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.

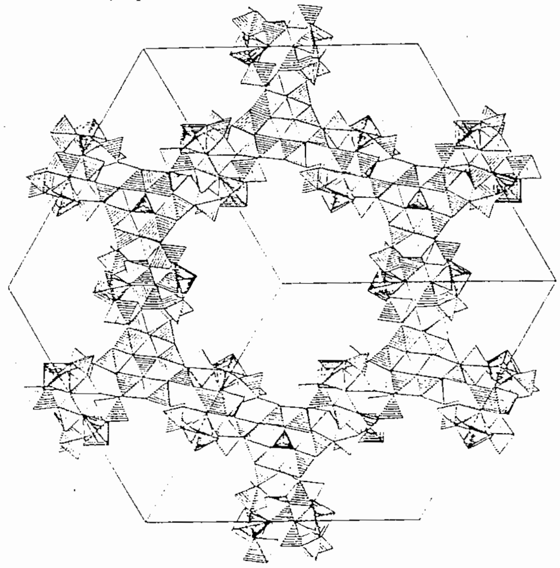

Figure 1 Cacoxenite crystal structure drawn by this system. $P6_3/m$,a = 2.7559nm; c = 1.055nm.

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 T_N 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.

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

The largest resonant enhancements have been observed for incident X–rays near the M_{IV} absorption edges of the actinides and near the L_{III} edges of the rare earths and transition metals. 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. Current experimental work is reviewed and perspectives related to the operation of new, third generation synchrotron radiation sources are discussed.

MS–01.04.04 MAGNETIC CIRCULAR X-RAY DICHROISM: PROBING LOCAL MAGNETIC STRUCTURES by Gisela Schutz , Experimentalphysik II, Universitat Augsburg, Germany, and Slike Stahler,* Fakultat Physik, E12, Technische Universitat Munchen, Germany

Circular magnetic x–ray dichroism in core–level absorption is the absorptive counterpart of magnetic resonance scattering. It is based on the same physical phenomenon, the difference in the imaginary part of the charge scattering amplitude for right and left circularly polarized photons in magnetic matter and a complementary element–and symmetry–selective methods to study the magnetic aspects of the electronic structure of solids. Typical magnetic absorption effects at K–and L–edges in the hard and soft x–ray range are presented. Their relation to the spin polarization of unoccupied bands as well as local magnetic spin and orbital moments are discussed in the frame of single–particle band–structure pictures and atomic multiplett theories. Focusing on magnetic multiayered systems as Co/Pt and Co/Cu it is demonstrated that the magnetic circular dichroism measurements yield important new informations on the exchange coupling mechanism especially the role of the –in the pure element non–magnetic–interlayer.
Also in the EXAFS range , the existence of a magnetic part (SPEXAFS) has been established to be an universal phenomenon, which allows to study local magnetic structures in ferro(i)magnetic materials. a comparison of the EXAFS allows a clear distinction between magnetic and nonmagnetic neighborhood also in case of non–magnetic absorbing atoms. Comparing the peak heights in the SPEXAFS strengths for various magnetic systems a direct correlation between the magnetic contribution to the EXAFS and the spin moment of the neighboring atom is found providing a new possibility of a quantitative investigation of local magnetic short–range order.

MS–01.04.05 SITE SPECIFIC MAGNETIC XANES. By H. Kawata, Photon Factory, National Laboratory for High Energy Physics, Tukuba, Japan.

