



The instrumental facilities at the ILL are shown in the schematic diagram on page 8.

Instruments are identified by the instrument's symbols which correspond to closely related experimental techniques:

- D Neutron diffraction:
- Powder, Single-crystal, & Small-angle diffractometers, Reflectometers
- IN Inelastic neutron scattering: Three-axis, Time-of-flight & High-resolution spectrometers
- PF & PN Nuclear and Particle physics

The list of instruments as of July 2005 is summarised below:

- powder diffractometers: DIA, DIB\*, D2B, D20, SALSA
- liquids diffractometer: D4
- polarised neutron diffractometers: D3, D23\*
- single-crystal diffractometers: D9, D10, D15\*
- large scale structures diffractometers: D19, DB21, LADI, VIVALDI
- strain imager: SALSA
- small-angle scattering: D11, D22
- low momentum-transfer diffractometer: D16
- reflectometers: ADAM\*, D17, EVA\*
- diffuse scattering and polarisation analysis spectrometer: D7
- three-axis spectrometers: IN1, IN3, IN8, IN12\*, IN14, IN20, IN22\*
- time-of-flight spectrometers: IN4, IN5, IN6, BRISP\*
- backscattering and spin-echo spectrometers: IN10, IN11, IN13\*, IN15, IN16
- nuclear physics instruments: PN1, PN3
- physics instruments: PF1, PF2

Besides the ILL instruments, there are 9 CRG-instruments (marked with an asterisk \*), which are operated by external Collaborating Research Groups. There are currently three different categories of CRG instruments.

- CRG-A in which the external group leases an instrument owned by ILL. The group has 50% of the beam time at their disposal and for the remaining 50% they support ILL's scientific user programme.
- The CRG-B category owns their instrument and retains 70% of the available beam time, supporting the ILL programme for the other 30%.
- Finally, CRG-C instruments are used full time for specific research programmes by the external group, which has exclusive use of the beam.

DB21, LADI and IN15 have a special status, since they are joint ventures of the ILL with other laboratories: in the case of DB21 and LADI with EMBL and for IN15 with FZ Jülich and HMI Berlin.

Details on the instruments can be found on the web under http://www.ill.fr/YellowBook.

# Diffraction Instruments

The ILL's diffraction instruments are divided into two main groups:

#### **Powder diffractometers**

D1A high-resolution powder and stress diffractometer D1B high flux PSD powder diffractometer D2B very high-resolution powder diffractometer D20 very high flux PSD powder diffractometer D4 liquid and amorphous materials diffractometer SALSA strain analyser for engineering applications

#### Single-crystal diffractometers

- D3 polarised hot neutron diffractometer
- D9 hot neutron 4-circle diffractometer
- D10 thermal neutron 4-circle & three-axis diffractometer
- D19 4-circle diffractometer with 2D PSD for large unit cells
- D15 thermal neutron normal-beam diffractometer
- D23 thermal neutron normal-beam diffractometer
- + polarised neutron option

#### **Powder diffractometers**

These two-axis diffractometers are used to investigate the structure of powders, liquids and amorphous materials. Diffraction group machines use relatively short wavelength neutrons (0.3 to 2.0 Å) to resolve structures to atomic resolution, in contrast to diffractometers in the Large Scale Structures group that use long wavelength neutrons for lower resolution of larger structures. Usually a large composite monochromator, up to 300 mm high, is used to select a narrow band of wavelengths and focus it onto the sample. The monochromator may be made from several crystals of pyrolytic graphite, copper or germanium. Large multi-detectors and linear position-sensitive detectors (PSDs) cover a large solid angle for maximum efficiency.

The two high-resolution powder diffractometers DIA and D2B are used mainly for Rietveld refinement, with scans lasting from 30 minutes to several hours. They are complemented by two high-flux medium-resolution powder machines, DIB and D20, which are used mainly for temperature scans and other types of fast experiment, especially on small samples. D4, on the short wavelength hot source, is used for liquids and amorphous materials, together with D20.

