ISIS

1987

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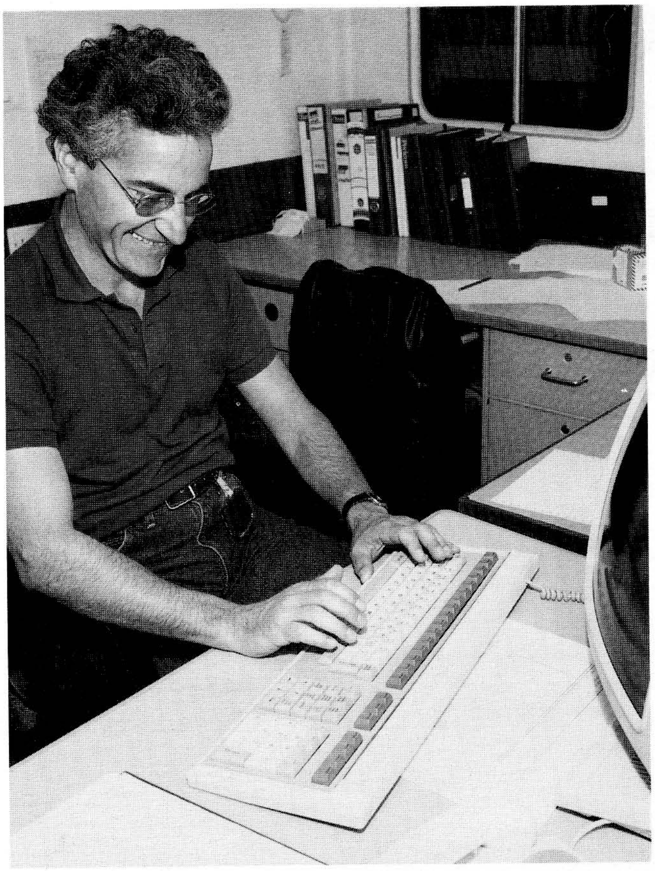
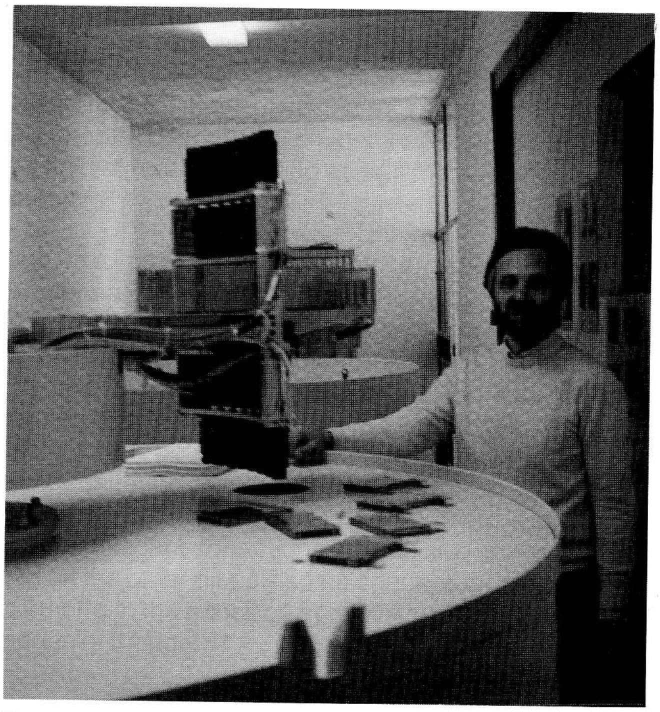


