THE MILLENNIUM PROGRAMME

PROPOSALS

FOR

ILL's

5-YEAR DEVELOPMENT PROGRAMME

ILL's Scientific Council – April 1999 – SC 99-1

ILL MILLENNIUM PROGRAMME

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ILL 5-YEAR DEVELOPMENT PROGRAMME

PREFACE

This document contains a collection of proposals on the future instrumentation at the Institute Max von Laue – Paul Langevin in Grenoble, and indicates new roads for pure and applied science that may open up in neutron research. The proposals (roughly three dozen, see table 1) were collected during the past few months both from within and from outside ILL. The document is intended to help the Scientific Council of ILL make recommendations to the Steering Committee on the subject of the next 5-Year Development Programme.

The various propositions range all the way from the evident to the exotic. It is evident that the numerous inventions done at ILL in recent years should be implemented on ILL machines on a larger scale (namely: CRYOPAD – 3D polarimetry, ^{3}He-polarisers and wide-angle analysers, « m = 4 »-multilayers, microstrip detectors, new crystal-optics devices, neutron image-plates, and others). In many cases the systematic implementation of these new devices will bring huge gains in efficiency, which in turn will make it possible to study problems which are not at all accessible with existing instruments.

Yet, the majority of proposals are new proposals in the sense that the instrument (or instrument option) proposed does not exist at ILL. Some of these new proposals are « exotic » in the sense that they are very intriguing, but their feasibility and their scientific weight still have to be proven. In any case there seems to be sufficient interesting material for a basic renewal of ILL's instrument park.

For about half of the proposals significant help from external laboratories has been offered, mostly in the form of equipment and manpower. In addition, there is a separate list of propositions (about one dozen, see table 2) for external help on ILL infrastructure and sample environment.

The proposals are arranged in order of the existing instrument groups at ILL. An instrument group on industrial applications and another group on general infrastructure have been added. The proposals have been widely discussed both in-house and within the Instrument Subcommittee, but have not been filtered yet (on the request of the Scientific Council).

The list of proposals presented here is not meant to be closed, and further proposals are welcome at any time. ILL Management proposes to first come to a decision on the proposals that can be realized in the years 2000 and 2001, see also the Technical Synthesis subsequent to the Summary.

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Table 1 : LIST OF PROPOSALS

Page N°		Proposed instrument	Position	Significant external input from	ILL-contact	Approx ILL costs MF	Priority
		1. Nuclear and Fundamental Physics					
21	New	« Miniball » rare-isotope spectrometer	PN1	U Munich/CEA/ISN Grenoble et al.	Faust et al.	5	
27	New	Cold neutron particle physics facility : efficiency x 10	H113	U Heidelberg/TU Munich	Nesvizhevski	2	
31	New	Ultra cold neutron source for neutron EDM : efficiency x 100	H53	Rutherford/U Sussex KEK/TU Munich	Butterworth		
		2. Diffraction					
35	New	Thermal LADI (image plate)	H22 ?		Wilkinson	3	
41		D2B (high resolution) : efficiency x 10			Suard, Hewat	4.3 + 2	
47		D19 (4-circle) : efficiency x 25			Forsyth, Mason	3.9	
53		D3 (hot neutrons) : 3D-polarimetry			Lelièvre, Tasset	3.3 + 1.5	
		3. Large Scale Structures					
59		Cold LADI : efficiency x 5	IH1 ?	EMBL	Myles et al.	1.5	
63		New SANS detectors : efficiency x 100	D11, D22		Lindner, May, Guérard	0.8+3.9+3.0	
67	New	Radical sites in biological macromolecules	D22	IBS Grenoble/ U Mainz/ U Heidelberg	Zimmer	0.4	
73	New	Microsecond SANS - TISANE	D11	TU Munich	Lindner, Gähler	1.5 + 5.3	
85		Ultra SANS	S18	U Vienna	Timmins		

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Page N°		Proposed instrument	Position	Significant external input from	ILL-contact	Approx ILL costs MF	Priority
		4. **Three-Axis Spectrometers**					
89		IN20 (polarised) : efficiency x 10			Kulda	1.9	
95	New	Multianalysers and PSD in TAS			Hiess	0.4 + 0.5	
101	New	Flat cone excitation mapping in TAS			Kulda et al.	3.1	
107	New	Spin-echo in TAS	IN3	TU Munich/HMI Berlin	Currat, Zeyen	0.5 to 1	
111		IN1 (hot neutrons) : polarisation option			Wildes, Ivanov		
113		IN1 (Be-Filter) : efficiency x 8			Ivanov	4.3	
		5. **Time of Flight and High Resolution**					
119	New	IN5 (TOF) : excitation mapping		U Bristol/ U Warwick	Schober, Kulda	9.7	
125		D7 (diffuse scattering) : efficiency x 30 …60			Stewart, Andersen	2 or 1	
131	New	PASTIS : large solid angle thermal polarisation analyser	H23 ?	U Mainz	Stewart	20	
137		IN15 (spin-echo) : higher efficiency and stability		FZ Jülich/HMI Berlin	Ehlers, Farago	1.7	
141		IN16 (backscattering) : efficiency x 10 … 32			Frick et al.	5.2 or 2.5	
147	New	Double precession spectrometer		TU Delft	Farago		
		6. **Industrial Applications and Engineering Science**					
151	New	Strain and stress in materials	D1A	U Manchester et al.	Leadbetter	3.5	
157	New	Purity control of materials	H24		Doll	1.5	
161	New	3D-imaging of technical objects	H9	(TU Munich)/U Heidelberg	Doll	1.2	
165	New	Imaging of hidden layers	H21	U Heidelberg	Dubbers	0.6	
169	New	Nuclear waste incineration tests (mini-Inca project)	Niveau D	CEA	Leconte, Faust		

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Page N°		Proposed infrastructure	Position	Significant external input from	ILL-contact	Approx ILL costs MF	Priority
		7. <u>Infrastructure</u>					
177		Cold super-mirror guide	H53		Wildes, Curat	1.5	
183		Thermal super-mirror guide	H24		Kaiser	5.8	
185		Hot source replacement			Bauer	5	
187		Superconducting magnet		CEA	Hiess	1	
189		Monte Carlo simulation of instruments		Risø	Anderson	2	
		8. <u>Reports on existing programme</u>					
191		Polarised ^{3}He project		U Mainz/CEA/EU	Leadbetter, Tasset		
195		Comparison of polarisation techniques			Tasset, Anderson		

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Table 2 : FURTHER EXTERNAL PROPOSITIONS ON INFRASTRUCTURE DEVELOPMENT

Diffractometer equipment and software	U Berkeley	USA
Single crystal TOF, Simulation and other software	HMI Berlin	D
Time-resolved SANS : sample environment	U Bristol School of Chemistry	UK
High pressure at 50 mK	U Cambridge, Chem. Phys.	UK
Emulsion studies development	U Canberra	Australia
Uniaxial stress at 50 mK, CRYOPAD, ^{3}He filter, detectors, etc	CEA Grenoble	F
Neutron imaging of polycrystalline material	DESY Hamburg	D
Reflectometry : development	U Leicester, Dept of Chemistry	UK
Scientific collaboration in TAS, TOF, ^{3}He filter, detectors	TU Munich	D
Strain scanning : neutron optics, software	U Newcastle, Dept. of Engineering	UK
Instrument simulation programmes	Risø	DK
Neutron optics, polariser and detector development	LLB Saclay	F
SANS : equipment development	ETH Zurich Applied Physics	CH

DD/bm 15/3/99

ILL 5-YEAR DEVELOPMENT

SUMMARY

The scientific work done at ILL is broadband in the sense that it covers many different and unrelated fields of science. Therefore, in the following summary the scientific justification will be developed case by case, covering particle physics, materials and life sciences all the way through industrial applications and engineering sciences. There exist interesting links between these different neutron applications which, however, are mainly methodological, and will not be discussed in the present context.

1. Nuclear and Particle Physics Instrument Group

Nuclear Physics at ILL is done on the two scheduled instruments PN1 and PN3. There exists a rich experimental programme which covers not only problems of nuclear physics, but also aspects of atomic, solid state, particle and astrophysics, as well as high precision metrology.

In the past, the main purpose of the fission product instrument PN1 (LOHENGRIN) has been the investigation of the nuclear *fission process*. The future of PN1 was intensely discussed among the respective subcommittee of the Scientific Council and ILL Management, and the following recommendations were given. In the future, the study of the fission process itself should have a low priority. Instead, high priority should be given to the study of the properties of the *fission products* because in this field exciting opportunities have opened up. The European Miniball Consortium has offered to install its high solid-angle gamma-ray spectrometer in regular intervals at ILL. In complement, it is proposed that PN1 buys for its own use a smaller number of gamma detectors compatible with Miniball. This very efficient instrument will then allow to routinely study the properties of isotopes which have typically 12 neutrons added to the last stable isotope of an element.

With this installation new scientific insight is expected on several topics : firstly, on the properties of nuclear matter near the « drip-line » where no further neutrons can be bound, and on which very little is known to this date ; secondly, on the mechanism of the « rapid » element-creation process which is believed to take place near this drip-line in the course of supernova explosions, and which is part of the huge element recycling process of our universe, but on which decisive data are still missing ; finally, on the practical problem of nuclear waste incineration. On this latter question various ILL user groups have lately done very useful work on PN1 and intend to continue this. A further proposal on waste incineration studies is found under the heading « Industrial Applications », at the end of table 1 in the list of proposals.

In recent years it has emerged that **Particle Physics** has many questions in common with **Cosmology**. The same is true for the particle physics programme run at ILL on the cold-neutron station PF1 and the ultra-cold-neutron (UCN) station PF2. In contradistinction to the experiments performed at accelerators, experiments at ILL are done at very low energies, but with extremely high precision (neutron energy : ΔE down to 10^{-22} eV, neutron momentum : $\Delta p/p$ down to 10^{-11}). About three dozen observables are accessible in neutron-particle physics, which address about two dozen basic questions related to particle physics and cosmology.

One on-going programme in particle physics is on free-neutron decay. As of today, all weak-interaction cross-sections involving nucleons must be calculated from measured neutron-decay data. In past years, these data have helped to provide a sound data base for big-bang calculations on primordial element production. They further have, in conjunction with arguments from cosmogenesis, allowed to fix the total number of particle families to three, in accordance with (and prior to) laboratory results from particle physics. Also solar-model calculations depend sensitively on neutron-decay data.

In the future, neutron-decay investigations will concentrate on high-precision tests of the Standard Model of Particle Physics. Here the open questions where neutron experiments do contribute are of the type : Was the manifest left-handedness of electroweak interaction built-in from the beginning, or is it an « emergent property » due to a phase-transition of the early universe's vacuum ? In electroweak quark-mixing, does every quark give as much as it receives? And so on.

To pursue neutron experiments on these and other questions a new type of supermirror cold-neutron beamline has been constructed and is at present being set up at ILL by two German universities. PF1 will move to this beamline after its completion. For the present development programme it is proposed that a rather avant-gardist supermirror neutron focusser be developed to be installed on this new beamline in order to obtain the highest possible flux density for the particle physics programme discussed above.

Another long-term programme at ILL tries to shed light on the unsolved question of why, after the big bang, so much more matter has survived than antimatter (the so-called baryon-asymmetry of the universe). The only known solution to this problem requires some Grand-Unification scheme beyond the present standard model, and, linked to this, the existence of an electric dipole moment (EDM) of the neutron.

Over the years, the experimental limit achieved on the neutron EDM has been reduced by eight orders of magnitude. This has already eliminated a good number of otherwise viable theories which predicted an EDM larger than this limit. The bulk of the remaining grand-unified theories to be killed or supported by this experiment lie only one or two orders of magnitude ahead of the present EDM limit. The next order of magnitude will be surpassed with a new UCN source to be developed by a British-Japanese-German consortium. (The conditions of the Japanese participation will have to be discussed separately by the Steering Committee).

2. Diffractometry Instrument Group

In most of natural science – in condensed matter physics and chemistry as well as in molecular biology – the main (though not only) approach is to try to understand matter on the basis of its molecular constituants. The first thing one needs to know about any new material or substance is its **Molecular Structure**. This is the domain of diffractometry and crystallography, which at ILL is done on seven scheduled instruments.

Like most fields of science diffraction started out with the study of simple systems. But most systems around us, be they natural or man-made, are far from simple. In recent years science has made great progress both in the experimental investigation of complex structures, and in the modelling and theoretical description thereof. Diffraction measurements nowadays are done on such complex problems as : the nanostructure of ceramic composites ; the filtering action of molecular sieves ; the orientation of particles during flow ; the study of colossal magneto-resistance; the fracture of animal bones, to name just a few recent examples from ILL.