	DIA		D2B		DIB-CRG		D20		D4		
λ (Å)	1.9	3.0	1.6	2.4	1.3	2.5	1.3	2.4	.35	0.7	
d <sub>min.</sub> (Å)	I	1.5	0.8	1.2	0.7	1.3	0.7	1.2	0.4	0.2	Q <sub>min.</sub>
d <sub>max.</sub> (Å)	27	42	22	34	36	70	12	23	34	17	Q <sub>max.</sub>
Time /dataset	5h	4h	lh	2h	lh	5m	lm	lm	10h	lh	
$\frac{\Delta d/d}{x10^{-3}}$	2		0.5 t	o I.5	(	5		4	20	)	ΔQ/Q

Resolution is given for D2B for high resolution and for high intensity mode. Values for D4 given in Q. Resolution of D20 for the new Ge monochromator.



**DIA** is still unique in being able to provide high resolution at long wavelengths, with shorter wavelength contamination eliminated by the guide tube. DIA is particularly suited to magnetic structures and other large d-spacing studies, such as zeolites. DIA-stress provides very high lateral resolution, and allows stress determination to within as little as  $50\mu m$  of a surface or interface.

**D2B** was designed to achieve the ultimate resolution, limited only by powder particle size ( $\Delta d/d \sim 5x10^{-4}$ ), but was built so that an alternative high flux option, with resolution comparable to that of D1A but much higher intensity, could be chosen at the touch of a button. D2B then has very high intensity at D1A resolution, or very high resolution at D1A intensity. Being on a beam tube in the reactor hall, it can use wavelengths as short as 1.05 Å, impossible on D1A. The D2B detector bank was recently replaced by a pseudo-2D detector with 6 times the solid angle, and data can now be collected on samples as small as 500 milligrams in a few hours, or normal samples of a few grams in a few minutes.

**DIB** has always been in very high demand for real time experiments, and for very small samples because of its high efficiency position sensitive detector (PSD). Although it is a CRG instrument, (run by a CNRS team and Spain), it is available 50% of the time for scheduled ILL experiments. Complete diffraction patterns covering 80° at moderate resolution can be collected in a few minutes.

**D20** has extremely high flux with a very large PSD and opens up new possibilities for real-time experiments on very small samples. The complete diffraction pattern at 1536 positions covering the whole scattering range can be obtained in as little as a few hundred milliseconds (or more typically a few seconds), and then repeated automatically as a function of temperature, pressure, magnetic field, etc. Higher monochromator take-off angles up to 120° provide good resolution over the complete diffraction pattern, which can be obtained in a few minutes, even with small samples.

**D4** on the hot source, is designed to use short wavelength neutrons to measure diffraction patterns over a large Q-range from non-crystalline materials (glasses, liquids, amorphous solids) with excellent accuracy and to characterise their local atomic order. D4 shares a beam with the three-axis spectrometer INI and is therefore only available for about 50 % of the time. However the complete scattering range is covered by a large array of microstrip detectors, making the machine very efficient and very stable for different measurements on small samples, with isotopic replacement used to enhance contrast of particular atomic species.

**SALSA** is the new ILL strain imager dedicated to the determination of residual stresses in a broad range of applications in terms of components and materials. It is in fact designed for diffraction measurements in "real" engineering components and optimised for stress determination in metallic components.



## Powder diffractometers Single crystal diffractometers

#### Single-crystal diffractometers

Single-crystal diffraction is a powerful method for the investigation of structural details in condensed matter. Hot neutrons are required to uncover the finest details in the nuclear positions and neutron spin polarisation is a handle to separate mixed components (nuclear polarisation, magnetic and electronic scattering).

A characteristic of the four-circle diffractometers is the use of Eulerian cradles for orienting the sample crystals, with the detector moving in a horizontal plane. Normal-beam diffractometers have a mechanism for tilting the counter out of the horizontal plane, thus enabling the installation of heavy equipment for special crystal environments (cryostats, magnets etc.).

These diffractometers can be used to find:

- average atomic positions. From these we can learn how the atoms are bound together to form molecules, and how the molecules are stacked;
- local atomic distributions. This gives information about the time averaged thermal motion or the local atomic disorder;
- magnetic structures and magnetic moment distributions.