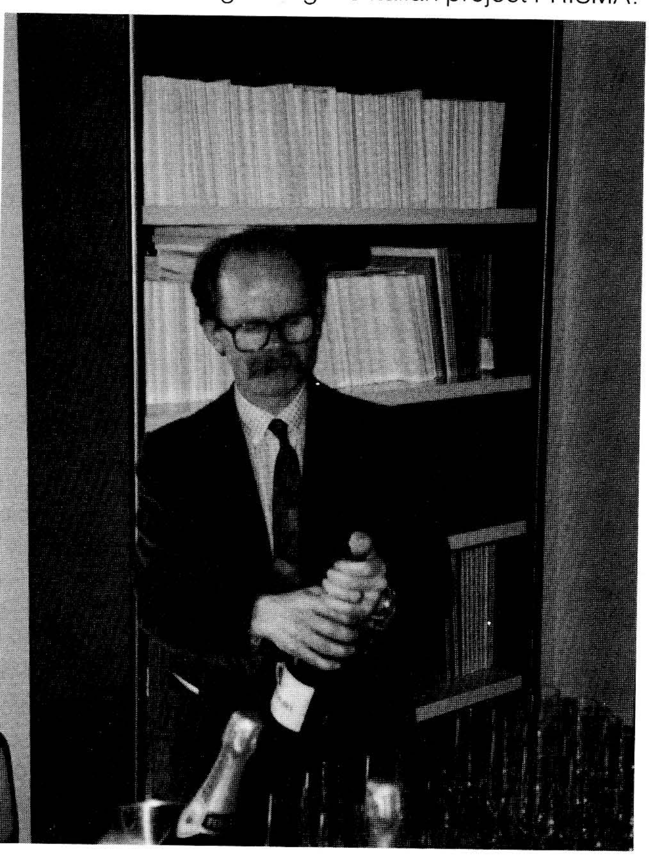
Fearless François (Dr F Fillaux from CNRS, Paris) laughs off the problems of data analysis on TFXA.

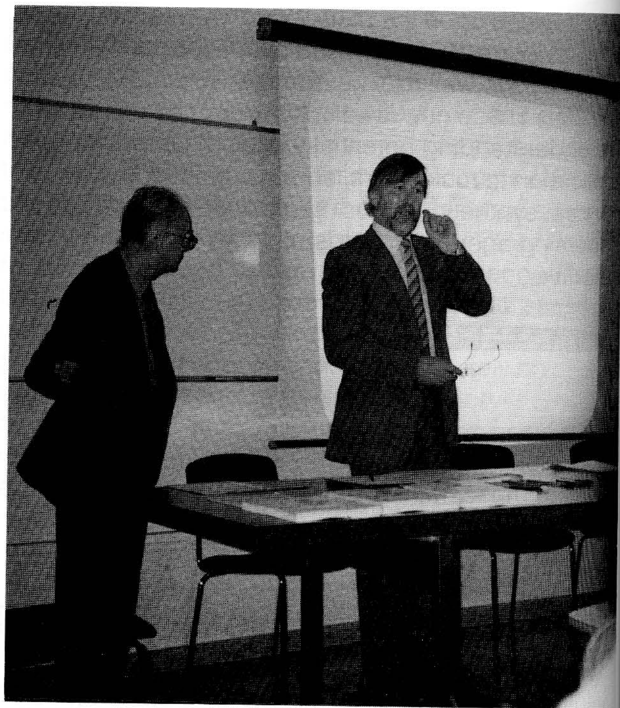
The TFXA team - Dennis Abbley, George Best, John Tomkinson, Bobby Moore, Scott Robertson, Pelé, Gordon Banks, Ulderico Wanderlingh and Jane Warren. Jane is the one wearing matching shorts and top.



Francesco Sacchetti next to the analyser arm of the Italian spectrometer PRISMA, before it was sent over to be installed at the Rutherford Appleton Laboratory.

Cesare Bucci inaugurating the Italian project PRISMA!





At a ceremony in Frascati, Alan Leadbetter thanked the Italian team for provision of the spectrometer PRISMA, and looked forward to a growing Italian participation in ISIS.

The components of the PRISMA spectrometer were delivered to RAL by lorry from Frascati. John Govans of the ISIS shift crew and Colin Carlile are giving advice whilst Denis Hilton drives the stacker truck. Instrument scientist Uschi Steigenberger is holding the camera!