In diffraction detailed maps of such structures are established as a function of external parameters like temperature, pressure, magnetic and electric fields, light irradiation, composition etc. Further, the phase transitions between different structures and their often universal features can be investigated in real time. Besides the molecular structure (defined by the position of the atomic nuclei), neutron diffraction also gives information on the **Magnetic Structure** of materials (carried by unpaired electrons). Many different types of more or less exotic magnetic structures are under investigation, many of them of actual or potential practical importance. – In short, diffraction is an immensely wide field, as rich as nature itself.

However, the more complex the system under study is, the more information one needs to extract from it in order to find a satisfactory description of the system. In neutron scattering one therefore should explore as large domains of reciprocal space as possible within one measurement, and this at as high a neutron countrate as possible. This is the strategy followed in the next three proposals.

The proposed « thermal » version of ILL's recently developed image-plate instrument LADI will cover almost full reciprocal space and will be ideal for rapid structural studies even on small single crystals. Similarly, the powder-diffractometer D2B will considerably gain by the installation of focussing monochromators and large linear position-sensitive detectors. This will enable researchers to study, for instance, the detailed progression of chemical reactions and precipitations in real time. The third instrument, D19, is mainly used to investigate disordered or weakly contrasting macromolecular structures. Its efficiency can be greatly enhanced by just adding a larger number of position-sensitive detectors to the one presently used.

The polarised hot-neutron instrument D3 is by far the world's most powerful machine for the study of magnetic structures in single crystals. Here, the installation of ILL's ^{3}He polarisers and of CRYOPAD will make it possible to investigate also very exotic magnetic structures. In *polarised* neutron work with CRYOPAD one can measure sixteen different scattering functions $S(\mathbf{q},\omega)$, instead of only one such function in *unpolarised* neutron work. At the same time, the countrate should be increased by a focusing monochromator. So the gain in information on the system under study will be considerable.

Neutron diffractometers at ILL are in high demand. Neither the advent of spallation pulsed-neutrons sources nor that of synchrotron sources have relieved the pressure on ILL instruments. To each problem there seems to exist a favorite method, and a great many problems need the information provided by all available methods. Certainly, the general situation needs continuous monitoring. Still it may be best to let people vote with their feet, as long as the quality of their work has a high standard.

3. Large-Scale Structure Instrument Group

The Large-Scale Structure group has six scheduled instruments (some of which run alternating on a half-time basis). Part of the studies of this group deals with the **Life Sciences.** Also here photon scattering and neutron scattering give different types of information. For instance, with synchrotron radiation one can obtain the detailed atomic structure of biomolecules, as long as these can be crystallized with a unique conformation. When this is not the case, then low-resolution neutron scattering enables to derive the overall shape and disposition of the constituent subunits of the biomolecules. Also, in hydrogen-bonding, the positions of labile protons, of importance for the function of many biomolecules, are determined preferentially with neutron scattering. Finally, most biological tissues have a high water content. The distribution of water molecules within biological structures is another important field of neutron applications in the life sciences. For more topics regarding the life sciences see Section 5 « High Resolution ».

The use of neutrons in the life sciences is somewhat hampered by their relatively low flux. But in many cases this disadvantage is compensated by the following neutron-specific advantages : contrast variation (by selective isotope substitution) is a powerful tool in neutron scattering from biomolecules; further, neutrons are important for the study of biological systems which, in solution are too fragile to support the high radiation damage induced by synchrotron radiation. We conclude that neutrons are indispensible in many studies in the life sciences, although ILL's total activity in this field (roughly 100 experiments per year) is lower than at ESRF (roughly 200 experiments per year).

Also some studies in the field of **Soft Matter** are closely linked to the life sciences, like the investigation of structure formation in multi-molecular aggregates. Thus, the structural transitions between micelles, vesicles, and other structures involving membranes and double layers can be investigated in neutron small-angle scattering in all detail. Other studies of the Large-Scale Structure group are more linked to the field of **Material Sciences**, like the studies of polymers, emulsions, precipitates and various nanomaterials.

In the life science sector there are several interesting proposals on new instrumentation. One proposal is evident : find more neutrons for cold LADI, the long-wavelength, high solid-angle image-plate machine on which important biological studies are being done. Another proposal is to equip at least one of ILL's small angle machines with high-countrate detectors, in order to make full use of the sometimes very high flux of scattered neutrons. SANS machines are of high interest both for the chemistry and the biology communities.

There are two new and « exotic » proposals in the field of the life sciences. Both could be realised on existing small-angle scattering machines. The first proposal is on the spatial localisation of paramagnetic electrons, which sometimes play a vital rôle in the functioning of bio-molecules. It is intended to surround each unsaturated electron in the probe with a cloud of polarised protons. That this is feasible has been proven in a recent NMR experiment at ILL. Small angle neutron scattering then can give information on the location of these polarisation clouds, and with it on the localisation of the paramagnetic centers in the molecule.

The other proposal is on externally triggered processes, like photo-induced processes in bio-molecules. If these processes are reversible, then, with the new scheme proposed, one can follow them via small angle neutron scattering at time scales down to 10 μsec. This is achieved by using a beam chopping sequence which is correlated in time to the triggering sequence of the probe. This method could close the gap between the time-scales accessible in neutron spin-echo (< 1 μs) and real-time diffractometry (> 1 μs).

Finally, with the proposed method of UltraSANS one can study the internal structure and size distribution of nanomaterials. Experience with such installations already exists elsewhere.

4. Three-Axis Spectrometer Instrument Group

When the structure of a new material, substance or composite system has been resolved, then the next difficult problem is to understand the movements of its atomic or molecular constituents. This also is a very rich field, full of surprises, which covers the vibrational, rotational, diffusional or tunnelling aspects of collective or single-particle quantum dynamics.

The 3.5 scheduled instruments of the Three-Axis group are used for single-crystal studies of atomic dynamics. Studies are both on structural excitations of the crystal lattice, and on magnetic excitations of the electronic spins.

The study of **Structural Excitations** gives valuable information on the form of the interatomic potential. Also, the coupling of conduction electrons to the crystal lattice (in particular in low and high-temperature superconductors) is of high current interest. Further, the dynamics of phase transitions between various aggregate states have been studied, and in many cases very subtle universality relations have been verified experimentally and compared to the predictions of renormalization theory.

In recent years the study of **Magnetic Excitations** in condensed matter has created much excitement. In particular in systems of low dimension (that is when the interactions are limited in space to lines or to planes) very strange phenomena occur. Seemingly very simple systems, like a collection of electrons arranged on a line, may show the most complex and exotic behaviour which often is not at all understood. For instance, although electrons are point-like particles, in low-dimensional systems their electric charge and their magnetism may be found on widely separated locations in space.

Such magnetic systems are best studied by polarised-neutron scattering with subsequent polarisation analysis. However, a polarisation option on an instrument always brings a strong loss in neutron intensity, which makes measuring times typically 30 times longer. Therefore, on an instrument like IN20, which is specialised on polarised neutron work, an increase in efficiency is highly welcome. This increase can be reached in various ways. Firstly, by installing CRYOPAD and (optionally) ^{3}He-polarisers. Secondly, by using large focusing polarising monochromators. Possible improvements of the secondary spectrometer of IN20 or other three-axis instruments at ILL are described in the subsequent proposals on multicrystal analysers and position-sensitive detectors, which may bring gains up to several orders of magnitude in counting efficiency. With such devices large regions of energy-momentum space can be measured in one go.

When a spin-echo option is made available for three-axis spectrometry, then the lifetimes of the various excitations in condensed matter can be measured with high precision. Several alternative spin-echo options are proposed. One alternative uses classical spin-echo in an optimised-field version, the other uses the zero-field spin-echo variant which was developed in recent years. These options should first be tested on the outphased three-axis instrument IN3.

For the hot-neutron three-axis spectrometer IN1 it is also proposed to install a ^{3}He-polarisation option. For the beryllium-filter downscattering version of this instrument the efficiency can be increased eight times by installing a corresponding number of detectors.

There are no serious competitors in this field of inelastic-scattering studies of atomic dynamics. Low-resolution inelastic measurements are also being done at synchrotron and spallation sources, but there is little overlap with the programme run at ILL.

5. Time-of-Flight and High-Resolution Instrument Group

In this instrument group there are 4 time-of-flight instruments and 3.5 high-resolution instruments.

One main subject of study on the time-of-flight instruments is the molecular **Dynamics of Disordered Systems**. Here the same remark can be made as in the section on diffractometry : the more complex the material and its lattice dynamics are, the larger the accessible reciprocal space must be. This is achieved by the installation of large position-sensitive multidetector systems on the time-of-flight instruments. Such installations would bring two further advantages : firstly, when you get the full picture, then you may find things that you did not look for - complex systems are always good for surprises ; further, signals from complex systems often are widely spread out, so that large solid angles are needed to cover them fully.

In the time-of-flight sector there are three proposals along these lines. One proposal asks to equip the existing time-of-flight machine IN5 with a large array of position-sensitive detectors. This would allow a fine-grain mapping of energy transfer in reciprocal space. This will open a new world of high-quality data on structural phase transitions, on strongly correlated electron-lattice systems, or on the dynamics of glasses and other disordered systems.

The polarised time-of-flight machine D7 has always been an avant-gardist instrument. It is able to do neutron-spin analysis over a large solid angle. With this instrument it is possible to study magnetic signals from very weak scatterers. It is also possible to separate coherent from spin-incoherent scattering, that is to separate uniquely the self-correlation function of a given system from its pair-correlation function. Here a high increase of efficiency can be reached by installing state-of-the-art components.

The newly proposed instrument PASTIS employs a similar principle as D7, but uses a large-angle ^{3}He polarisation analyser, and works for much larger neutron momentum and energy transfers. This instrument would bring a completely new quality to the studies of crystal field excitations, of spin fluctuations in amorphous systems, as well as of exotic quantum fluids.

On the high-resolution instruments of ILL the **Very Slow Dynamics** of molecular systems can be studied. There are two types of instruments, the so-called backscattering instruments which work in the frequency domain, and the spin-echo machines which work directly in the time domain. A recent success of the spin-echo instrument IN15 was the clear experimental distinction between various competing theories on polymer dynamics. Here the subtle theory of de Gennes on reptation dynamics has been verified experimentally for the first time. Another example is the spin dynamics of mesoscopic magnetic particles or « super-paramagnets ». It is proposed to improve the efficiency and stability of IN15 considerably by renewing several of its components.

During the past years, on the backscattering instrument IN16 a whole catalogue of atomic-potential data has been established for a large number of organic compounds. These data serve as a valuable basis for comparison with molecular-dynamic simulations. There are many other programmes run on the backscattering machines, but let us focus on the life sciences.

Very recently in the field of **Biomolecular Dynamics** it became possible to link the measured dynamics of certain bio-molecules to their biological function : the *slow* molecular motion is linked to weakly bound molecular sites which are prone to large conformational changes, that is have high biological activity ; this motion could clearly be separated from the *fast* molecular motion which is linked to strongly bound molecular sites, typical for a stable stereo-specific conformation of the molecule. With this type of measurement the function of the light-driven « proton pump » in purple membranes has been clarified. As a second example, the mechanism of the protection of biostructures against dehydratation was studied. It was found that this protective effect is correlated with the trapping of proteins in a deep harmonic potential where they are stable even at high temperatures. It is now proposed to increase the efficiency of IN16 to enable better and new experiments to be carried out.

Finally, there is a new but preliminary proposition to measure high-resolution diffraction patterns without the need for highly collimated beams. This is achieved by labelling each neutron of the incident beam, via its Larmor precession angle, with its wavelength and its scattering angle. The experimental feasibility of this proposal still has to be worked out.

To summarise, by far the best and often only method to study the fast and slow molecular dynamics of matter is the inelastic scattering of low energy reactor-neutrons.

6. Industrial Applications and Engineering Science

At ILL a good number of studies are of industrial relevance. So far, however, no instrument is wholly dedicated to industrial applications. But, as neutrons are only available at publically funded facilities, neutron-related methods that are useful to industry should also be offered to industry.

Five new installations in the field of industrial applications and engineering science are being proposed here. We call « engineering science » all **Studies of Prototype Devices**, whether they are done by industry or by universities. Instruments for engineering science will not necessarily be fully self-supporting financially. Under « industrial applications » we subsume all other activities paid for by industry or other organisms. These applications should be self-supporting and pay back their share of ILL running costs.

The first proposal is to rebuild the diffractometer D1A so it can be used exclusively as a strain-scanning instrument. This engineering-science project is well defined and has repeatedly been discussed in the Scientific Council. It probably will not be self-supporting financially, but will produce generally useful results.