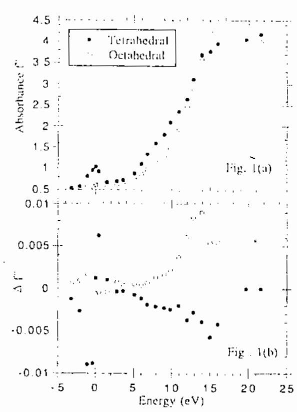
Magnetic X-ray Absorption Near Edge Structure (XANES) using circularly polarized X-rays gives on the spin-polarized unoccupied electron states [1,2]. Recently, the study for ferro- or ferri-magnetic materials by using this experimental method have been rapidly developed. In a case of ferri-magnetic materials, however, there are two different sites for magnetic atoms; for example in the case of $Y_3Fe_2(FeO_4)_3$ (YIG), the magnetic ions Fe^{3+} have two different sites. One is an octahedral site and another is a tetrahedral site. The directions of magnetic moments on these sites are opposite to each other. It is naturally expected that the magnetic XANES spectra of Fe K-edge for Fe^{3+} ion at the octahedral site is different from that for the tetrahedral site, because of the different chemical bonding and the different direction of the magnetic moment. Therefore, it is necessary to identify the site-specific magnetic XANES in order to study these materials. Here we present the first measurement of the site-specific magnetic XANES of YIG by mean of the following two methods.

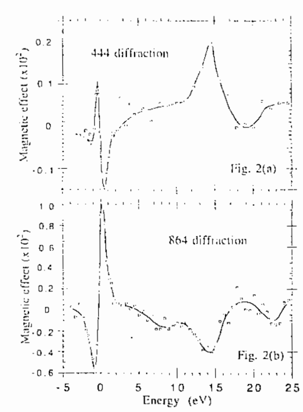
<Magnetic XANES under a standing wave field>
The standing wave field method, which is obtained by exiting a dynamical Bragg diffraction in a crystal, gives us site-specific information. Therefore, magnetic XANES measurement under a standing wave field gives us the site-specific magnetic XANES[3]. Figure 1(a) and (b) show the site-specific XANES and magnetic XANES at Fe K-absorption edge. The black dots and open circles in each figures are these of the octahedral site and tetrahedral site, respectively. As shown in this figure, the characteristic structure at the pre-edge is mainly given by the tetrahedral site.

<Resonant magnetic Bragg scattering>
Recently, Stragier et al. presented the site-specific normal XANES by mean of DAFS[4]. The resonant magnetic Bragg scattering corresponds to the magnetic DAFS. Therefore, the resonant magnetic Bragg scattering from the different diffraction indexes also brings us the site-specific magnetic XANES. Figure 2(a) and (b) show the results from (444) and (864) diffraction. The structure factor of these indexes are as follows;

$F(444)=-12f_Y+8f_{Fe}^O-12f_{Fe}^T,$
$F(864)=-8f_Y-8f_{Fe}^T.$

Here, f_Y, f_{Fe}^O, and f_{Fe}^T are atomic form factors of Y, Fe at the octahedral site, and Fe at the tetrahedral site, respectively. In the case of 864 diffraction, Fe at the tetrahedral site only contributes to the structure factor, and the spectrum of Fig. 2(b) is well explained by the magnetic XANES of the tetrahedral site in Fig. 1(b).





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PS–01.04.06 MAGNETIC STRUCTURAL STUDIES USING LONG-WAVELENGTH PULSED NEUTRONS. By J. B. Forsyth, C. J. Carlile and P. S. R. Krisna, Rutherford Appleton Laboratory, Chilton, Oxon. OX11 0QX, U.K.

Powder diffractometers at pulsed neutron sources such as ISIS can provide very high resolutions in backscattering, $\Delta d/d \sim 5\times10^{-4}$, which are almost constant over the whole range of d-spacings down to d ~ 0.3 Å. Whilst this is very effective for atomic structural studies, it is less adapted to the measurement of magnetic scattering since this intensity falls off rapidly with increasing $\sin\theta/\lambda$ due to the magnetic form factor. The low order reflections of interest occur at low $\sin\theta/\lambda$ and are weak due to the paucity of long λ neutrons from the 90 K moderators normally used. We now report measurements in which the incident beam came from a 25 K liquid H_2 moderator. The enhanced long λ flux gives powder patterns having good intensity, excellent