Structural data of this kind are required for a large number of systems, ranging from organic molecules to high temperature superconductors. Often studies are made as a function of temperature, pressure and magnetic field which may lead to important modifications of the crystal structure.

	D3	D23-CRG	D9	DIO	DI5-CRG	DI9	Vivaldi
λ (Å)	0.3 –0.85	1.0-3.0	0.3-0.9	1.3-2.4	0.85-1.54	0.8-2.4	1.3-2.4
Q <sub>min.</sub> (Å-1)	?	0.15	0.06	0.004	0.12	0.015	
Q <sub>max.</sub> (Å-1)	20		20	8.5	12.6	10	
Beam size (mm)	20	20	6	10	10	10	
Expt.time (days)	8	7	7	7	7	14	
Remarks	Polarisation analysis	Special environments Pol. neutrons	High spatial resolution	Special environments	Special environments	Big 2D PSD Large cells	lmage plate Large cells

### D 3 and D 9 use neutrons from the hot source with wavelengths as short as 0.3 Å.

It is therefore possible, using D3, to measure magnetic structure factors up to  $\sin\theta/\lambda = 2 \text{ Å}^{-1}$ . D3 is a diffractometer with a polarised incident neutron beam. In practice, the instrument is set at a Bragg peak of an already known crystalline structure. Then, by simply reversing the beam polarisation, D3 performs a highly sensitive measurement of the spin-dependent nuclear magnetic interference amplitude term which is present in the Bragg scattering of polarised neutrons from a small single crystal specimen magnetised in a field. With polarisation analysis and Cryopad, D3 carries out spherical neutron polarimetry experiments. In the case of magnetic structures, this leads to the direct determination of the magnetic interaction vector. Hence, D3 is a very powerful tool for solving complex AF structures that had proven to be intractable with other techniques. Moreover, when the magnetic and nuclear scattering occurs at the same position in reciprocal space,

D3 allows a precise determination of the AF magnetisation distributions. D3 can also be used for many purposes other than diffraction experiments, e.g. the search for the T-odd asymmetry of light particle emission in 239-Pu ternary fission.

For structural analysis beyond the determination of average atomic positions, high-resolution nuclear density maps are required. D9 is ideally suited for this purpose. Because of the short wavelength very small atomic displacements can be identified, accurate to typically 0.001 X. A two-dimensional multidetector is employed.

Various models of anharmonicity are used, involving many parameters that can only be determined by including reflections at high momentum transfers.

Structural data from D9 are also used:

- to help in the analysis of magnetic structures, especially if magnetic and nuclear reflections are not superimposed as with antiferromagnets;
- for the determination of magnetic structures of absorbing elements as Sm, Gd, etc;
- for various fundamental studies of the nature of diffraction from single crystals;
- for combined neutron and Xray analyses to get the electron distribution in atoms and molecules;
- to get a model for the extinction correction by measuring at different wavelengths.

#### The three-axis diffractometer DI0

D10 is unique in being the only four-circle diffractometer with optional energy analysis as on three-axis spectrometers. It also possesses a unique four-circle cryostat for temperatures as low as 0.1 K, and offers high reciprocal space resolution and low intrinsic background, to medium real space resolution.

It is intended primarily for conventional crystallography, detailed study of modulated structures, quasielastic scattering and diffuse scattering.

#### The two-axis diffractometer D23

D23 is a double-monochromator two-axis diffractometer with a lifting detector mounted on an arc (normal beam geometry). It is installed on the thermal neutron guide H25 that is equipped with a supermirror-coating, and thus offers a high flux and a very good signal to noise ratio. D23 is designed to work with or without polarised neutrons, with wavelengths in the range I - 3 Å. It can support special sample environments (high field cryomagnets up to 15 Tesla, pressure cells, dilution fridges etc.) and is well suited to the determination of magnetic structures, magnetic phase diagrams and magnetization distribution maps.

#### The large structures diffractometer D19

D19, with its 120° x 30° position sensitive detector, is the monochromatic thermal neutron single crystal/fibre diffractometer of choice for determination of crystal structures with unit cells in the range of 10<sup>3</sup> to 10<sup>5</sup> Å<sup>3</sup>.