The « industrial » instrument proposed for purity control « in-beam » will do trace analysis by prompt gamma-ray spectroscopy. In contrast to the conventional neutron activation analysis « in-pile », prompt analysis « in-beam » is also sensitive to the lighter elements. On a first preliminary installation it will be tested whether this instrument can really become self-supporting. One main application will be in **Quality Control**.

The three-dimensional imaging of technical objects has been developed to a high precision tool at the small Munich reactor FRM in Garching. There are interesting applications in industry, related to the **Optimisation of Fabrication Procedures** (like the control of gluing processes), or related to the Quality Control of industrial products of high commercial value. This installation will be allocated somewhere between engineering science and industrial applications.

The imaging of hidden layers via neutron autoradiography has, in the past, been applied on smaller reactors to the study of paintings. Here it is proposed to extend this method such as to make it possible to image the hidden layers separately for each element. Main applications will be in the **Fine Arts.**

At present, a number of incineration schemes for the destruction of long-lived nuclear wastes are under study. Some of these schemes require the investigation of specific nuclear neutron-induced processes. It is proposed to install an irradiation facility into the heavy water moderator of ILL's reactor dedicated to studies on **Nuclear Waste Incineration.**

Our aim is that most of the funds spent in the « industrial application » sector will eventually return to the investor. The main task here will be to create a structure adapted to the needs of the customers.

7. Infrastructure

A number of projects in the renewal programme are of common interest to all instrument groups. ILL must ensure that its basic installations like neutron guides, beam tubes and neutron moderators are renewed when necessary and improved when possible. Further, larger investments on high-field superconducting magnets, or on the further development of ^{3}He polarisers, are of high interest to many ILL users. These proposals have been subsumed under the heading « Infrastructure » at the end of Table 1 in the list of proposals. More external propositions on help with infrastructure development are listed in Table 2 of the list of proposals. ILL will be happy to collaborate with these external proposers for the mutual benefit.

FINANCIAL CONSIDERATIONS

1. The finances available for the Millennium Programme in the ILL budget over the coming 5 years can be estimated on the basis of the latest multiannual financial estimates as follows (MF) :

1999	*2000*	*2001*	*2002*	*2003*	*2004*
0	3.3	6.7	9.1	9.6	9.6

Total = **38.3**

2. In addition we may expect further contributions from a variety of other sources which in an optimistic scenario might amount to 20 MF.

3. The total cost of the proposals exceeds 110 MF. Furthermore the available manpower will limit the number of projects which can be undertaken. Hence it is clear that hard choices will have to be made. On the other hand additional financial and manpower contributions from the community would make it possible to include more of the proposed new developments.

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Technical Synthesis

N.B. : External proposals have not been scanned through by DPT

Proposed instrument	*Feasibility*	*Cost MF*	*Manpower*	*Possible starting date*	*Duration*	*Impact on DPT*
Nuclear and Fundamental Physics						
« Miniball » rare-isotope spectrometer	Well defined	5	3 months BE 1 month LEE	2000	2 years	Low impact, Design vacuum, cryostat..
Cold neutron, Particle physics facility : efficiency x 10		2		2001	1 year	No load
Ultra cold neutron source for neutron EDM : efficiency x 100					Several years	No load
Diffraction						
Thermal LADI (image plate)		3		2000		No load.
D2B (high resolution) : efficiency x 10 1) Detector	Straightforward. Gain 6 guaranteed	4.3	3 months design	2000	1.5 year. No stop of the instrument	Rather low Collimator design
2) Monochromator	To be proven	2				Large impact on LON
D19 (4-circle) : efficiency x 25	Success of μ strip ? Two steps process Background protection to be studied	3.9	9 months LD 4 months BE	Decision 2000	2.5 years	Large impact on LD
D3 (hot neutrons) : 3D-polarimetry 1) Phase 1	Eulerian cradle not standard. Local expertise.	3.3	3 years LEE 1 months BE	2000	3 years	Major development work for LEE
2) Phase 2	Local expertise	1.5		2003	2 years	Large impact on LON

LD = Detector Laboratory, SCI = Electronics, SMAE = Mechanics, LEE = Sample Environment Laboratory, BE = Design Office.

Proposed instrument	***Feasibility***	***Cost MF***	***Manpower***	***Possible starting date***	***Duration***	***Impact on DPT***
Large Scale Structures						
Cold LADI : efficiency x 5	To be defined	1.5	?			?
New SANS Detectors : efficiency x 100	2 steps process 18 months prototyping	Proto 0.8 D22 : 3.9 D11 : 3.0	12 months LD 2 months SCI 4 months SMAE	Proto 2000 Then start 2001	Proto 18 m. Detect 2 y Total 3.5 y	Load on LD + SMAE. Collaboration with CERCA and ISIS
Radical sites in biological macromolecules		0.4		2000		No load
Microsecond SANS - TISANE		1.6 + 5.3		2000	3 + 2 years	Not evaluated
Ultra SANS	To be evaluated	?	?	?	?	Not evaluated
Three-Axis Spectrometers						
IN20 (polarised) : efficiency x 10	Check beam tube renewal plan. Impact on cycle duration Well defined.	1.9	6 months BE 2 months LON 1 month SMAE	At will 2000	18 months	SMAE + LON, Normal activity
Multianalysers and PSD in TAS	Choose µstrips or wires	0.4 studies 0.5 later	6 months SCI LD or ext.	2000	2 years	Normal activity
Flat cone Excitation mapping in TAS	Background ?	3.1	8 months BE 1 month SMAE	2001	2 years	Load on BE and SMAE
Spin-echo in TAS	Choose between coils or RF	0.5 → 1	Not evaluated	2000	3 years	?
IN1 (hot neutrons) : polarisation option tests	Straightforward		Not evaluated	2000	1 year	Low impact
IN1 (Be-Filter) : efficiency x 8	Find Be at reasonable price (Russia ?). Find molten Cd supply ?	4.3 or 5.9	6 months BE 6 months DS Techn	2000	2 years	BE + SMAE + LEE

LD = Detector Laboratory, SCI = Electronics, SMAE = Mechanics, LEE = Sample Environment Laboratory, BE = Design Office.

LD = Detector Laboratory, SCI = Electronics, SMAE = Mechanics, LEE = Sample Environment Laboratory, BE = Design Office.

Proposed instrument	*Feasibility*	*Cost MF*	*Manpower*	*Possible starting date*	*Duration*	*Impact on DPT*
<u>Time of Flight and High Resolution</u>						
IN5 (TOF) : excitation mapping	Cone shaped lines and straight detectors : (computed corrections and paths in air.	9.7	6 months BE 4 monts SMAE 2 months SCI	2000	2 years	Load on SCI + scientific computing
D7 (diffuse scattering) : efficiency x 30 …60 Option 1 : mirrors Option 2 : ^{3}He	2 steps process One quarter first	Option 1 : 2 Option 2 : 1	3 years LON 2 months BE	2002	3 years	300 m^2 or 70 m^2 Strong load on LON
PASTIS : large solid angle thermal polarisation analyser	Totally new instr. TEST on IN4 To be redefined	20	Comparable to IN4	2003	5 years	Major work
IN15 (spin-echo) : higher efficiency and stability	Non-magnetic selector ? without precession coils	1.7	9 months	2000	2 years	Small
IN16 (backscattering) : efficiency x 10 … 32 1) Non-moved	Check the gain ? Feasibility Doppler machine ?	2.5	4 months BE 3 months SMAE 1 month LON	2001 but study now new Doppler	2 years	Design + mechanics
2) Moved after PF1 position	X32 ?(10)	5.2	16 months	Not too early	2.5 years	Large impact
Double precession spectrometer	Not evaluated					
<u>Industrial Applications and Engineering Science</u>						
Strain and stress in materials	New position recommended	To be invested partially from outside. 3.5	6 months BE 4 months HE 2 months SCI	2000	2 years	Can be Subcontracted
Purity control of materials	Straightforward	1.5	Low	2000	1 year	Low
3D-imaging of technical objects	Straightforward	1.2	Low	2000	1 year	Low
Imaging of hidden layers	Detector development needed	0.6	Low	2000	2 years	Low
Nuclear waste incineration tests (mini-Inca project)	Test proposed		Reactor manpower	1999	2 years	Impact on reactor

LD = Detector Laboratory, SCI = Electronics, SMAE = Mechanics, LEE = Sample Environment Laboratory, BE = Design Office.

Proposed infrastructure	*Feasibility*	*Cost MF*	*Manpower*	*Possible starting date*	*Duration*	*Impact on DPT*
Infrastructure						
Cold super-mirror guide	Big effort small gain on IN14	1.5	SMAE	2000	1 year	Normal load
Thermal super-mirror guide		5.8				
Hot source replacement		5				
Superconducting magnet (CEA pays half)	State or the Art	1 (+1 from CEA)		2000	2 years	low
Monte Carlo simulation of instruments	Collaboration with other laboratories	2		2000	2 years	low

LD = Detector Laboratory, SCI = Electronics, SMAE = Mechanics, LEE = Sample Environment Laboratory, BE = Design Office.

Thermal LADI - An Image Plate Diffractometer For Physics and Chemistry

C Wilkinson and G J McIntyre

Introduction.

A detector employing neutron-sensitive image plates is comparatively cheap, is capable of high spatial resolution, has good homogeneity, a large dynamical range, extended linearity and no dead-time, and can be constructed to subtend very large angles at the specimen. The neutron-sensitive plates are based on the same storage phosphor (BaFBr doped with Eu^{2+} ions) used for X-ray image plates, but with Gd_2O_3 added. This enables the Gd nuclei to act as neutron scintillators by creating a cascade of γ-rays and conversion electrons.

The on-line single-crystal cylindrical neutron image-plate Laue diffractometer (LADI, an ILL/EMBL collaboration) which has been constructed for macromolecular crystallography has been shown to give good quantitative structural information e.g N. Niimura, et al. Nature Structural Biology **4** (1997) 909; A. J Habash, et al. J. Chem. Soc. Faraday Trans., **93** (1997) 4317; P Langan et al. Acta. Cryst. **D 55**, (1999) 51. It is now in scheduled operation for visitors at an end-beam position on a cold neutron guide.

The present proposal is to construct a machine using already proven components to investigate problems in physics and chemistry (small unit-cell materials). Using the Laue technique with single crystals and a thermal beam, the two-dimensional projection of large volumes of reciprocal space can be seen in a single exposure. This allows structural and magnetic phase transitions (which often result in complex incommensurable structures) to be observed and followed as a function of temperature or pressure. Since the flux in a white beam can be considerably greater than a monochromatic beam, data can be obtained in a significantly shorter time (between one and two orders of magnitude) than in a monochromatic experiment, with only a modest loss in precision. It will provide a tool for development of new diffraction experiments and will be complementary to existing ILL diffractometers.

Scientific case.

While not optimised for small unit-cell investigations, LADI has occasionally been moved to the thermal beam H22 for test experiments on problems in physics and chemistry. An outline of the variety of applications which have so far been investigated is given below.

Magnetism.

LADI is equipped with a small Joule-Thompson expansion refrigerator, which was used to study temperature-driven magnetic transitions in 4 % Ga doped $FeGe_2$ (figure 1). The large detector surface combined with the white beam allowed rapid investigation of extensive regions of reciprocal space (J. B. Forsyth et al. J. Mag. Magn. Mat. **177-181** (1998) 1395). Due to the high spatial resolution of the detector, even very subtle changes in the positions of the reflections could be followed as the temperature changed, a dramatic departure in style compared with previous experiments on a monochromatic beam.