POTASSIUM HYDROGEN CARBONATE: THE INTERACTION CONSTANT FOR THE OUT-OF-PLANE VIBRATIONS

Potassium hydrogen carbonate $KHCO_3$ forms cyclic dimers in the crystal phase. These dimers are held together by hydrogen bonds, as shown in the inset to Fig. 1. The inelastic neutron scattering (INS) spectrum of $KHCO_3$, at 5 K, was obtained on TFXA. This is shown in Fig. 1. The dimer has a centre of symmetry. Therefore the vibrational bands of the molecule can be excited either by infrared absorption (Au, Bu modes) or Raman scattering (Ag, Bg modes). In the INS technique optical selection rules do not apply and all vibrational modes can be excited. This can be seen in Fig. 1(a). The two bands are due to the symmetric deformations of the carbonates $\delta_s(CO_3)$. We observe the vibrations at 634 and 666 cm^{-1}, whilst optically they are observed at 639 (Raman) and 661 (IR) cm^{-1} respectively.

In the INS technique those vibrational modes which involve significant displacement of the hydrogen atom will have most intensity. (This is because of the very large scattering cross-section of neutrons from hydrogen atoms.) The geometry of the dimer is well known from crystallographic studies and the vibrations can be modelled. This can be achieved by the use of the CLIMAX program. This program provides values for the force constants that best reproduce the observed spectrum, both for band **positions** and **intensities**. Initially the true molecular geometry was approximated to an HCO_3 moiety. The curve shown in Fig. 1 is the best fitting curve produced by this approximation. It is seen that above about 1800 cm^{-1} the spectrum is providing detailed information on overtones and combinations. This ability has already proved useful in examining the harmonicity of molecular vibrations. Furthermore this spectrum demonstrates the unique ability of the INS technique to examine interaction constants directly.

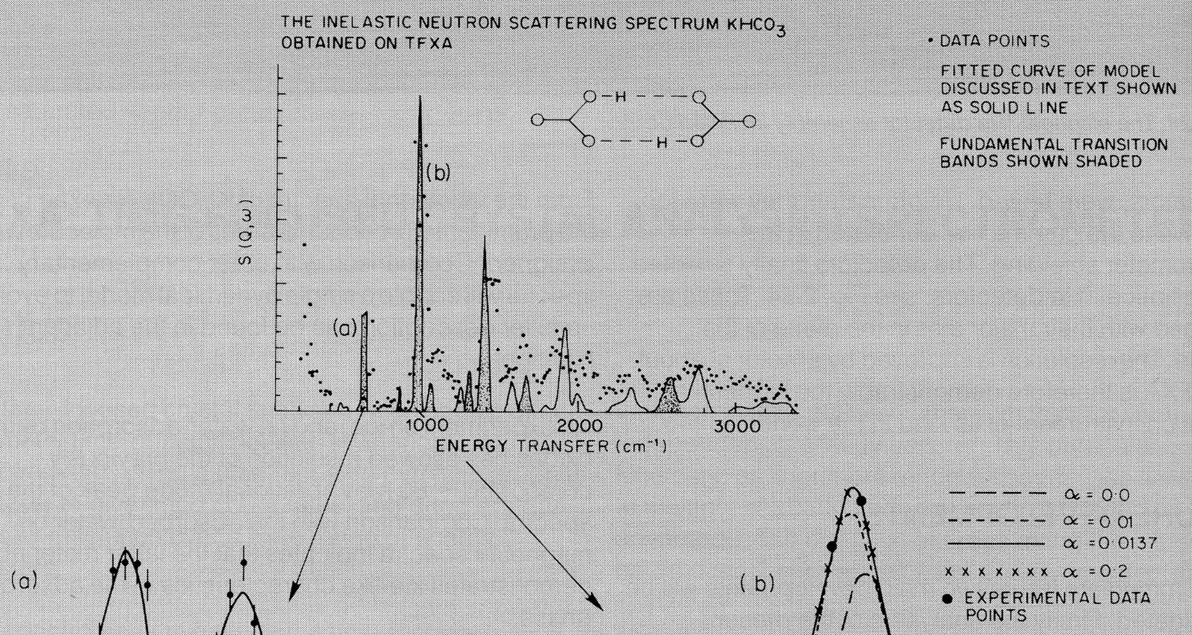
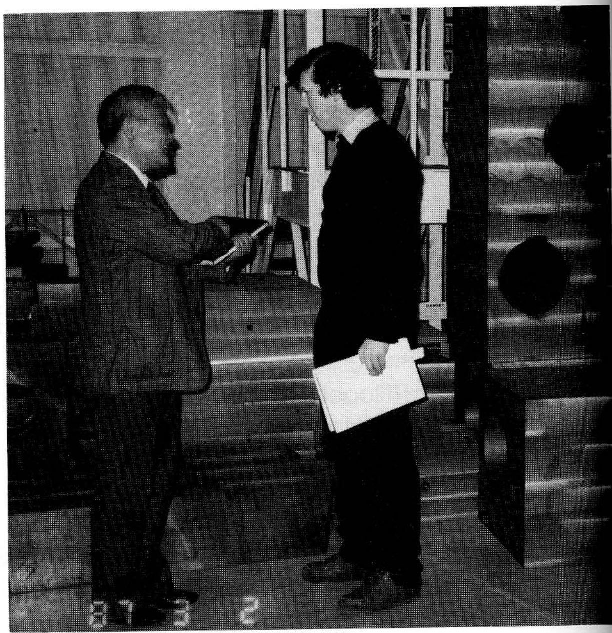