Examples of single crystal studies include organometallic complexes, proteins, helium single crystals, acetylene polymers, liquid crystals, Vitamin B12, cyclodextrin complexes. Fibre work includes studies of DNA, cellulose, filamentous viruses and many industrial fibres.

## Large Scale Structures Instruments

The instruments of the Large Scale Structures group are all dedicated to measuring structures on the scale of 1 to 100s of nanometers. A vast range of science is covered: from magnetism to polymers and colloids to biological structure, in solution, in the solid state or in very thin films.

Information on these large scales is obtained by measuring at especially low Q exploiting neutrons from each of the ILL reactor's cold sources.

Although the instruments all exploit cold neutrons they fall naturally into three classes, reflectometers, diffractometers and small angle scattering instruments.

#### Reflectometers

There are three reflectometers at ILL; D17 is an ILL owned instrument and ADAM, is a CRG-B contributing 30% of its beam-time to ILL scheduling. EVA is a CRG-C and as such is does not provide time for allocation to the ILL.

The three instruments are largely complementary and work in rather different modes:

**D17**, on the vertical cold source, can operate in three different modes: timeof-flight, monochromatic and polarised. It has a white flux at the sample position of 9.6 x 10° n.cm<sup>2</sup>/s. Highly variable resolution may be achieved by varying the separation and phasing of the choppers in time-of-flight mode. The monochromatic and polarised modes each use multilayer monochromators ( $\lambda = 5$  and 5.5Å respectively). Polarisation analysis can be performed with either a large supermirror for specular studies or a He<sup>3</sup> cell for off-specular measurements.

**ADAM** is a fixed wavelength reflectometer using a focusing pyrolytic graphite monochromator to access neutrons of 4.4Å or 2.2Å wavelength. Polarisation and polarisation analysis are available as options.

**EVA** is also a fixed wavelength reflectometer, being built originally for grazing incidence diffraction and serving now as CRG-C spectrometer mainly as a test bed for "Spin-echo resolved grazing incidence scattering (SERGIS)"

	DI7		ADAM	EVA		
	Tof	Mon		Reflec	Diff	
Qmax. (Å <sup>-i</sup> )	4.0	1.5	5.4	0.4	4	
Qmin. (Å <sup>-i</sup> )	0.002	0.005	?	0.06	0.1	
Resolution $\Delta\lambda/\lambda$	.0012	0.04	.006		0.12	
Polarised neutrons		yes	yes	yes	yes	
Polarisation analysis		yes	yes	yes	yes	

#### Small angle scattering instruments

In DII and D22 the ILL possess the world's most powerful small-angle neutron scattering instruments.

**D11**, situated on the vertical cold source was one of the first instruments at the ILL to come into operation in 1972. It has been continuously refurbished and has maintained its foremost position in the field. Using its longest sample-

detector distance of 36.7m (180 m from the reactor) it is possible to make measurements at momentum transfers, Q, down to  $5 \times 10^{4} \text{\AA}^{-1}$ .

**D22**, commissioned in 1995, operates on the horizontal cold source where it benefits from the slightly higher flux and increased guide area. The high flux, combined with a detector allowing count-rates of up to  $2 \times 10^6$  n/s make it particularly attractive for kinetics experiments. Polarised neutrons are also available on D22.

	DII	D22
Qmax. (Å-1)	0.44	1.0
Qmin. (Å <sup>-1</sup> )	5 x 10⁴ (17Å, 36.7m)	10 <sup>-</sup> ³ (25 Å, 17.6m)⁴
Qmax./Qmin in one setting	7	25
Maximun flux on sample at lowest resolution (n.cm <sup>-2</sup> /s)	3.2 × 10 <sup>7</sup>	1.2 × 10 <sup>8</sup>
Max. count rate (10% losses) n/s <sup>1</sup>	105	2 x 10°

#### Diffractometers

The LSS group runs three diffractometers each fed by neutrons from the vertical cold source.