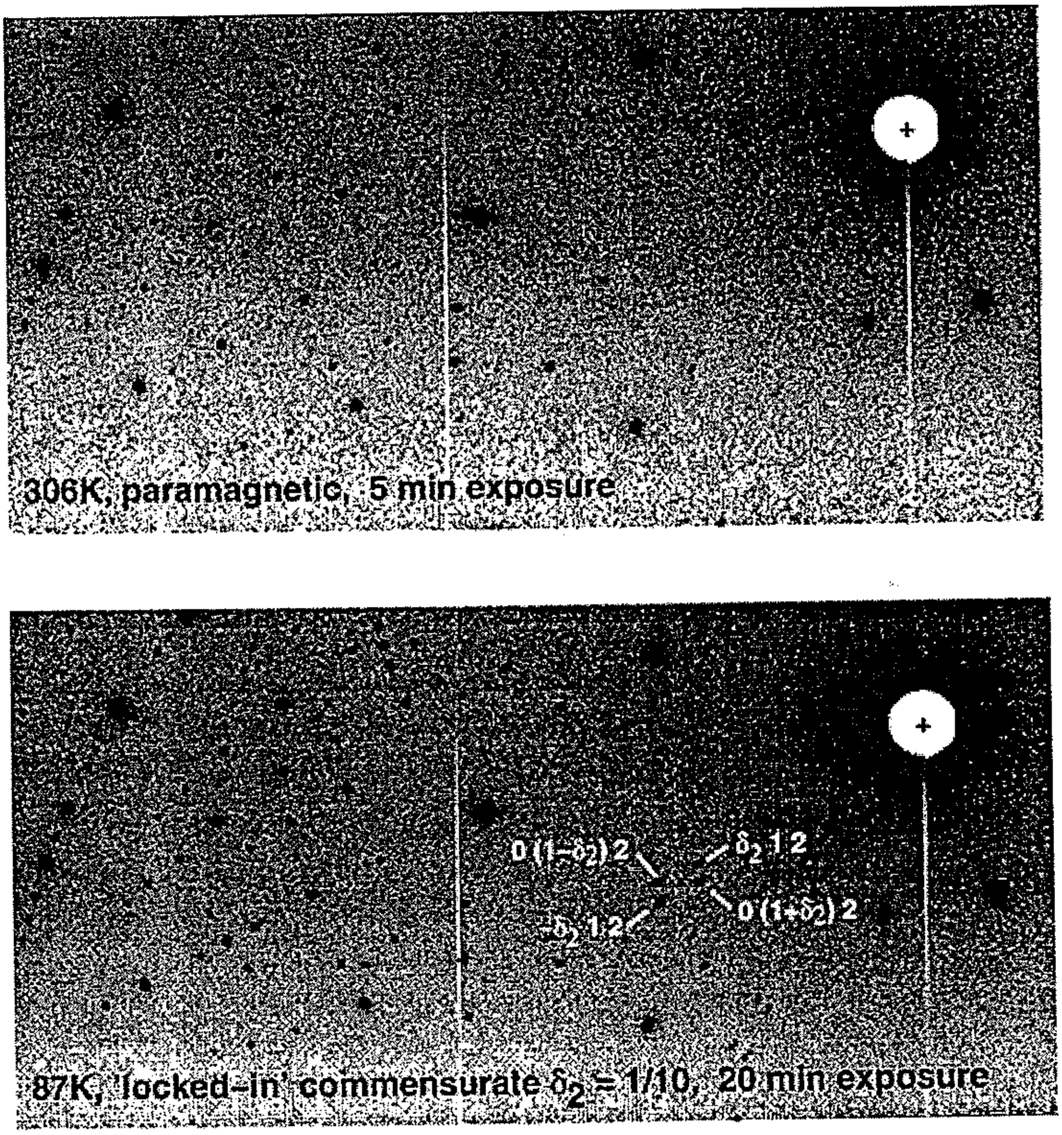


Figure 1. the paramagnetic-antiferromagnetic phase transition in 4% Ga doped $FeGe_2$. The first picture shows part of the room-temperature Laue diffraction pattern. This material undergoes a number of magnetic transitions and below 180K it locks into a non-harmonic spiral phase with a propagation vector of exactly 1/10. This gives rise to additional Bragg-peaks, which are shown in the second picture. The recording times of a few minutes are sufficient to give integrated intensities of good statistical quality.

Charge-density Waves.

The puzzle of the diffuse layers of reflections in monochromatic diffraction patterns from hexagonal single crystals of $La_2Co_{1.7}$ has been solved using the ability of LADI to survey rapidly large volumes of reciprocal space, and found to be due to a charge (nuclear) density wave with a propagation vector τ =0.113a*,0,0.203c*. The relative strengths of the groups of satellites associated with fundamental reflections show that the displacement of nuclei is close to the **c**-axis direction and that the effect persists from room temperature down to 15K (P. Schobinger-Papamantellos et al. Collected Abstracts, ECM, Prague, August 1998).

High Pressure Experiments.

Large gains in speed can also be obtained for high-pressure experiments, and the first test with a diamond anvil cell on a known sample, a small 0.04 mm^3 crystal of KH_2PO_4 at 2 GPa, gave an estimate of a factor 100 above similar measurements on a conventional diffractometer equipped with a position-sensitive detector (Kuhs and Ahsbahs, ILL report, 1997). In addition, the combination of the large detector surface and Laue techniques alleviated the problems that often occur due to changes of crystal orientation during the pressure experiments. From this experiment it was concluded that with a modified cell approximately 10 GPa can be reached using this set-up, pressures presently inaccessible in single-crystal neutron-diffraction experiments at the ILL.

Rapid structural studies.

Due to the large wavelength range and increased detector area over conventional monochromatic experiments, Laue diffraction data can be collected on LADI on smaller crystals and in times which are typically one tenth of those needed for the equivalent monochromatic experiment. Due to the increased background levels in Laue diffraction , the weak reflection data are normally less precise than those of a monochromatic experiment, but the crystal-structure parameters obtained are sufficiently accurate for most purposes.

A typical example of the data quality was the measurement on asparagine monohydrate, done in 12 hours using a 1.5 mm^3 crystal and a white beam with a useful wavelength range from 1.1 to 1.9 Å (D.A.A. Myles et al. Physica **B241-243** (1998) 1122). The final crystallographic agreement factor $\Sigma(F_o-F_c)^2/\Sigma F_o^2$ was 0.029 for 1060 reflections and while the data were collected fifteen times faster on a crystal of only one tenth of the volume, the precision of the bond lengths (figure 2) was almost as good as in a previous monochromatic experiment.

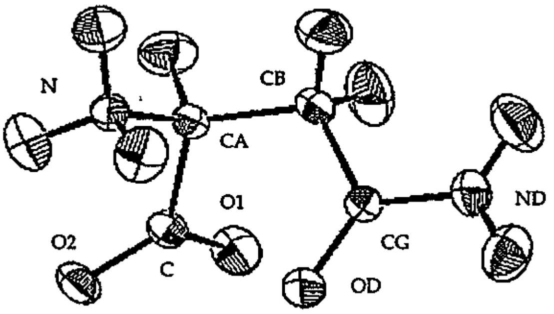


Figure 2. Asparagine monohydrate. Errors on bond lengths are 0.002 to 0.003 Å. This should be compared to the original measurement done at the Brookhaven high-flux reactor (J.J. Verbist et al. Acta Cryst. **B28** (1972) 3006) which took over a week on a 15 mm^3 crystal.

The increase in measurement rate was also evident in a study of ND_3-density distributions in the oriental disorder of $Ni(ND_3)_6Cl_2$, where again a factor of 100 in combined speed and crystal size was observed (Schiebel, Büttner and Kearley, ILL report, 1997). For these compounds it is of interest to compare the crystallographic observations with molecular dynamics modelling, and with the proposed new detector this could be done as a function of temperature - for example near a phase transition - thus adding a completely new dimension to these types of studies.

User Base.

Such an instrument would have a wide user base, covering fields such as magnetism, charge (nuclear) density waves, high pressure studies and structural phase transitions, as outlined above. When (even small) single crystals of a material are available, it provides a tool more powerful than powder diffraction for the preliminary investigation of a system. In many cases the data collected would be adequate to give an answer of sufficient precision to render subsequent experiments unnecessary. Using a monochromatic beam, such a detector would be ideally suited for many types of diffuse scattering experiments, but these applications have yet to be explored .

Proposal.

We propose the following unit (see figure 3 in Technical Annex), which is a vertical detector cylinder covered on the inside with neutron-sensitive image plates; the reader head is also placed on the inside. This will give the improved detector quantum efficiencies measured for 'front' exposure and readout tests on the LADI detector. There will be free access from the top to insert many different sample holders such as cryostats, furnaces, magnets and pressure cells (this is not possible with LADI, which is horizontally mounted). The sample holder is integrated into a high-precision sample rotation unit, which sits above the detector and can be lowered into this for the measurement.

Dimensions: 40 cm high, 100 cm circumference.
Pixel dimensions: variable at 200, 400 or 800 μm
Read-out time: 2 minutes

The detector will be controlled either by VME electronics connected to a HP workstation (the same as on the two present instruments - a 16-plate, automatic reader of large X-ray plates in operation at the ESRF and LADI at the ILL - which have identical, fully-developed sets of electronics), or by Windows NT and a PC. The user-friendly data-analysis software developed on LADI will be used for most experiments.

We propose that the machine be positioned at the end of the thermal guide tube H22 (behind D1A/D1B) in the position used for the small-unit-cell tests with LADI. The data collected show that a clean neutron beam with low γ-ray background can be delivered to this position (image plates are γ-ray sensitive and would otherwise need extensive protection).

Technical Annex.

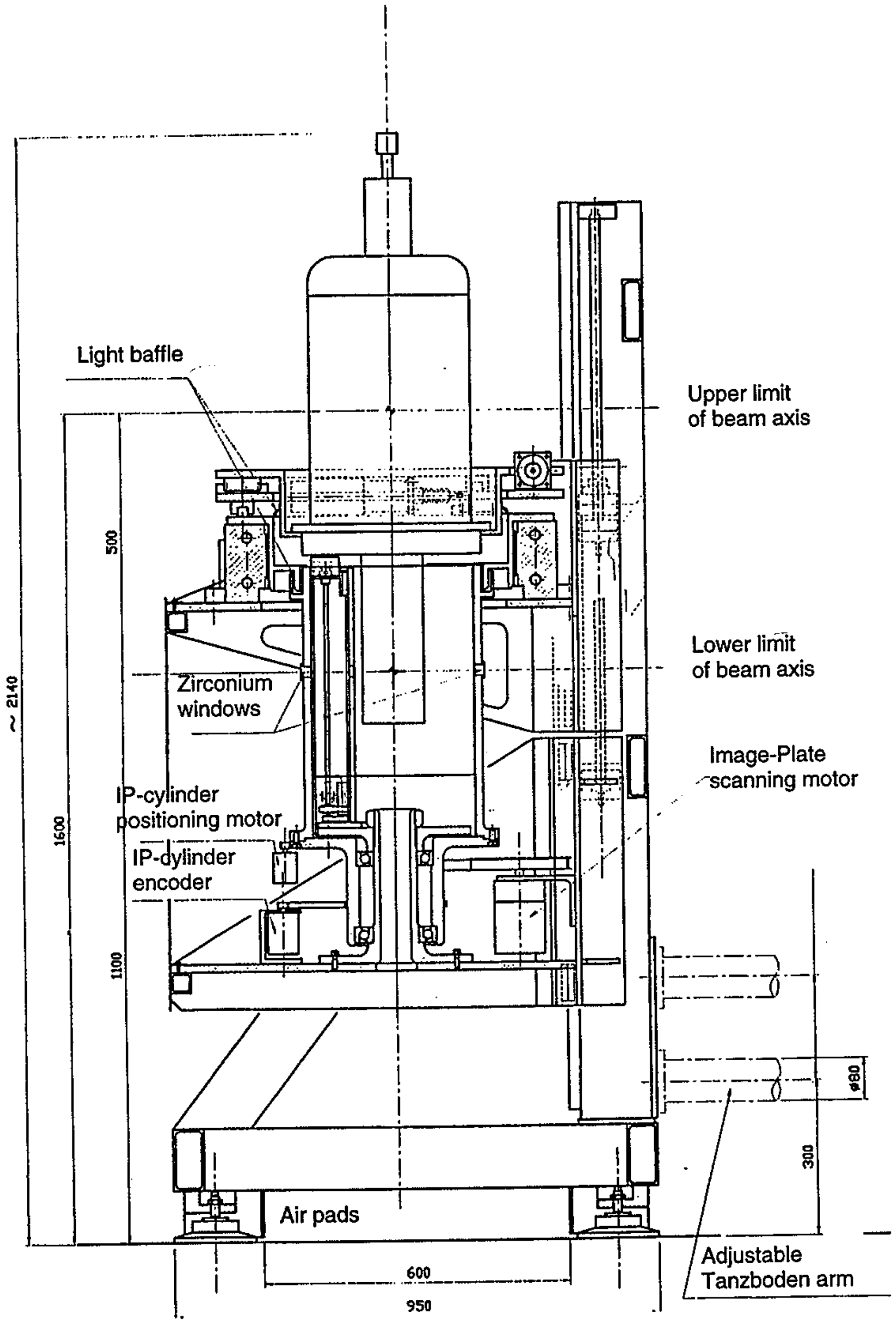


Figure 3. The proposed thermal LADI diffractometer

Technical Feasibility and Costs.

A detailed design study has already been undertaken by an external company, who can construct and deliver a complete turnkey instrument for a fixed price (2.9MF). Demand on ILL technical services for design and installation will be minimal. The data-treatment and analysis software will be based (as with the present LADI) on the CCP4 Laue suite, which is available as freeware.

Manpower.