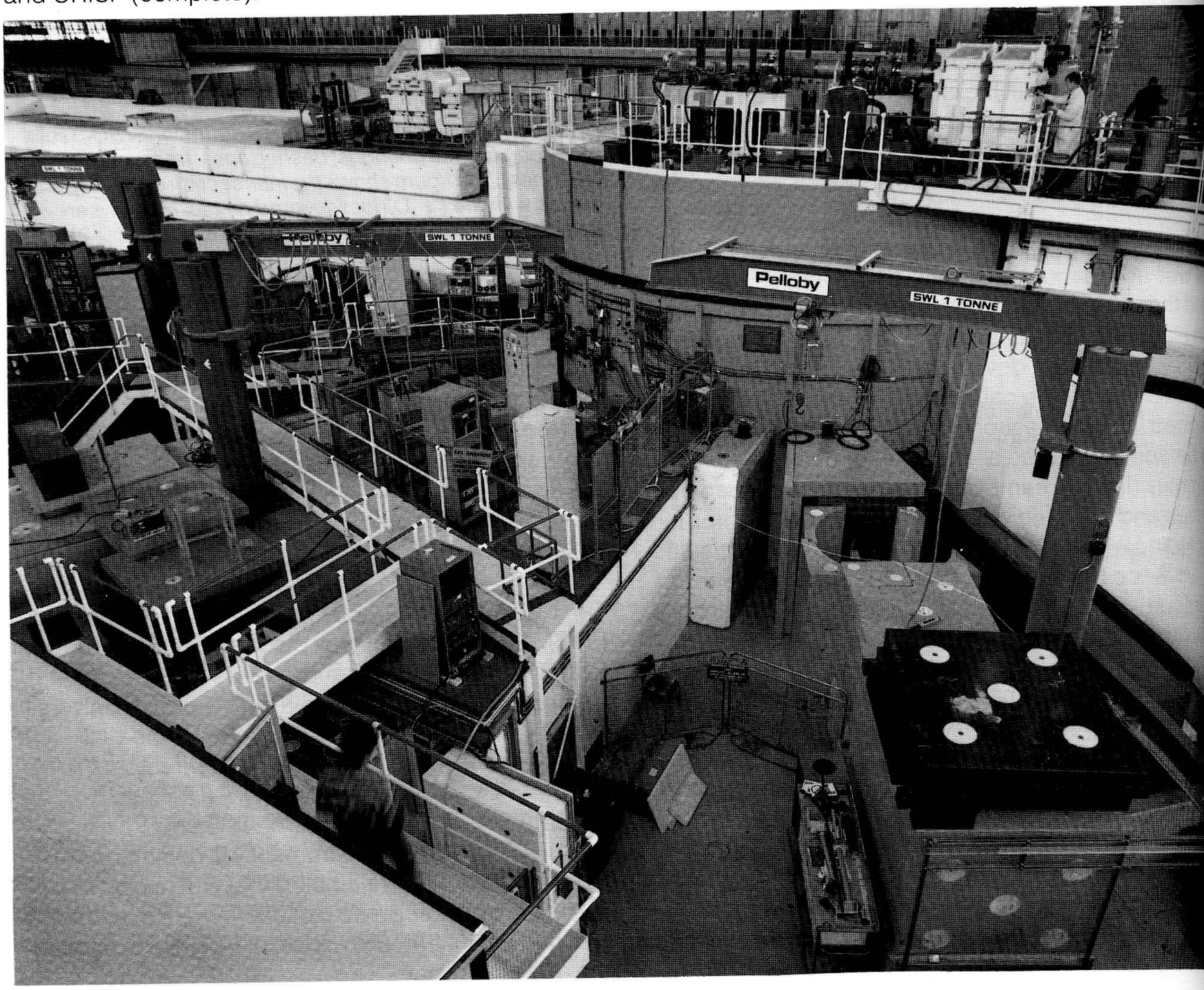
Fig. 1. The inelastic neutron scattering spectrum of $KHCO_3$ obtained on TXFA, at 5 K. The data points are shown with a fitted curve. The best fitted curve is shown as a full line and includes contributions from fundamentals which are shaded. The inset at the top right shows the molecular structure of the dimer. (a) Detail of the spectrum in the region of the δ_S(CO vibrations, showing the resolving power of the spectromet (see text). (b) Detail of the spectrum in the region of the out- plane vibrations. The variation of the best fitting curve, as th parameter α is changed, is demonstrated.