**D16** is a 2 or 4 axis diffractometer specialized in the study of partially ordered systems such as stacked membranes or intercalated layers. The vertically

focusing pyrolytic graphite monchromator can deliver beams of 4.5 or 5.6Å wavelength with good  $\Delta\lambda\lambda$ . With its 256 x 256 mm position sensitive detector it is ideal for the study of structures of around 50Å periodicity. D16 may also be used for small-angle scattering and has been used for reflectivity studies. **LADI** is a diffractometer for macromolecular crystallography built and operated jointly with EMBL. It exploits the "quasi-Laue technique" whereby a



### Large Scale Structures Instruments



broad band of neutrons from 2 - 4 Å wavelength, supplied by a multilayer monochromator, is incident upon the sample stimulating simultaneously a very large number of Bragg reflections. The scattered neutrons are detected on a cylindrical neutron sensitive image plate subtending a solid angle of about  $2\pi$ . In this way diffraction patterns from unit cells up to ~10° Å<sup>3</sup> can be measured in a reasonable time from crystals of ~1mm<sup>3</sup>.

A very similar instrument operating on a thermal beam, VIVALDI, is available in the Diffraction Group.

**DB21** is a 4-circle diffractometer for low resolution biological crystallography built and operated jointly with EMBL. It is designed to study single crystals of biological macromolecules using the contrast variation technique to visualize parts of the structure, such as detergent in membrane protein crystals, which may be invisible in classical X-ray crystallography. Using a 7.56Å beam from an intercalated graphite monochromator DB21 can measure data from unit cell up to ~400Å to a minimum d-spacing of ~10Å. Experiments are usually long (several days per contrast) but may only require moderately large crystals (~0.1mm<sup>3</sup>)

	D16	DB21	LADI
Qmax. (Å-1)	2.4	1.2	3.0
Qmin. (Å <sup>-i</sup> )	0.025	0.2	.2
Resolution $\Delta\lambda/\lambda$	.01	.03	.082
Typical sample size	10 x 30 mm	0.1 mm <sup>3</sup>	I mm <sup>3</sup>
Max. flux on sample n.cm <sup>-2</sup> /s	~ 107	1.7 x 10 <sup>6</sup>	3 × 10 <sup>7</sup>

#### Sample environment

A wide range of sample environments is available for the LSS instruments. Many are interchangeable between the various instruments and special usersupplied sample environments may be installed but the appropriate instrument responsible or local contact should be consulted in advance of experiments to determine whether this is possible. For details of sample environment consult the individual instrument pages.

	DI7	ADAM	EVA	DII	D22	DI6	DB21	LADI
Sample changer: -10 – 70°C (in air)	x			x	x	x		
Vacuum sample changer				x				
Heatable sample changer 30-250°C				×	x			
T control by water both 10 70°C								
T control by water bath -10 = 70 C	X	x	X	X	X	X	X	
Displex		x	x					x
Cryostat I.2 – 300K	x	x		x	x			
Dilution fridge	x	×		×	×			
r							1	
Furnace	x	x		×	×			
Cryomagnet	x	x		x	×			
Electromagnet	×(<1,5T)		×(<0,5T)	×(<1,2T)	×(<1,2T)			
Polarised incident beam possible	x	x	x		x			
Polarisation analysis possible	×	x	x		projet			
Pressure cell			×	~	×	×		
			~	^	~	~		
Couette shear cell				x	x			
Humidity cell						x		
Bohlin Viscometer/shear				x	x			
Stopped-flow apparatus	x			x	x			
Humidity chamber	×					x		
Robot				x	x			
4-circle						х	standart	

# Time-of-flight spectrometers

#### Time-of-flight and high-resolution group

The mission of the time-of-flight and high-resolution (TOF-HR) group consists of providing the best possible experimental conditions for the investigation of excitations over as wide a range in energy and momentum transfer as possible. The ensemble of TOF-HR instruments allows the study of the motion of matter in a more or less continuous way from fractions of a picosecond up to nearly a microsecond. Many scientists fully exploit this wide range by combining medium-resolution time-of-flight with high-resolution backscattering or spinecho experiments. The CRG-instruments play an important role by extending the space and time regions accessible.