For operation, technical assistance from ILL would be limited to sharing the technician presently employed on the neighbouring D10. It is proposed that scientific support would be provided by external scientists (including students and post-docs) detached from user laboratories in return for beam time to develop new applications of the machine. Several laboratories have already expressed an interest in such an arrangement.

Time-scale.

The design study was completed in January 1999 and is therefore up to date. Construction of the machine could start as soon as finance is available and contracts are placed.

A Super-D2B High Resolution Powder Diffractometer

E. Suard and A.W. Hewat, ILL

The Scientific Case and the User Base

D2B was proposed as part of the ILL "2eme souffle" with D19 and D20, and was the first machine operational, in 1984. The design was based on that of D1A, using commercial detectors and collimators. D2B is often the most requested of all ILL machines in terms of the number of proposals, and it has also resulted in the most scientific publications.

Of the more than 5000 papers produced by ILL since 1981, 50 experimental works were cited more often than others[1]; as much as 20% of this high profile work was done using D1A/D2B ! (Zeolites, Superconductors, Giant Magneto-Resistive materials, Ice-phases etc).

The success of neutron powder diffraction is due to the power of the method for the study of subtle changes in structure and magnetism with temperature and pressure. It is one of the first techniques to be applied to new materials, which are often available only as impure samples and in small quantities. These advantages are illustrated by the following examples.

1) High temperature oxide superconductors

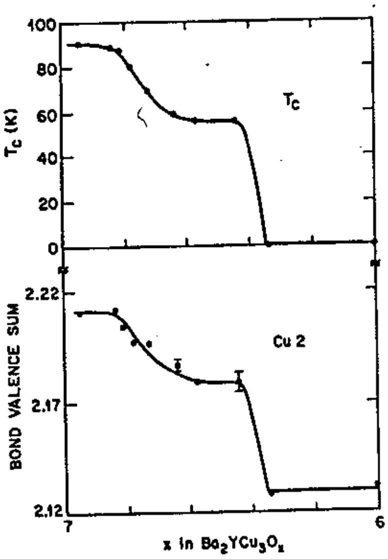


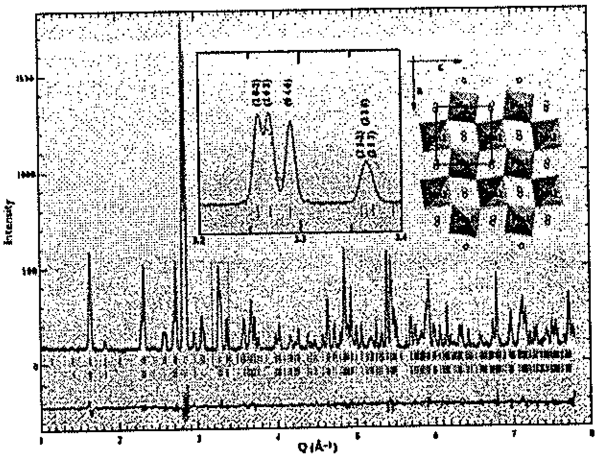
Fig. 16. Comparison of T_c and bond valence sum around the plane copper as a function of oxygen stoichiometry.

The most cited of all ILL publications[2] was work done on D2B with Bell laboratories and CNRS Grenoble to establish the "charge reservoir" concept of high temperature superconductors. While this work does not explain the physics of high Tc superconductors, it has been very useful in understanding the chemistry to produce new materials.

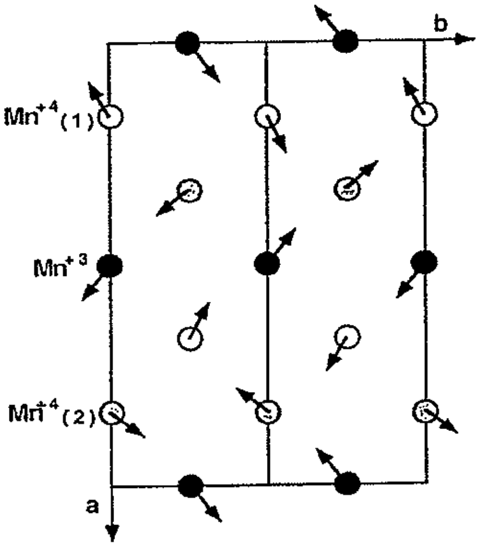
By studying small structural changes as a function of the oxygen stoichimetry, it was concluded that oxidation-reduction of a "charge reservoir" layer could control the hole doping in copper oxide layers responsible for super-conductivity. This idea lead immediately to a successful search for new materials with different "charge reservoir" layers, such as oxides of bismuth, thallium and mercury. These subtle effects in heavy metal oxides are much better studied with neutrons, which are more sensitive to scattering from oxygen, especially since new materials are at first available only as powders.

2) Mixed Valence, Charge Ordering and Giant Magneto-Resistance

High temperature superconductors are only one example of the many interesting materials found in recent years whose properties depend on order-disorder of the mixed valence states of one or more of the atoms. A recent example is that of charge and magnetic ordering in GMR manganites. Ordering is only within domains, so the average structure of a "single crystal" appears unchanged, and again it involves subtle movements of the heavy and light atoms, which are best seen with neutrons. Whether ordering appears as "stripes" or "ladders" has generated great interest, and neutron powder diffraction, coupled with synchrotron powder diffraction, has been essential to answer these questions[3,4].



3) Magnetic structures from neutron powder diffraction



Not only has the charge ordering mechanism responsible for the GMR effects been understood, but neutron powder diffraction has also been essential for understanding the magnetic structure[5]. Of course if single domain single crystals can be grown, more complex magnetic structures can be studied using other neutron techniques, but often this is simply not possible. Even when single crystals can be grown, the first work has usually been done with powders.

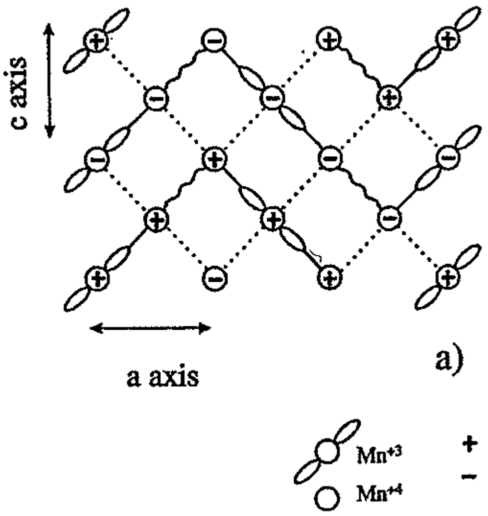
High resolution neutron powder machines operate at high scattering angles, and this means that long wavelength neutrons can be obtained - 2.4 Å is routinely used with the new graphite filter, and up to 6 Å is available with a beryllium filter. High resolution at long wavelengths is increasingly useful for the study of complex magnetic structures, such as magnetic spirals.

4) Structural phase transitions

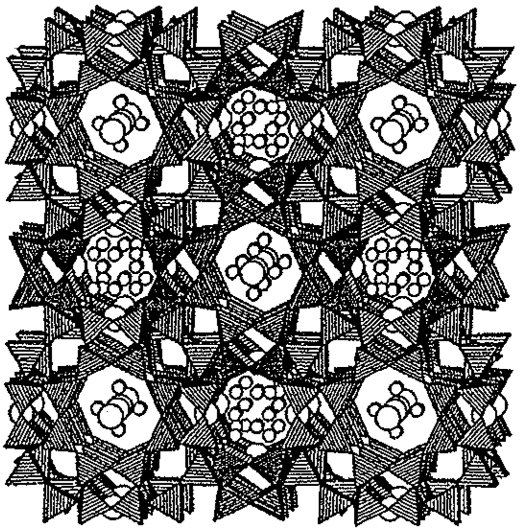
Neutron powder diffraction has been important for establishing that structural phase transitions at low temperature are much more common than had been thought. Clearly it is important to understand the 'ground state' structure of a material, but this has often been difficult for two reasons. First it is more difficult to perform precise single crystal measurements at low temperatures; it is easy to miss the subtle splitting of reflections, or the appearance of superlattice reflections indicative of a phase transition. Second, such structural transitions are often 'destructive', so that a single crystal no longer exists, but only a collection of domains with different orientations. Both of these fundamental problems are addressed by powder diffraction.

The study of structural phase transitions has contributed much to our understanding of the stability and dynamics of crystal lattices.

"Wigner crystal" model

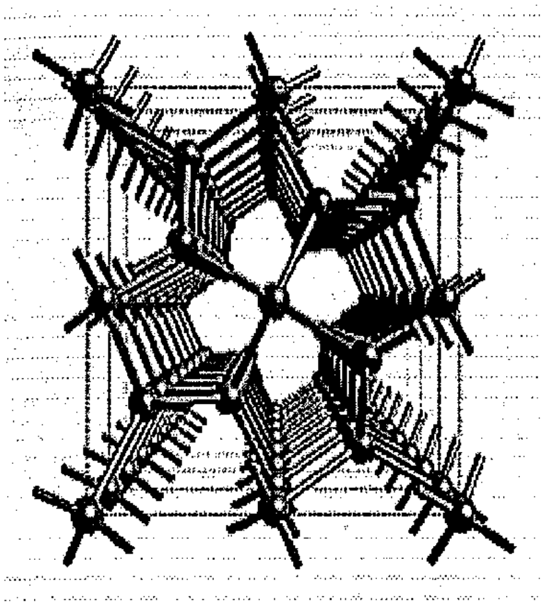


5) Zeolite Structures and Adsorbed Molecules



The study of zeolites has been another important application of neutron powder diffraction[6], since synthetic zeolites are only available as powders. Resolving the difference between Si and Al is much easier with neutrons, and the contrast between hydrogenated and deuterated components can also be very useful. The basic framework structure is first obtained with X-rays, and then the location of organic molecules introduced into the zeolite can be studied with neutron powder diffraction using difference Fourier techniques.

6) The Structures of High Pressure Ice and Geological materials



Higher resolution means that more subtle, yet often crucial changes, can be measured, and higher efficiency means that these changes can be followed over a larger range of temperature and pressure. Often, higher resolution has revealed the existence of new phases, for example with new high pressure forms of ice[7]. Hydrogen bonding is very important for many materials, and hydrogen bonding in water is the most fundamental example.

All of these studies benefit from higher resolution and higher efficiency. The case is similar to that made for a high resolution powder diffractometer on the European Spallation Source, except that an upgrade of D2B would be relatively inexpensive, risk free, and possible within a short period of time. Neutrons are the most effective diffraction probe of condensed matter; they would always be superior if it were not for their intensity, and addressing this problem will have a major impact.

The proposal

The proposal is to increase both the resolution and the efficiency of D2B by replacing the detector, with a bank of 128 commercial high pressure He3 detectors and collimators, and the monochromator, with a vertical and horizontally focusing composite, an extension of the design already proved on D2B and triple axis machines. This will result in an order of magnitude gain in efficiency, a significant gain in resolution, and zero loss of operation of the machine; the new detector bank and monochromator will be constructed and tested off-line, and installed during a winter or summer long-shutdown.

A super-D2B high resolution 2D detector using commercial components

A factor of x6 will be obtained in detector solid angle by constructing a high resolution '2D' detector from a stack of 128 vertical position sensitive wire detectors, such as those developed at ISIS. An array of 128 mylar collimators will be used to obtain high resolution with scattering angle, and the vertical resolution will be used to integrate over the diffraction cones.

The 128 collimators of 5' divergence would be mounted at 1.25 degree intervals on a circle of radius 917 mm from the sample, so that a complete 160 degree powder scan will be obtained with only 25 steps of 0.05 degrees - as little as 15 minutes for a high resolution pattern. The collimators will be 350 mm long, as at present on D2B, permitting the use of standard 1 inch He3 high pressure detectors. The collimators and detectors would have an active height of 300 mm, x3 greater than at present on D2B. The only compromise would be that the maximum sample diameter would be reduced from 20 mm to 15 mm, but available sample volumes are usually small anyway. This would leave only 2.5 mm for the collimator side plates at the front, increasing to 6mm at the rear. Such a high efficiency collimator, using Gd_2O_3 coated mylar plastic foils, has already been designed by EuroCollimators (see drawing); the height is greater than usual, but in fact 300 mm high collimators are already used in the primary beam of D2B, so there is little doubt that they can be made.

A much greater vertical divergence will also require more serious corrections for the geometrical effect of cutting the diffraction cones with a vertical 'slit'. These corrections are easy if we also measure the vertical point of intersection with the diffraction cone. For this reason we propose to use linear position sensitive wire detectors, with the vertical position of neutrons determined by charge division at the ends of each detector; this is a standard technique and provides a resolution of 2 mm, much better than needed. Such detectors can be purchased commercially, but have also been developed at ISIS.

