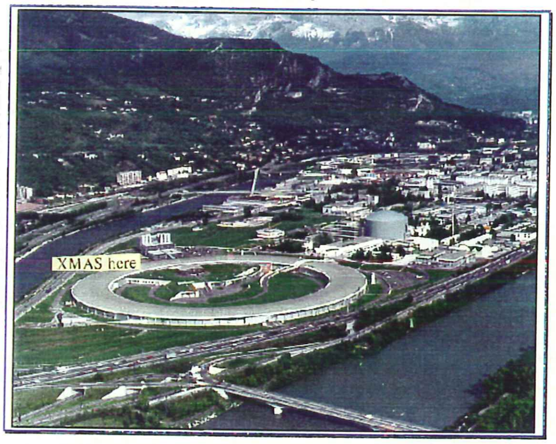
XMaS newsletter

September 1995

X-ray Magnetic Scattering

The UK's Collaborative Research Group (CRG) project at ESRF .....

..............for magnetic and high resolution diffraction.



This newsletter is the first of what we hope will be a short series describing progress on the planning and construction of the beamline and station. It should be a limited series given that we expect to have user beam in the autumn of 1997, but that is time enough to keep you informed, to solicit your opinions on the options that we have before us at various stages and to generate your enthusiasm for using the beamline.

First things first, we've got an acronym - XMaS - and the obvious slogan "XMaS is coming", both thanks to the fertile imagination of Bruce Forsyth. After arguing over that, building the beamline should be a piece of cake.
The story so far (in a nutshell) is that after inumerable iterations of the basic application over four years by Bill Stirling and Malcolm Cooper, we convinced SERC/EPSRC that their money (£M2.3 of it) would be safe in our hands and that magnetic and high resolution x-ray diffraction would be an enduring hot topic. The design study phase finished in September of last year with a simplified, more conventional design for the optics than the one on which we originally based our application. The pros and cons of being adventurous and being conservative are described in the paper entitled "Design of an x-ray beamline..." by D. F. Paul, M. J. Cooper and W. G. Stirling which appeared in Rev Sci Instrum **66** p1741 1995.

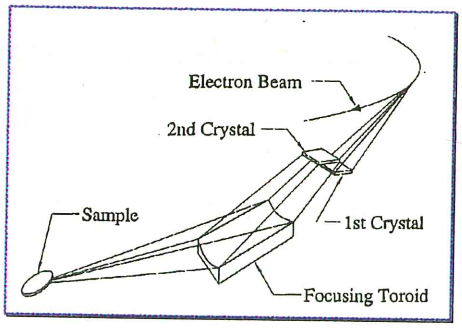


Fig. 1

The simplified design that we adopted is shown schematically in figure 1. Basically it consists of two elements, a non-focusing two bounce monochromator followed by a toroidal mirror. With a slope error of 1 arcsec on the mirror the focal spot will have dimensions 0.17mm x 0.24mm (height x width - sigma values).

The first monochromator crystal absorbs the heat load (about 200W if the ESRF is operating at 200mA and we accept 3mrad onto the monochromator) and is water cooled. The second crystal is independent and the relative orientation of the two can be 'tweaked'. The mirror, which is made from a silicon single crystal is ground to a cylindrical radius of 116mm and bent to a radius of 5.7km to form a toroid which will give 1:1 focusing at the diffraction station some 25m further down the beamline.

We also took a decision to use the "soft" end of the dipole magnet. This was based upon the desire to ensure that, despite the beryllium windows in the beamline, we have the maximum flux available at the low energies (3.5-5keV) associated with the actinide M-edges where much of our in resonant exchange scattering interest lies and will remain (resonant exchange scattering is the phenomena that enhances the magnetic signals by many orders of magnitude and converts the immeasurably small into the significantly large). Incidentally "our" beamline -D28- is quite close to the bridge across from the ESRF central building and will be conveniently close to the office/laboratory space to be built for the new CRGs. Everything has to have an acronym of course; those spaces were called PLUOs by ESRF for reasons that escape me. They are now to be called SLOMs (small laboratory and office modules); fortunately the British managed to resist a move to call them small laboratory and office buildings!

The work that has been done since last September has been to translate that outline design into specifications that allow us to place orders. For example what are the exact dimensions of the two hutches (one for the optics and the other for the diffractometer) and where exactly do they sit? In outline the beamline is as in figure 2

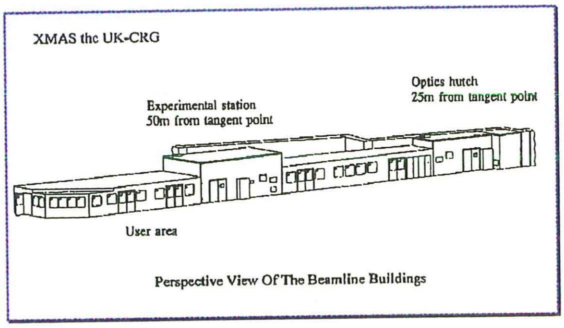


Fig. 2

The team assembled so far is as follows:

Malcolm Cooper - - who is based at Warwick, his job is
(a) to write newsletters;
(b) to worry about the budget, especially when the pound sinks without trace compared to the currencies of other European countries from which we are intending to purchase goods and (c) to coordinate and manage the efforts of the following unfortunates:

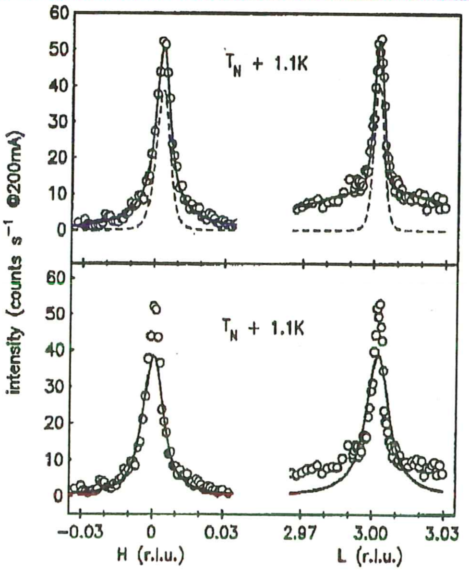
Bill Stirling - - whose job is to ensure that we do not forget the scientific requirements that govern the specification of the equipment and to worry about Malcolm worrying about the budget. Bill is the person in this motley group who is leading magnetic x-ray diffraction experiments at ESRF, NSLS and HASYLAB; he has built up an x-ray Laboratory for high resolution diffraction at Keele University, from December onwards Bill will be based in the Physics Department at Liverpool University.

David Paul - - who is our Project engineer. Thankfully he is a real engineer and understands all those things about which scientists display a charming naivety. He carried out the design study for the beamline (see the Rev Sci Instrum. paper referenced above) and then set about translating this concept into a detailed design compatible with (a) ESRF regulations, (b) manufacturers' capabilities and (c) the budget limits - in other words doing the impossible! In this task he is aided by the following persons.

David Laundy - - who is our beamline scientist. Many SRS users will know David in his previous incarnation as a Daresbury Laboratory staff scientist where he became an expert on beam polarisation and was involved in the first white beam magnetic diffraction experiments on ferromagnets. Not a lot of people know that previously he worked with Malcolm Cooper at Warwick as a Compton scatterer and was involved in the first magnetic Compton scattering experiments that the Warwick group performed at the SRS. Having seen sense and turned to diffraction he is now our expert on matters to do with the beamline.

Simon Brown - - who is our instrument scientist/engineer, having designed and built a number of magnetic and optical instruments. His main job is to worry about the hardware inside the experimental hutch. In particular he has been evaluating the diffractometer options that we have and deciding how to turn what is commercially available into what is scientifically desirable.

The corresponding critical exponents and the anisotropies of these two components are currently being extracted from the data. Particular care is being taken to allow for instrumental resolution effects in a reliable and robust manner. **See Figure 3** (to be submitted to Phys. Rev. B).



Two-component lineshape of the (0,0,3) magnetic peak in USb; the bottom panel shows the best fit obtainable with a single component scattering function (convoluted with the instrumental resolution), the top panel shows a similar fit with a two-component scattering function (the dashed lines demonstrate the separate components of the fit).

Fig. 3

Nd, X22C, NSLS
(Watson, Forgan, Nuttall, Stirling)

High resolution XRES studies of the AF ordering of the light rare-earth metal neodymium have been made at the L_{II} and L_{III} absorption edges. A single domain of the double-magnetic structure has been observed directly for the first time (in zero field). Precise measurements of the temperature-dependence of the modulation wavevector showed no sign of lock-in behaviour, inferred from neutron measurements. These experiments demonstrate the power of this technique in revealing detail not possible with neutron diffraction. (Submitted to Phys. Rev. B).

Tb, W1, HASYLAB (Perry, Costa, Bruckel, Mannix, Stirling)

The L_{II} and L_{III} resonances in terbium have been studied with analysis of the scattered polarisation as part of a systematic study of rare-earth antiferromagnets. Whereas there is a clear "double" peak in energy in the total scattering at the L_{II} edge (at the (0,0,2+q) satellite), this is not apparent in the sigma -> pi polarisation. In addition precise determinations of the variation with temperature of the modulation wavevector and satellite width have been made. A decrease in the magnitude of q has been observed at the lowest temperature in the narrow antiferromagnetic phase. Higher-order satellites have been observed at 2q and 3q. (Paper in preparation).

GdSe, 9.4, Daresbury
(Costa, Almeida, Nuttal, Cooper, Forsyth, Tang, Stirling)

The rock-salt structure compound GdSe has been investigated using resonantly-enhanced magnetic x-ray scattering. Relatively little is known about the magnetic structure of this material due to the large thermal neutron absorption cross-section of gadolinium. The 9.4 diffractometer at the Daresbury SRS has been used to examine magnetic satellites with modulation wavevector (½, ½, ½) at the L_{II} and L_{III} absorption edges of Gd. Evidence has been found for a magnetic phase transition at about 40K. (To be submitted to J. Phys. C: Condens. Matter).