Richard Ward and Masa Arai admiring the MARI insert steel shielding.



Noboru Watanabe and Andrew Taylor discussing the MARI collimation.

View of the north west corner of the experimental hall, showing the SANDALS beamline (collimator only), PRISMA (shielding complete awaiting spectrometer) and CRISP (complete).



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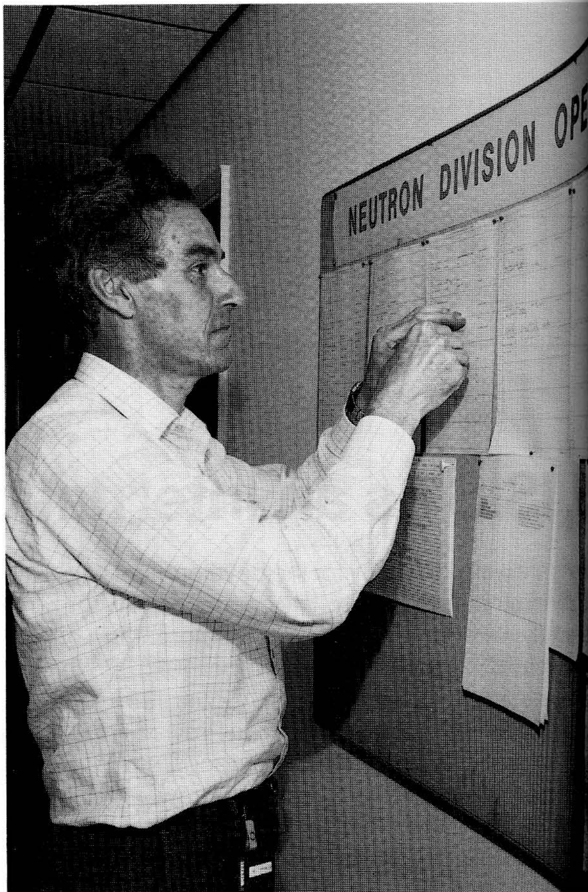
Ruth Taheri (left) and Pam Butler involved in work of the University Liaison Secretariat.



Brian Boland, in charge of Operations.

Participants at the Rapallo meeting on ISIS as an international facility, November 1986.

HIGH TEMPERATURE SUPERCONDUCTIVITY

Introduction

Observation of superconductivity at temperatures approaching twice the previous highest temperature at the end of 1986 has spawned a vast world-wide effort, both in searching for higher transition temperatures and in understanding the physics and chemistry of the original materials. So far the results of this effort have been to produce liquid nitrogen temperature superconductors, which should have large technological repercussions, and experimental results which cast great doubt on the role of traditional mechanisms of superconductivity in the new materials. ISIS has played a key role in this exploration in at least three ways. Firstly it has elucidated the crystal structures of the new materials; secondly it has provided the first density of states measurements for phonons in the materials; thirdly it has provided absolute measurements of the distance of penetration of a magnetic field into the superconductors in **two** different ways.