The new D2B will then have a high resolution 2D detector using a stack of linear wire detectors, similar to 2D detectors proposed for small angle scattering. Each of the 128 detector/collimator elements is estimated to cost up to 30 kF including primary electronics, for a total cost of up to 3.84 MF. The existing D2B detector support mechanics will be re-used, but a new B_4C/expoxy detector box will be needed for a total cost of 4.34 MF. The existing D2B detector might be re-sold to cover part of this cost.

A proposed new D2B double-focussing composite monochromator

This is a second proposal that would further double the efficiency of the machine; it is independent of the proposal to replace the detector.

The resolution $\Delta d/d$ of modern powder diffractometers such as D2B is already much better than the neutron waveband $\Delta\lambda/\lambda$; high angle focussing geometry is designed to reduce line broadening due to this wavelength spread, which is otherwise needed to obtain high intensity. This second proposal is to further increase the waveband to double the intensity. Although this will not degrade the resolution near focussing, it will have an effect especially at low angles. By using horizontal as well as vertical focussing we plan to limit this reduction in resolution, while we will also control the effective waveband using a simple aperture after the monochromator. At the same time we plan to have a greater choice of useful wavelengths so that we can move the d-spacings that interest us most, to higher angles, where focussing is better.

Clearly this proposal needs much more development than the proposal to rebuild the detector, and unlike the new detector, the new monochromator will have to be made at ILL. A large part of the cost of such a monochromator would be for manpower. However, DPT-LON is very successful in developing new types of monochromator, and we believe that this proposal would further encourage such development in the 5 year time scale of the millenium programme.

Conclusions

Such an upgrade to D2B would be consistent with ILL strategy of improving the resolution of our high intensity machine, and the intensity of our high resolution machine. (The resolution of D20 is ultimately limited by the sample dimensions for a PSD design, while the intensity of D2B is ultimately limited by the soller collimator design). The two machines would then dominate the whole range of applications of neutron powder diffraction, for at least the next decade.

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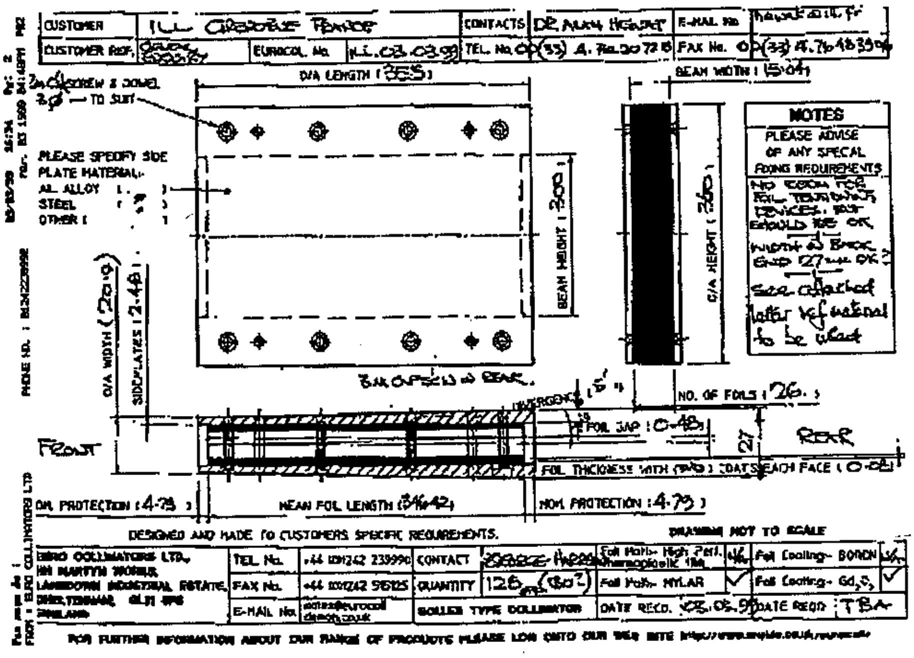
The structure of a new phase of ic

A Super-D2B High Resolution Powder Diffractometer

Technical Annex with Costs

The 128 high resolution soller collimators are already designed by EuroCollimators (Cheltenham) and estimated to cost 10 kF each. The active aperture would be 15 x 300 mm high, with side plates tapering to the front. Little ILL manpower would be needed for design or construction, and no interuption to the measuring schedule would be required.



CUSTOMER	ILL Grenoble France			CONTACTS	DR. ALAN HEWAT	E-MAIL No.	hewat@ill.fr
CUSTOMER REF.	[illegible]	EUROCOL. No.	[illegible]	TEL. No.	00(33) 4.76.20 72 13	FAX No.	00(33) 4.76.48.39.06

NOTES

PLEASE ADVISE OF ANY SPECIAL FIXING REQUIREMENTS

No room for foil tensioning devices, but should be OK.

Height at back end 27 mm OK?

See attached letter ref material to be used

EURO COLLIMATORS LTD., [illegible] LANSDOWN INDUSTRIAL ESTATE, CHELTENHAM, GL51 [illegible] ENGLAND	TEL. No.	+44 (0)1242 235990	CONTACT	[illegible]	Foil Matl.- High Perf. thermoplastic film	½	Foil Coating- BORON	½
	FAX No.	+44 (0)1242 [illegible]	QUANTITY	126 (180?)	Foil Matl.- MYLAR	✓	Foil Coating- Gd2O3	✓
	E-MAIL No.	[illegible]	SOLLER TYPE COLLIMATOR		DATE RECD.	[illegible]	DATE REQD.	TBA

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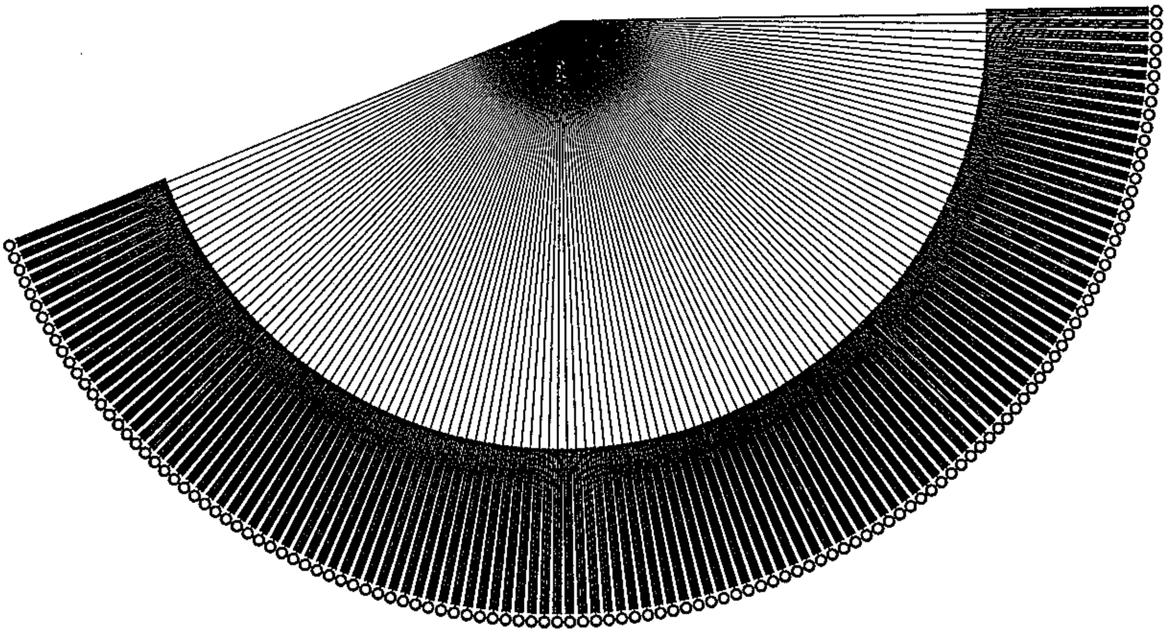
The high pressure linear-sensitive wire detectors would also be commercial types or else the type developed at ISIS. The cost of each of the 128 collimator/detector/electronic modules is estimated at 30 kF, for a total price with shielding of 4.34 MF for the complete 2D detector. The second project, independent of the detector, would consist of improving the efficiency of the monochromator, at a cost of up to 2 MF, mainly in manpower.



Super-D2B with its high resolution 2D collimator-detector array

A New Large-Area Detector for the Diffractometer D19

V.T. Forsyth and S.A. Mason

D19 is a diffractometer equipped with a 2-d multiwire detector that has an aperture of 4° by 64°. The instrument has proven applications in biology, chemistry, physics, materials science and polymer science. It is the only instrument at the ILL that can record single crystal diffraction data to atomic resolution from small samples with relatively large unit cells; it is also the only instrument in the world that can perform high-angle neutron fibre diffraction experiments.

The limited size of the existing detector means that at any given instant of time, approximately 95% of the available diffraction data is unrecorded. Our proposal is to replace this detector by an array of 8 area detectors, producing a gain in efficiency of up to a factor of 25. The benefits for the user community in each of the areas where D19 is heavily demanded are clear and quantifiable. The development will have a huge impact on the quality of D19 experiments and will considerably widen the scope of both single crystal and fibre diffraction experiments that can be carried out on the instrument.

1.1 Scientific Background. D19 is unique because it combines a high flux monochromatic neutron beam and an area detector. This provides the user community with the only instrument capable of surveying reciprocal space for small samples with large unit cells, for d-spacings from 100Å to 0.5Å.

1.1.1 Small Molecules. In single crystal work on small molecule systems, D19 allows the determination of the location of light atoms amongst heavy ones and the accurate characterisation of liganded H and H_2 and of hydrogen bonding and hydrogen disorder in studies of organic and inorganic molecules, complexes, solvates, and adducts. Such work has been the mainstay of D19 in the 1990's; examples are given in section 1.2.2 from the fields in chemistry and physics that are most likely to be affected by this proposal.

1.1.2 Larger Molecules. Some larger molecules of biological interest have also been studied on D19, such as vitamin B_{12} (Jogl *et al*, 1999), lysozyme (Bouquiere *et al*, 1993), and haemoglobin (Waller, 1989). The interest here is obvious – information on proton positions and hydration is vital for understanding biological processes. As can be seen from Figure 1, data from monochromatic neutron diffraction studies allows H or D positions to be determined at a much higher level of significance than is obtainable with x-rays. Although it is true that such information can be obtained from high resolution x-ray diffraction when crystals diffract to 1.2Å or better, it is also true that only a small fraction of crystals diffract to this resolution.

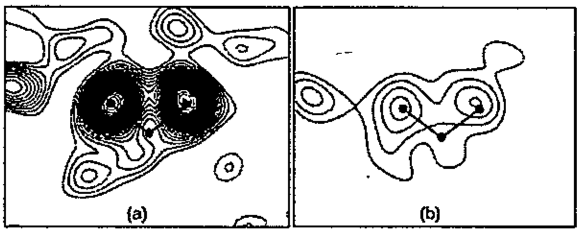


Figure 1: "Omit" density maps calculated for a D_2O molecule located in the crystal structure of coenzyme B_{12}. (a) 1A map showing the density determined from the D19 data and (b) 0.9A map showing the density from a synchrotron x-ray study (Langan et al, 1999).

Paradoxically it may in many cases be easier to grow crystals to neutron size than to produce crystals that diffract to 1.2Å resolution. Neutron diffraction allows proton positions to be determined with high precision using crystals that diffract to much lower resolution of the order of ~2Å. Where isotopic replacement of H_2O by D_2O is possible, it allows centre of gravity positions for water molecules to be unambiguously located from difference maps at even lower resolution.

Although neutron experiments on small proteins are at the limit of what can be achieved in reasonable beamtime allocations using the current detector, the use of a monochromatic beam and fine step scanning in omega, with frame readout times as small as 5 or 10 seconds, has clear advantages in situations where the sample background is high (*e.g.* for samples with high H content where deuteration is either not desirable or not feasible).

1.1.3 Fibre Diffraction. The availability of an area detector has also meant that D19 can be used to record high-angle neutron fibre diffraction patterns. The first experiments of this type were on DNA hydration and provided the first information on hydration in polymeric DNA. The studies are also important because fibres allow the study of DNA conformations that have not been observed in oligonucleotide single crystals and also of stereochemical changes that occur during conformational transitions (see Shotton *et al*, 1997). The same techniques have since been used to study hyaluronic acid, filamentous viruses, and have recently produced some outstanding results from cellulose (Nishiyama *et al*, in press). Similar methods have been used to study hydrogen atoms in aromatic polymers (Mahendrasingam *et al*, 1992) and are currently being developed for the study of polymers such as Nylon 66. There is increasing interest from industrial collaborators in the use of fibre diffraction methods in combination with specific deuteration to study changes in polymer structure as a function of chemical composition, temperature, and drawing processes. All of the neutron fibre diffraction studies provide information that cannot be obtained from complementary x-ray fibre diffraction studies.

