studies. The possible use of the relative advantages and disadvantages of each will be considered in this talk. We conclude that neutrons remain the most powerful tool for studying the broad range of magnetic properties. There is, however, an important supplementary role for x-rays in specific cases.

MS-01.04.02 X-RAY MAGNETIC CRITICAL SCATTERING. By Doon Gibbs, Department of Physics, Brookhaven National Laboratory, Upton, NY 11973.

During the last several years, x-ray resonant magnetic scattering techniques have been exploited in a variety of interesting physical settings. For example, the polarization and energy dependence of the resonant cross-section has provided a new spectroscopy of magnetic states, which is only beginning to be developed in both scattering and absorption geometries. The existence of large resonant enhancements has also made possible experiments for which the signal rates were formerly thought too weak, for example, in studies of thin films, multilayers, and surfaces. In this talk, we describe the results of recent experiments concerned with x-ray magnetic critical scattering in rare earths and actinides. In some cases, it has been found that the magnetic fluctuations which occur within about 1 Kelvin above Tn exhibit two length scales, reminiscent of the structural-to-cubic transitions of the perovskites. The results obtained by x-ray scattering are compared to those obtained by neutron diffraction.

The speaker is indebted to his collaborators in these experiments, especially T. R. Thurston, G. Helgesen, J. Hill, B. Gaulin, G. Shirane, S. Langridge, W. Stirling, G. H. Lander, C. Vettier, F. de Bergevin, P. Dalmas, and J. B. Hastings. Work performed at Brookhaven is supported by the U.S. DOE, Division of Materials Science under contract No. DE-AC02-76CH00016.

MS-01.04.03 REVIEW OF MAGNETIC X-RAY DIFFRACTION EXPERIMENTS

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The first magnetic X-ray scattering experiments were performed in 1972 by de Bergevin and Brunel in NiO following the original calculations by Platzmann and Tsoar. Limited by the weak scattering cross-section the technique remained in the shadow of powerful neutron scattering until it was shown, both theoretically and experimentally, that a significant enhancement of the X-ray magnetic scattering intensity can be obtained by tuning the photon energy near distinct absorption edges of the atoms in the respective magnetic systems. Since then resonant and non-resonant magnetic scattering studies have been carried out in most of the heavy rare earth metals, rare earth magnetic multilayers and in a variety of actinides and transition metals.