In terms of structure, ISIS has an unparalleled instrument in the high resolution powder diffractometer, HRPD, which yielded the first correct structural measurements of both the 40 K and 90 K superconductors. To see why the structural measurements are important, we need to note that the high temperature structures of the superconductors are highly anisotropic, both being layered materials. They consist of sandwiches of superconducting materials, in the form of copper-oxygen layers between insulating rare earth layers. One can view them as naturally occurring analogues of the artificial semiconducting heterostructures, which are revolutionising the microelectronics industry. The consequence of these structures on the materials' electrical properties is that their quasi two dimensional nature leads to infinite singular 'densities of states' from the electrons in the Cu-O layers - there are an infinite number of ways to place an extra electron in the materials.

The infinite density of states implies that they should be highly susceptible to structural and/or magnetic phase transitions as the temperature is lowered. In the La-Ba materials, HRPD found an orthorhombic-tetragonal transition at ~180 K which doubled the unit cell, as theoretical analyses predicted. However the nature of the distortion was not of the predicted 'breathing mode' symmetry, where the Cu-O squares along the (110) direction are alternately expanded and contracted. Moreover, the amplitude of the orthorhombic distortion behaved in an anomalous manner, by decreasing as the temperature decreased, in the region 35-70 K - i.e. near the superconducting transition temperature. There are a number of possible explanations of this - ranging from antiferromagnetic fluctuations coupling to the lattice (as the stoichiometric La_2CuO_4 is believed to be antiferromagnetic), to an effect of 'unbinding' of the Cooper pairs above T_c. The latter idea fits in with bipolaronic theories where the transition temperature of the superconductors is not determined by the binding energy of the Cooper pairs, but by their Bose condensation temperature. This is quite unlike conventional superconductivity, and is due to the possible very small size of the pairs in these materials.

A complementary tool is the HET spectrometer which measures the motion or vibration of the lattice. The importance of this is that near an instability (or phase transition) in the structure (e.g. the orthorhombic-tetragonal transition in La-Ba) the lattice can barely decide which structure to be in, so that if the lattice is distorted away from the equilibrium in the direction that it will distort in the other plane, the force which pushes the atoms back is very small. Thus the atoms vibrate very slowly - there is a 'soft mode'. The HET data are interesting in this context and they show an increase in the number of very 'slow' or low frequency modes near the temperature of the anomalous decrease of the amplitude of the orthorhombic distortion. This agrees with the notion that the material almost wants to go back to the tetragonal phase. Another interesting - and mysterious - feature is that there is a large difference at **high** energies (~100 meV) between the La-Ba and the parent compound, see Fig. 1.

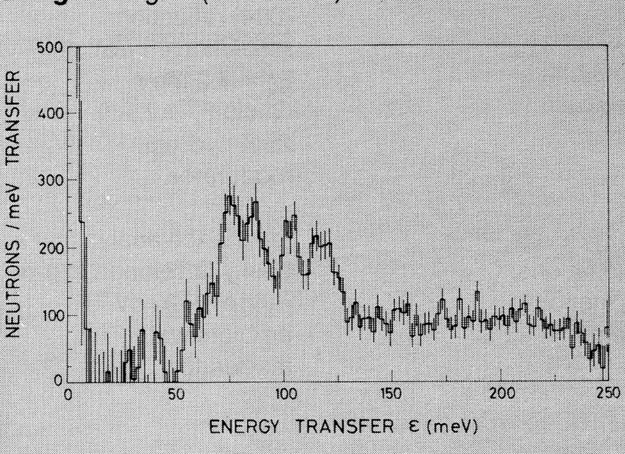


Fig. 1. The difference in high energy inelastic scattering intensity between the high temperature superconductor $La_{1.85}Ba_{0.15}CuO_4$ and its non-superconducting parent compound La_2CuO_4 at 12 K. These features may be associated with Cu-O breathing modes.