1.2 New Scientific Opportunities. The limited size of the area detector means that D19 is much less efficient than it should be. This has been repeatedly pointed out by users, who see the loss of data as indefensible given the notional costs that are attached to the use of neutron beams. This was most recently pointed out in the survey conducted for the Scientific Council Review of ILL single crystal diffraction instruments (K. Yvon, 1998). In the following sections, we demonstrate the implications of our proposal for scientific work on D19 by outlining some recent projects at the present limits of viability.

1.2.1 Biological Systems. For reasons that are evident from section 1.1.2, a gain of a factor of ~25 will have an enormous impact on the scope of biological neutron crystallography. Results comparable to those currently obtained in a two week experiment will be obtained in half a day, and very substantial improvements will therefore be possible in reasonable allocations of beamtime. This will open the way to new projects (smaller crystals, larger units cells) that cannot be considered at the moment.

The implications are equally significant for fibre diffraction studies. This is very simply illustrated in Figure 2 which shows two neutron fibre diffraction patterns recorded from DNA.

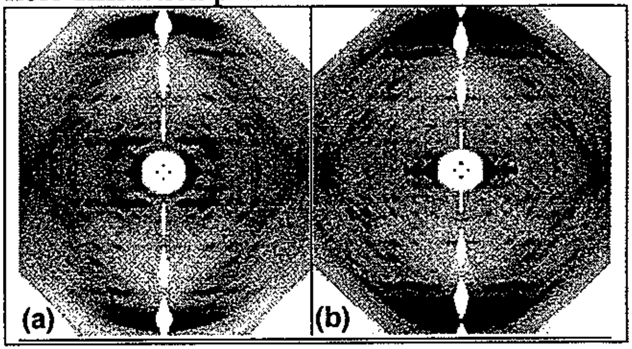


Figure 2: Neutron fibre diffraction patterns recorded from B-DNA hydrated (a) with H_2O and (b) with D_2O.

The counting statistics in each pattern are relatively poor and the individual "strips" corresponding to each detector position are clear. The new array will allow all of this data to be recorded in two exposures. Such a gain will be invaluable for work on crystalline fibres, but will be absolutely crucial for work on samples that give continuous layer line diffraction. This type of diffraction is very common in biological fibres - for example in conformational transitions in nucleic acids (Shotton *et al*, 1998), filamentous viruses, and in industrial polymer systems.

1.2.2 Chemistry and Physics.

1.2.2.1 Supramolecular Organic Complexes.

Detailed structural information on hydrogen atoms comes mainly from neutron diffraction. As new areas are explored there is a growing demand for such studies e.g. of N-H...π intermolecular interactions in the aminophenol crystal structures (Allen *et al*, 1997). Another application is work aimed at understanding how in compounds containing acidic C-H groups, weak C-H...X or C-H...π bonds aid in building up supramolecular arrays. Such compounds, for example alkyl (triphenyl) – phosphonium aryloxides, may contain 100 or more atoms in the asymmetric unit, and at present can be studied only if large crystals are available.

1.2.2.2 Inorganic and organometallic complexes. Here, accurate positions of light atoms such as hydrogen are sought in the presence of heavy atoms. A typical example is the successful location of and determination of bond lengths for H atoms in the non-octahedral hexanuclear cluster $H_2Os_6(CO)_{18}$ (Bau *et al*, 1997). However, anisotropic refinement was not possible because of the small crystal size, and the precision in bond lengths was barely adequate. Even more difficult, because of the high hydrogen content, poor crystal quality and larger asymmetric unit, was the study by Muller *et al* (1998) of a uranium complex, $C_{36}H_{53}BF_{15}N_3Si_6U.\ 3.5C_6D_6$. Again, the lighter atoms were all found, and the neutron refinement proved that a μ_2-H_2 ligand was not present. The electron deficiency of the uranium atoms was explained as effectively compensated by the formation of multi-centre bonds between U and S-CH_2 units. However, the precision, *e.g.* 0.008Å for a U-H distance, was only four times better than in the very accurate X-ray study, and a factor of 5-10 worse than ideal. A dramatic increase in detector area is needed.

1.2.2.3 Liquid Crystals Studies. One of the aims of studies of liquid crystals is to link liquid crystalline properties to molecular structure. A study of 4-n-pentyloxybenzylidene-4'-n-heptyl quiline on D19 has shown that, unlike other techniques, neutrons can provide information on both molecular structure and orientation distribution by exploiting the difference in scattering from H and D (Richardson *et al*, 1990). The quality of the data was limited by the time available for data collection; one day for each H/D mixture.

1.2.2.4 Quasicrystals Of the 30 or so known quasicrystalline compounds, many are of technological interest, *e.g.* as hard, high-temperature resistant substitutes for teflon. Models of the atomic structure are not as accurate as for conventional 3-d periodic structures, partly because, on a conventional diffractometer, only a small proportion of the available number of reflections in a given volume of reciprocal space can be observed. Recent measurements on $Al_{70}Pd_{20}Mn_{10}$ on D19 have for the first time allowed whole volumes of reciprocal space to be measured, giving over five times the number of unique reflections previously recorded with a dynamic range of more than four orders of magnitude. Because of the 6-d lattice needed to describe quasicrystals, a monochromatic beam is vital. A related application is observation of diffuse scattering and incommensurate satellites, as done for the decagonal phase of $Al_{65}CO_{15}Ni_{15}$ (Frey *et al*, in press). Only a high-quality large area detector will enable such measurements to be extended

2. User base. The table below gives a breakdown of D19 experiments by subject area.

Analysis of D19 experiments 1995-98	
Chemical Crystallography	30 (total)
Inorganic chemistry	15
Organic chemistry	15
Biological Structures	20 (total)
Fibre diffraction	15
Coenzyme cob(II)alamin & cyclodextrins	4
RNA octamer crystals	1
Physics & Materials Science	10 (total)
Phase transitions, super- & incommensurate structures & quasicrystals	7
Other	3

Although extrapolation from the present user base is hazardous since a factor of 25 in detector area will alter the scope of experiments on D19, it is obvious that this proposal will have a large impact on each of these main areas. In particular, the development will widen the user base for single crystal studies of large organic compounds, inorganic complexes, and small proteins, as well as for small molecule work where only small crystals can be obtained. The fibre diffraction user base will also be dramatically affected. Until now neutron fibre diffraction experiments have been carried out by users who are able to prepare large samples; for their part this requires a considerable investment in time and effort. It has been very clear from the last few annual CCP13 (BBSRC-funded collaborative computing project for fibre diffraction) meetings that the fibre diffraction community has interest in experiments of this type and that the general area will develop rapidly once the sample requirements change.

3. Proposal: the D19 detector upgrade. State of the art thermal neutron psd's are either multiwire or microstrip (Velletaz *et al*, 1996) gas detectors or image plate detectors. We have selected the ILL's microstrip technology because many D19 applications require rapid step-scan readout times, and because tests on H-containing compounds with the LADI image plate detector on D19 gave an unacceptably low peak to background ratio (Langan *et al*, 1997).

We propose to replace the D19 detector by an array of eight 2-dimensional microstrip PSDs. Each module will be 230 x 230 mm with a detection area of 192 x 192 mm, a resolution of 3mm, and an efficiency of 50%. The eight detectors will be mounted on a curved surface of either 60cm or 90cm radius (see Figure 3). This relatively large maximum radius is chosen to increase the signal to incoherent background ratio for hydrogen-containing samples. At this radius the detector array subtends an angle of 34.4° x 34.4° at the sample. When the incoherent background is small enough, the distance from the sample can be reduced to 60cm, in order to increase the number of reflections striking the detectors. At 60cm the angle subtended at the sample will be 51.4° x 51.4°. The projected gain in efficiency over the present D19 is a factor of up to 25. This is greater than the increase in solid angle (4.63 at 90 cm and 10.33 at 60 cm) because of large edge effects in the present narrow detector.

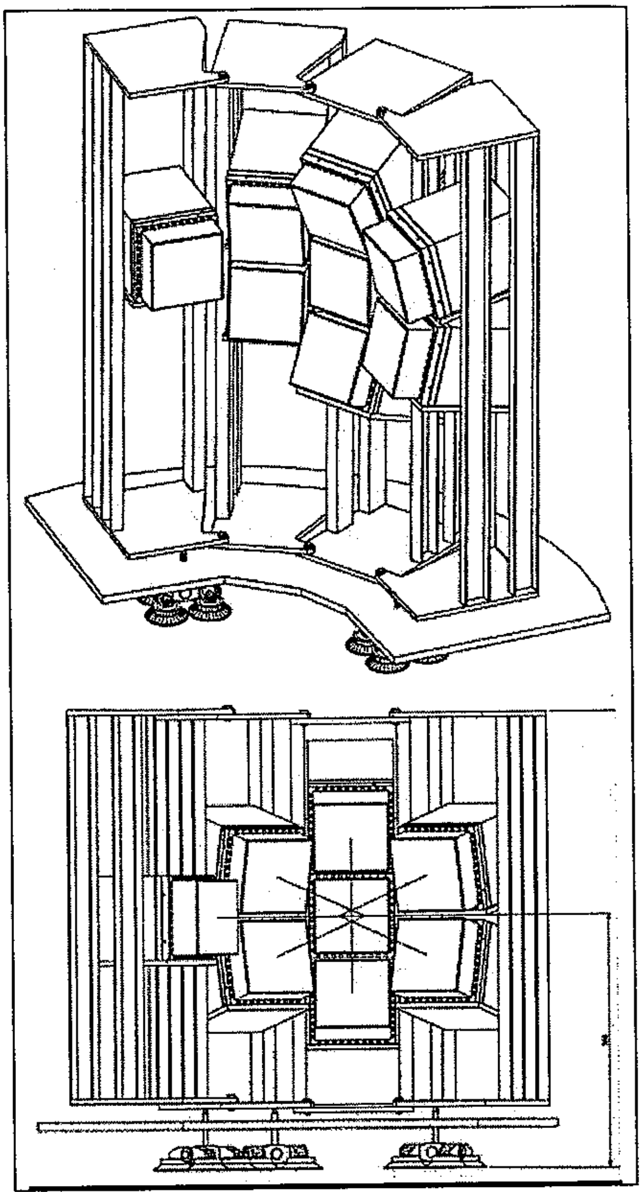


Figure 3: *Views taken from the designs for the new D19 detector system. Bottom: the detector array as seen from the sample position, illustrating the large solid angle that will be captured. Top: the detectors will be arranged in a curved array about the sample position.*

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We thank Paul Langan, Michael Walsh and Garry McIntyre for their contributions to this project.

D19 Technical Annex

A1.1 Technical feasibility & risks

The construction consists of 3 main parts, each using only technology already known at ILL.

- The 8 modular position sensitive detectors (PSD's) will use in-house designed 2-d microstrip technology very similar to that adopted for D4C: such a module has operated for 1 year with no sign of deterioration; a D19 prototype PSD will be tested on d19 in summer 1999. The modular design of the D19 array means that PSD's can be interchanged e.g. for calibration, temporarily removed for inspection or repair, or replaced as required. New-generation detectors, e.g. using small-gap microstrip technology, can be smoothly integrated into the array after testing and calibration elsewhere, without interrupting the d19 experimental program.
- Neutron shielding and mechanical mounting of the complete array will be analogous to that for the existing D19 banana PSD. The mechanical design – allowing for a change in sample-detector distance – is straightforward since D19 is already equipped with a Tanzboden floor. It is well advanced.
- Electronics and computing are completely standard PCI-VME and Unix based. Data processing software will be extended in-house as required.

A1. 2 Costs The unit cost of one PSD module including encoding electronics is 350KF.

	KF
Detectors : 8 new PSD's including psd electronics	2800
Mechanical support & shielding for the array (includes polythene & B_4C)	500
Electronics (standard commercial modules)	160
Senior technician (12 months)	400
TOTAL	**3860**

A1.3 Manpower

Construction manpower for PSD's: outside technician for 12 months. This includes 3 months for design modification if required after testing the prototype, and 9 months spread over 18 months for assembling the PSD's

A1.4 Time-scale

The prototype PSD will be installed on D19 in September 1999 and tested with user experiments until December 1999, in parallel with the existing D19 detector, so that modifications can be proposed if required. Components for the 8 new PSD's will be delivered in September 2000. Assembly will be completed within 12-18 months, depending on manpower. Detector modules will be used on D19 as soon as available, and the array will be completed by March 2002 at the latest.