UO_2, 8.4, Daresbury
(Collins, Laundy, Tang and Cernik)

The first successful measurement of a magnetic x-ray peak from a powder have been made. The measurement was made at the L_4 resonance of uranium in a powder sample of UO_2. As expected, the peak was only present below the Neel temperature and showed resonant behaviour. Published as "magnetic x-ray powder diffraction from antiferromagnetic UO_2", Collins et al, J. Phys. Condens. Matter, 7, 16, L223 (1995).

Bruce Forsyth - - who is our expert on diffractometer hardware and acquisition/control. Bruce remains on the staff of CLRC (the Rutherford Appleton Lab and Daresbury to you and me) and brings a wealth of experience from magnetic neutron diffraction and an ability to invent better acronyms than anyone else!

Michael Hart - - who up to now has helped us with understanding the critical requirements of the x-ray optics and synchrotron radiation projects in general. He has just disappeared across the pond to become chairman of the Brookhaven Light Source for five years.

In addition we have two further posts that we will be looking to fill shortly. One is for an engineer/scientist to reinforce the effort of David/David and Simon as we move over to a Grenoble base within the next 9 months and the other for a technician to help with the installation at ESRF. If you have names to suggest please contact Malcolm Cooper.

The plan of campaign is roughly as follows: Simon moves over to Grenoble at the end of this year when the hutches should be delivered. This is the signal for on-site activity (at least we shall have somewhere safe to store things). Simon will be followed a few months later by David Laundy. Everyone will be based in Grenoble for the final 12 months (October '96 to September '97). We are in the process of placing orders for the hutches, which involves detailed approval of various ESRF bodies and would be impossible without the help of Ian Kilvington who is the ESRF's Liaison Engineer for the CRGs. We shall shortly place the order for the monochromator goniometer, where the prime considerations are the accuracy of the angular setting (sub arcsecond for accuracy and reproducibility) and of course the price. We shall produce our own crystal cage and contract the cutting of the monochromator crystals. The mirror and the bending mechanism will be ordered from Zeiss in the near future. We are close to deciding which diffractometer will suit best the requirements for vertical and horizontal diffraction, polarisation analysis and high resolution. Therefore all the major decisions on equipment should be settled within the next few months.

Members of the CRG team have continued their programmes of x-ray scattering with experiments in a number of areas and just to prove that we have continued to push back the frontiers of science here are a few notes on our scientific highlights!

UAs, ID10, ESRF
(Langridge, Lander, Nuttall, Stirling, Bernhoeft, Stunault, Vettier, Grubel, Sutter)

Polarisation analysis studies of the non-resonant X-ray magnetic scattering from antiferromagnetic (AF) uranium arsenide have been performed at the TROIKA beamline, ESRF. A number of commensurate magnetic reflections were examined in pi -> pi and pi -> sigma geometries to assess the separate spin (S) and orbit (L) contributions to the cross-section. The intensities observed are qualitatively consistent with the predictions of standard theory; a detailed analysis is being pursued. This experiment further extends the application of polarisation analysis to off-resonant 5-f magnetism. (Paper in preparation).

USb, X22C, NSLS
(Perry, Nuttall, Lander, Stirling)

Complex "two-component" lineshapes in x-ray critical scattering measurements have recently become the subject of intense interest and controversy. Either the conventional theory of phase transitions requires profound reassessment or the effects of changes in the surface-layer structure are more important than previously realised. USb is a much studied triple-q antiferromagnet which was among the earliest actinide compounds studied by X-ray magnetic diffraction. We have re-examined the critical magnetic paramagnetic-AF transition of USb at 210K. The lineshape observed is composed of 2 components; the broad component is of the same width as that measured using neutrons, while the sharp central component exhibits a very different temperature dependence.

US, 8.4 Daresbury
(Collins, Laundy, Tang and Van der Laan)

Magnetic x-rays dichroism has been measured in ferromagnetic US at the M_4 and M_5 edges of uranium. The dichroism has been modelled using an atomic calculation and, by making use of the optical theorem, the data have been compared with resonant magnetic x-ray diffraction data. To be submitted for publication as "magnetic circular dichroism at uranium M-edges in uranium monosulphide".

Magnetic Compton Scattering, AR Japan

Although this is a diffraction beamline Malcolm Cooper would not like you to get the impression that he has given up Compton Scattering (leopards never change their spots). At KEK Japan the Warwick group have studied $CeFe_2$ (to some purpose) and UFe_2 (let's do it again). In $CeFe_2$ we have shown that the Ce 4f spin moment is indeed smaller than that calculated by the Uppsala group in agreement with the deduction of our neutron scattering colleagues (Kennedy, Brown and Coles, J. Phys. Cond. Mat. 5, 5169, 1993). It cannot really be more than one quarter of the predicted value.

Meanwhile at headquarters (ESRF) we have made the first magnetic scattering study on the high energy beamline (ID 15) on cobalt. That work was at 117 keV which is about twice the energy of other magnetic Compton scattering studies and we are set to push upwards even before the superconducting wavelength shift becomes operational. The band theory model for hexagonal cobalt was shown to be lacking in several respects (submitted to J. Phys. Cond. Mat.).

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