Fig. 6.1. Participants at the Course on Neutron Scattering at a Pulsed Source, September 1986, outside the ISIS experimental hall.

1 Dutch, 1 Indian); and 5 UK research assistants. Figure 6.1 shows the participants during a break from their work.

The principal aim was to present an overview of neutron scattering techniques to a very mixed audience. The theory lectures by Mike Gunn (RAL) were well received, drawing on insight and intuition rather than relying on mathematics. The initial aim to provide 'hands on' experience for the students turned out to be complicated but, with the cooperation of Neutron Division staff, 17 distinct activities were devised, mostly involving data reduction and fitting of stored spectra. Most students were able to tackle 4 or 5 separate practical exercises.

The course was generally regarded as a success. The feedback from questionnaires issued to students was positive, although there was a bias towards physics which in future should be corrected, with greater emphasis on chemistry; longer practical sessions would also be desirable.

Lecture notes are to be published by Adam Hilger, with Bob Newport as editor.

ICANS IX

The ninth meeting of the International Collaboration on Advanced Neutron Sources was held at SIN, Switzerland. About ten members of ISIS and Neutron Division staff attended and presented papers and posters, giving details of their work on accelerator design; target station design and upgrade; and neutron scattering instrumentation and science.

The proceedings are being published as a SIN report.

UK NEUTRON BEAM RESEARCH COMMUNITY MEETING

This user meeting was organised by SERC Central Office, and held at the Rutherford Appleton Laboratory. It was attended by 205 users and potential users of ISIS and ILL, coming from either UK universities and polytechnics - postgraduate and permanent staff - or industry, which was also well represented by, for example, ICI, Rolls Royce and British Rail Engineering. The disciplines represented ranged over physics, 5

5. ISIS as an International Facility

Plans are well underway for the development of ISIS as a fully international facility. The connections with France and Italy were forged through a Memorandum of Understanding agreed in December 1985, to which Sweden became a signatory in August 1986. This provided for the establishment of a Provisional Council to execute the terms of the Memorandum of Understanding, a Project Group to draw up technical plans for the future development of ISIS as an international facility, and a Science Advisory Committee to advise on matters concerning the scientific exploitation of the facility. At its meeting in December 1986, the Provisional Council considered legal documents for the establishment of a fully international ISIS Institute, together with proposed institutional arrangements under which the Institute would operate and relate to RAL. The Project Group has prepared a set of costed scenarios for future development of the facility, and these have been assessed by the Science Advisory Committee and presented to the Provisional Council.

WORK OF THE PROJECT GROUP

The Project Group first met at RAL in May 1986 and considered future options in accelerator design, target station development and neutron scattering instrumentation. This work continued throughout the Summer in collaboration with UK university groups and other European experts in the field and culminated in a week long workshop held in Rapallo, Italy, in November 1986, with about 60 members from half a dozen countries participating. A detailed report was prepared, presenting the various options for future development of the facility, and this was presented to the ISIS Provisional Council in December 1986.

Three scenarios were proposed, all of which started by ensuring maximum performance of the initial ISIS machine and its full exploitation with neutron and muon instrumentation (see Fig. 5.1) and all included the subsequent extension of the facility to two target stations. The simplest development is to add a second low repetition rate non-fissile target using one pulse in five from the current machine. Such a source would be particularly attractive for those instruments which suffer from frame overlap on the 50 Hz source. A second, technically more difficult, option is to enhance neutron production on this target by introducing fissile material. For this option a nuclear site licence would be required. The third major option would be to increase the proton current by a factor of eight to 1.6 mA taking 1.3 mA onto a new target station and modifying the first target to take 300 μA and 10 Hz. This would require building an 800 MeV linac and using the current synchrotron as a storage ring. It would be the most expensive option but holds out the prospects of a really major development of ISIS in the long term future.

The Science Advisory Committee and the Provisional Council have now considered the conclusions of this report, which will be incorporated in eventual submissions of proposals to Governments for the creation of an international ISIS Institute.