D3 Project

E. Lelièvre-Berna

Introduction

In order to improve the characteristics and extend the fields of science investigated on the present polarised hot-neutron diffractometer D3B, we propose the project D3C. Taking advantage of the novel ^{3}He neutron spin filter presently available at the ILL, we can: 1) improve the peak count rates by optimising the monochromator irrespective of the spin selection process; 2) add polarisation analysis of the scattered beam. By featuring the best polarised flux at short wavelength in combination with a 10 Tesla cryomagnet for optimised flipping ratio measurements and uniaxial polarisation analysis, or a dedicated zero-field neutron polarimeter Cryopad for carrying out 3-dimensional polarisation analysis experiments, D3C will be the most powerful and flexible neutron machine in the field. Among the new fields of science, there are determination of exotic magnetic structures and the precision measurements of antiferromagnetic form factors in large Q range.

Scientific Case

The diffractometer D3B uses the polarised neutron diffraction (PND) technique to determine precise quantitative magnetisation distributions of single crystals that are magnetically ordered in a ferro- or ferri-magnetic phase under an applied magnetic field. The PND technique is a very sensitive method to observe the distribution of unpaired electrons in the whole unit cell. It reveals unambiguously the spin delocalisation, the polarisation sign, the density shape and the effects of magnetic interactions. It applies successfully to molecular compounds (3d transition metal complexes and free radicals), heavy fermions, high-T_c superconductors, transition metals and actinide alloys. The versatility of this instrument also permits unusual polarised neutron experiments to be carried out such as the study of the parity-violation in the vicinity of the p-wave neutron resonance of ^{139}La.

The basic improvement to the instrument through the decoupling of the optical functions and spin selection will give higher resolution and better flux. This will lead to more precise determination of ferro- and para-magnetic densities by providing better data at higher $\sin\theta/\lambda$ where the magnetic signal weakens. This will further improve the world lead held already by D3B.

In order to open this instrument to new fields of science, we propose to add polarisation analysis and to take advantage of new polarised neutron techniques. In elastic mode, the use of a ^{3}He neutron spin filter is simpler and better compared to a polarising crystal (flux x 5). Other advantages are the possibility to use a position sensitive detector and to compare directly spin dependent cross-sections (no convolution by a third axis). Uniaxial polarisation analysis may also be used with a large energy window to investigate the paramagnetic scattering of 3d transition metals using single crystals made of single isotopes. Short-range magnetic orders are expected well above the ordering temperature as an outcome of the very fast hopping processes, which will lead to a scattering function in sharp contrast to that of insulators or any other localised magnetism.

By adding polarisation analysis, this will also make possible the use of a Cryopad to carry out spherical neutron polarimetry (SNP) experiments. This unique technique gives access to the 16•measured quantities related to the 16 independent correlation functions involved in the most general nuclear-magnetic scattering process. Using SNP, we measure both the longitudinal and transverse components of the final polarisation vector, which is not possible with uniaxial polarisation analysis (with the sample in a magnetic field, transverse components are cancelled and only longitudinal components are accessible). In the case of magnetic structures, this leads to the determination of the direction of the magnetic interaction vector. Hence, SNP is the most powerful tool for solving non-trivial magnetic structures. Furthermore, because transverse components contain most of the information related to the nuclear/magnetic interference terms, SNP is the best method to study antiferromagnetic compounds for which Bragg peaks contain both magnetic and nuclear information. Among the new fields of research that will be opened are the following:

- Antiferromagnetic ground states in frustrated lattices: these are the subjects of numerous discussions. In principle, there are an infinite number of degenerate ground states in an ideal "spin-liquid". Neutron powder diffraction studies of various pyrochlores have discovered diffuse magnetic scattering that appears similar in form to a liquid structure factor. Recently, we investigated successfully the magnetic ground state of the Jarosite $KFe_3(OH)_6(SO_4)_2$. Contrary to neutron powder diffraction results, we could solve unambiguously the magnetic structure and compare it to the theoretical model.

- Magnetisation densities of canted antiferromagnets: we have shown recently on IN20 and later on D3 that we are able to determine precise antiferromagnetic form factors. Providing a Cryopad with a rotating sample environment giving 3D access to Bragg peaks, we expect to generalise this for the first time to the magnetisation determination.

- Investigation of non-trivial magnetic structures: chiral spin configurations, complex helices, configurations in which symmetry centres are lost, domain populations, etc... For the past few years, most of the magnetic structures solved using the SNP method were in disagreement with what was obtained previously with other techniques.

This will also contribute to the further developments of spherical neutron polarimetry.

User Base

With the new 10 Tesla cryomagnet, we expect a small increase of the present overload of D3 (actual average of about 1.7). By adding polarisation analysis, we will open new fields of science and it is difficult to evaluate the growth of the user base. However, we guess that part of the kind of experiments that was performed on D5 with the polarisation analysis option can be considered.

Regarding the SNP, since the restart of the reactor, the number of experiments has increased by a factor 3. Table 1 shows that the number of experimental days allocated for SNP experiments is now of about 100. It mainly concerns 5 collaborative groups: P.J. Brown et al., G.H. Lander et al., Schweizer et al., Regnault et al., McEwen et al. Because SNP is a novel technique, there is no way to determine how this growth will behave. The

SNP is able to give access to the whole information contained in the most general nuclear-magnetic neutron scattering process and the potential user base is wide open.

Table 1: Number of allocated days for SNP experiments

Year	*IN20*	*D3*	*Total*
1995	33 / --	--	33
1996	35 / --	--	35
1997	30 / 14	--	44
1998	75 / 14	12	101
1999	14 / 14 (+14)	18 (+30)	46 (+44)

Elastic / Inelastic scattering, (submitted proposals)

Proposal

In a PND experiment, the data measured are the ratios between the intensities observed for both polarisation states of the incident neutron beam at the peak of Bragg reflections. The incoherent scattering is subtracted from the Bragg intensity by measuring the background intensity away from the peak. In order to improve the quality of the dataset, one must increase the peak count rate, i.e. the incident flux and the energy resolution. Because Heusler polarising crystals are flux limited and provide a poor energy resolution, we propose to decouple the neutron spin selection from the optical functions by using a focussing monochromator combined with a ^{3}He neutron spin filter. The global improvement is given by the quality factor Q_R defined for flipping ratio measurements. This quality factor is proportional to the inverse of the standard deviation of $\gamma = M/N$ where M and N are respectively the magnetic and nuclear structure factors. For $\gamma << 1$, one have $Q_R = P\sqrt{\Phi \cdot T \cdot f}$ where P, Φ are the polarisation and the flux of the incident beam, T is the total transmission of the ^{3}He spin filter and f the resolution function. Roughly, with a Cu [200] focussing monochromator and $P_{3He} = 70\%$, simulations show that the standard deviation of the data may be divided by 1.5 to 1.9 (depending on the wavelength) when the magnetic signal weakens, i.e. for $0.2 < \sin\theta < 0.6$. Just as I'm writing this proposal, another alternative with ^{58}Ni monochromators points out. This could lead to a quality factor multiplied by 2.1 to 2.7.

As mentioned earlier, we also propose to add polarisation analysis using a ^{3}He neutron spin filter. Compared to the use of a Heusler crystal, it leads to a nice increase of the flux into the detector: ×4.7 for $P_{3He} = 55\%$, ×5.9 for $P_{3He} = 70\%$ and more at shorter wavelengths. The difficulty of this project resides in the ability to shield the inhomogeneous and large stray field coming from the new 10 Tesla cryomagnet in order to maintain the ^{3}He cell in a homogeneous magnetic field necessary for long relaxation time. A new device called Cryopol and being developed in collaboration with the CEA-Grenoble should clear up this difficulty. Briefly, the Cryopol is a superconducting cylinder surrounded by a µ-metal box in which we trap a homogeneous magnetic field. Tests recently performed with a prototype show that it is a very promising device.

The Cryopad-II, developed and uniquely existing at the ILL, is presently the only device which can accomplish SNP measurements. However, in order to determine magnetic structures and distributions, we need general 3D access to Bragg reflections in a large Q range. To carry out SNP experiments, we propose to build a new Cryopad optimised for short wavelengths (large Q range) and able to host a fully non-magnetic, four-circle helium flow, low-temperature cryostat.

To summarise, the D3C project consists in building a new Cryopad hosting an Eulerian cradle and envisage the use of a focussing Cu (or ^{58}Ni ?) monochromator combined with a ^{3}He neutron spin filter as soon as ^{3}He polarisation reaches 70 %. I propose to build the Cryopad and the rotating sample environment in the coming three years. Then, in a second step, the ^{3}He polarisation should be improved (about 70 % with the new compressor) and there will be strong motivations to modify the primary spectrometer of the instrument (better resolution and higher flux).

Technical Annex

D3C Project

Technical feasibility and risks

The main difficulty of this project resides in building a non-magnetic cradle and a larger Cryopad.

- Cradle: I propose to fix a D10 like cryostat to a first circle called $(\chi + k\varphi)$ and to add another circle called φ which is connected to the axis of the cryostat with a gear. Both rotations can be controlled from outside the zero-field chamber with limited plays. I expect a resolution of about 0.02°.
- Cryopad: calculations show that 2 screens (100K, 40K) will be needed to keep the whole surface of the two Meissner shields below T_c. Several designs are envisaged: cryogenerator + LHe bath, 2 cryogenerators, 3 coils + pillars.

Costs and time-scale

Table 2: Part I - 3 years - Cryopad & cradle

Cryopad cryostat (inner Ø65 cm)	~ 61 k€ (400 kFF)
Two Nb cylinders (Ø75 cm × 100 cm)	~ 46 k€ (300 kFF)
NbTi wire + manpower	~ 4.5 k€ (30 kFF)
Toroidal flange	~ 7.5 k€ (50 kFF)
μ-metal shield to cool down Cryopad	~ 18 k€ (120 kFF)
μ-metal shield for operation	~ 7.5 k€ (50 kFF)
Two nutators + VME card (QCL)	~ 6 k€ (40 kFF)
Two rotating plates	~ 14 k€ (90 kFF)
Two power supplies + NIM cards	~ 10.5 k€ (70 kFF)
Non-magnetic Eulerian cradle	~ 198 k€ (1300 kFF)
Cradle cryostat + siphons	~ 38 k€ (250 kFF)
Two LHe dewars	~ 30.5 k€ (200 kFF)
Total	~ 442 k€ (2900 kFF)

Table 3: Part I - 3 years - Cryopol (spin-analyser)

Cryopol cryostat	~ 18.5 k€ (120 kFF)
Nb cylinder (Ø30 cm × 70 cm)	~ 7.5 k€ (50 kFF)
μ-metal shields for operation	~ 3 k€ (20 kFF)
Coil + support	~ 7.5 k€ (50 kFF)
Nutator	~ 1.5 k€ (10 kFF)
^{3}He cells (high pressure)	~ 7.5 k€ (50 kFF)
Plate with air-pads	~ 0 k€ (0 kFF)
Support for detector + coil + nutators	~ 7.5 k€ (50 kFF)
Total	~ 53 k€ (350 kFF)

Table 4: Part II - 2 years - Flux and resolution improvement

Cu crystals ([200] – transmission geometry)	~ 30.5 k€ (200 kFF)
Mechanics + electronics	~ 46 k€ (300 kFF)
Carousel including shutters, monitor, λ/2 filters	~ 61 k€ (400 kFF)
Cryopol cryostat	~ 18.5 k€ (120 kFF)
Nb cylinder (Ø30 cm × 70 cm)	~ 7.5 k€ (50 kFF)
µ-metal shields for operation	~ 3 k€ (20 kFF)
Two nutators	~ 3 k€ (20 kFF)
^{3}He cells (high pressure)	~ 7.5 k€ (50 kFF)
Magnetic shields & nutators'box	~ 46 k€ (300 kFF)
Total	~ 223 k€ (1460 kFF)

To summarise, the estimated costs for this project are about 500 k€ (3.3 MFF) for the first part: Cryopad, Cryopol, Cradle; and 225 k€ (1.5 MFF) for the performance improvement. If ^{58}Ni monochromator tests are positive, an extra cost must be planned (300 k€ ?).

Manpower

- Zero-field chamber simulations by M. Thomas, F. Tasset. We will take advantage of the previous simulations done for Cryopad-II.
- Cryopad and Cryopol design by E. Bourgeat-Lami, S. Pujol, F. Tasset and F. Thomas. AS Scientific will certainly do the job (C. Hilier). They built Cryopad-II and Cryopol prototype successfully.
- Cradle, Carousel and Monochromator mechanics design by E. Bourgeat-Lami, S. Pujol, F. Tasset, F. Thomas and the help of the "Bureau d'Etudes". I propose to make the general assembly drawings at the ILL and to ask for detailed drawings and construction outside.
- Cu crystals (or ^{58}Ni ?) prepared by I. Anderson's team.