TOF-HR instruments cover practically all branches of modern science that require information on the motion of atoms or molecules including nano-science and biophysics. The excitations studied range from high-frequency vibrations in carbon nanotubes to long-range diffusion in zeolites. A large part of the experimental program is dedicated to magnetic fluctuations. While three-axis spectrometers excel in obtaining detailed information on single excitations, time-of-flight machines perform best when a rather complete coverage of  $(Q,\omega)$ -space is required. This is generally the case for liquids and disordered materials and systems displaying low-dimensional magnetic correlations. Even in investigations of single crystals, exciting questions of current interest strive for information over the entire excitation spectrum.TOF-HR instruments perform very well in this area, in particular, when they are equipped with position sensitive detectors.

Experiments on TOF-HR spectrometers profit from a wide range of sample environments. Sub-Kelvin temperatures may be combined with magnetic fields. There are several dedicated high-temperature furnaces as well as specially adapted highpressure cells. The instruments are designed such that they facilitate the installation of ancillary equipment like shear and stress-cells, optical pumping devices or controlled humidity chambers.

The TOF-HR group together with the Scientific Computing group maintains an extensive suite of data analysis software.

TOF-HR instruments can be **classified** as follows:

- I. The time-of-flight instruments IN4, IN5 and IN6 as well as the CRG instrument BRISP
- 2. The diffuse scattering instrument D7
- 3. The high-resolution spin-echo instruments IN11 and IN15
- 4. The high-resolution backscattering instruments IN10, IN16 and the CRG instrument IN13
- **IN4** is the thermal time-of-flight spectrometer with the highest flux in the world. It is particularly suited for studies at low temperatures or over very extended Q-regions where a high incoming energy is required e.g. to study excitations in neutron energy loss mode. Typical scientific examples are the temperature dependence of structural and magnetic excitations in superconductors.
- **IN5** is currently the world's highest-flux cold neutron timeof-flight instrument. It has a large dynamic range and perfect resolution function. IN5 allows the study of excitations and relaxations from about 10  $\mu$ eV to 10  $\mu$ eV (and even 100  $\mu$ eV in energy gain mode). It thus connects directly to ILL's highresolution backscattering instruments on the low-frequency side and to IN4 on the high-frequency end. The secondary spectrometer of IN5 is currently being redesigned and will in the future host position sensitive detectors.
- Due to time-focusing the cold time-of-flight spectrometer IN6 offers extremely low background coupled with a very high counting rate. **IN6** thus provides unrivalled conditions for studying kinetic processes, small samples or tiny intensities. First single crystal experiments have been done successfully on IN6. IN6 will soon be upgraded from moderate to high magnetic fields offering even better flexibility for the study of magnetic excitations in powder and single crystal samples.
- **BRISP** is the worlds only dedicated neutron Brillouin-spectrometer and the only one in the thermal region (The Brillouin options on IN5 and NEAT work with cold neutrons, and that at PHAROS works with epithermal neutrons). BRISP is currently in its final commissioning stage. It must be expected that it will contribute new insight into liquids and glass dynamics as well as magnetic and critical scattering.





### Time-of-flight spectrometers

- **D7** is on a cold guide and permits 3-directional (X,Y,Z) polarisation analysis on a multidetector spectrometer. It offers unprecedented possibilities in the study of magnetic disorder and paramagnetic scattering, where any non-magnetic contribution can be separated out. The completion of two more new supermirror analyzer banks and the addition of a new Fermi-chopper will transform D7 into the world's only time-of-flight spectrometer with full polarization analysis.
- INII is the world's leading medium-resolution spin-echo instrument and combines high flux with exceptional flexibility. Structural and magnetic relaxations are measured as a function of Fourier-time. The high counting rates and an angular coverage of 30 degrees offered by the wide-angle secondary arm (INIIC) is highly appreciated and requested by the users.
- IN15 is the spin-echo instrument with the longest Fourier times and highest flux in the world. Optimized for long wavelength neutrons, it is particularly adapted to study slow processes up to a fraction of a ms at low Q scattering vectors. IN15 is jointly operated by the FZ-Jülich, the HMI and ILL. IN11 complements IN15 in the high Q range using shorter wavelength neutrons.
- **IN16** is the world's most sensitive back scattering instrument. It equally has the world's highest resolution (0.4 meV using polished Si<111> analysers). A new Doppler drive will increase the dynamic range (presently  $\pm$  14  $\mu$ eV). IN16 is currently undergoing a major upgrade based on the concept of phase space transformation.
- **IN10** was ILL's first pioneering backscattering spectrometer. Presently it is used as a complement to IN16. The heated monochromator option IN10B allows for high-resolution measurements at appreciably larger energy transfers.
- The CRG **IN13** is the world's only thermal backscattering spectrometer. It has largely been turned into an instrument dedicated to the investigation of biological systems, but equally serves other communities.