FOREWORD

Our second year of operations has again been one of intensive activity. Commissioning of the machine towards full design performance continued along with strenuous and successful efforts to improve the reliability of the injector system. The user-based neutron scattering programme has now acquired considerable momentum while at the same time new instruments are in design, construction or commissioning stages. Also, first muons were produced at ISIS in March, appropriately in the 50th anniversary year of the discovery of the muon.

Detailed preparations for the creation of an international ISIS Institute continued through the year culminating in agreements on legal and institutional arrangements and presentation of costed options for the future development of ISIS prepared by the International Project Group with participation by scientists from many countries. Further progress now awaits submissions to the governments of potential partners. The last year has also seen the start of real industrial involvement in ISIS with the signing of agreements with both BP and ICI, and the start of work on applications of resonance radiography in collaboration with Rolls Royce and Bristol University.

From April until August 1986, there was a shutdown during which vigorous efforts were made to identify and correct the faults leading to unreliability of the injector; the final two radio frequency cavities, required for 800 MeV running, were installed; three new beamlines were opened and the intermediate target station prepared ready for the installation of the muon target early in 1987. The period from September until the end of the year saw the injector performance much improved and, by November, proton currents of up to 25 μA at 550 MeV were routinely being delivered at the target. ISIS then had a wonderful start to its running programme in 1987, with currents greater than 50 μA being achieved. In March, a total of some 17,000 μA-hr of 550 MeV protons were transported to a fully working target station, and during the last four days of this user run the average current was 42 μA. This performance means that ISIS is already almost three times as powerful as any other pulsed neutron facility in the world. During the machine development period right at the end of the financial year, the muon target was installed and the muon beam commissioned. The accelerator was successfully run at 750 MeV and this gave the expected increase in neutron yield compared with 550 MeV of about 50% in the upstream moderators and a factor of two in the downstream moderators.

During the year a large number of user experiments were carried out over a wide range of science. A significant proportion (~ 15%) of these involved overseas scientists as ISIS was opened up to international participation as part of the lead up towards creation of an international Institute.

The experimental programme on the scheduled instruments HRPD, LAD, HET, TFXA and IRIS (where the higher resolution analyser system is now being commissioned) is proceeding very well, with the instruments performing well up to design expectation and producing many novel results. Especially notable has been work on the new ceramic high temperature superconducting materials where data of unique quality have been obtained on structure and vibrational properties. In addition, the ISIS 'instrument of the year' - the reflection spectrometer CRISP - was built and commissioned and is now producing results in a wide area of surface science, including surface magnetism, not obtainable anywhere else in the world. The small angle scattering instrument LOQ has been rebuilt to incorporate a LETI multiwire detector to improve the spectrometer performance. Initial commissioning results have been obtained and are most encouraging. Also, progress on the three first development instruments, for polarised neutrons (POLARIS), high energy transfers (eVS) and single crystal diffractometry (SXD), has been highly satisfactory, with SXD expected to become a fully scheduled instrument during the next year. In June 1987, the Italian instrument for measuring excitations in single crystals (PRISMA) was delivered to ISIS from Frascati where it was built. An Agreement was signed in December with Japan for provision of about one million pounds for a versatile multi-angle rotor spectrometer (MARI). Finally, the design and construction of SANDALS, the small angle diffractometer for liquids and amorphous materials, have proceeded steadily over the last year.

The year again finishes on a note of optimism despite continuing difficulties arising from a lack of resources. This positive outlook is due to the enormous hard work, dedication, skill and initiative of all the staff involved in the commissioning and operation of ISIS and its instruments. We look forward in the next year to the approach to full specification of the accelerator, a growth in the number of operating spectrometers, a continued scientific achievement of the highest quality and the creation of a fully international ISIS Institute.

Alan Leadbetter

A J LEADBETTER
July 1987

SSOCIATE DIRECTOR FOR SCIENCE BOARD - **A J Leadbetter**

he personnel of the two RAL Divisions principally concerned in the construction and operation of ISIS are listed elow for information. It should be noted, however, that major contributions in the construction of ISIS and its nstruments have also been made by the RAL Service Divisions.

NEUTRON DIVISION STAFF - March 31, 1987

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