#### **Three-Axis Spectrometers (TAS)**

The Three-Axis Spectrometer is one of the most versatile instruments for neutron inelastic scattering studies of condensed matter. It is designed, primarily, to investigate the collective motion of atoms and that of their magnetic moments in single crystalline samples.

#### How does it work?

The name refers to the three axes of the monochromator, sample and analyser crystals, the orientation of which can be varied independently. The neutrons emerging from a reactor beam tube or from a neutron guide have a broad distribution of energies. A single crystal monochromator mounted inside the primary shielding selects a beam of neutrons in a narrow energy band by means of Bragg diffraction. The diffracted beam impinges upon the sample, which is mounted on the sample table. The neutrons are generally scattered by the sample in all directions. In the scattering process the neutrons may conserve their energy - elastic scattering - or they may gain or lose energy - inelastic scattering. The analyser is positioned to select a particular scattering direction. Varying the angle of Bragg reflection from the analyser crystal scans the energy of the neutrons entering the analyser. The neutrons passing through the analyser – with an energy determined by the analyser position - are finally counted in a detector. In short, this measuring technique allows the determination of the energy transfer between the neutrons and the sample, as a function of scattering angle, which itself is related to the momentum transfer.

#### What is studied?

The neutron scattering from single crystals is limited by selection rules, which connect the scattering in a particular direction with momentum transfer Q to a certain change in energy  $\eta\omega.$  The measured intensity as a function of  ${\bm Q}$  and  $\omega$ is mainly determined by two factors: the resolution of the instrument, and the dynamic scattering function  $S(\mathbf{Q},\omega)$ . In general terms,  $S(\mathbf{Q},\omega)$  corresponds to the Fourier transform of correlations in space and time of atomic positions or magnetic moments. Three-axis spectroscopy provides information on the atomic force constants and interaction potentials, and also on the nature of the elementary excitations in the solid. Harmonic excitations such as phonons and magnons give a sharply peaked scattering function and  $S(\boldsymbol{Q}, \boldsymbol{\omega})$  describes the phonon or magnon dispersion curve. Other excitations are short-ranged and short-lived, and hence less well-defined in Q- and  $\omega$ -space. Some current scientific examples are given on the instrument pages; those cover research into anharmonic phenomena near phase transitions, excitations in liquids and noncrystalline materials, excitations in low-dimensional magnets and exotic magnetisation dynamics observed in strongly correlated electron systems like hightemperature and heavy-fermion superconductors.

#### Advantages of Three-Axis Spectroscopy

The unique power of Three-Axis Spectroscopy for the study of excitations in condensed matter is due to the fact that it is possible to perform selected scans to explore specific sections in  $\mathbf{Q}$ - and  $\omega$ -space. One outstanding advantage is the ability to perform constant  $\mathbf{Q}$ -scans, as normally a  $\omega$ -spectrum for a constant value of  $\mathbf{Q}$  can be calculated theoretically. But generally any scan in  $\mathbf{Q}$ - and  $\omega$ -space can be performed, limited only by scattering kinematics due to the inherent relation between momentum and kinetic energy of the neutron. The relevant quantities for a Three-Axis Spectrometer, operating in a certain energy range, are luminosity, resolution width and the signal-to-noise ratio.

### NEUTRONS FOR SCIENCE

#### How does it compare to other experimental techniques?

Neutron inelastic scattering is a unique tool for several reasons. Principally, the magnetic dynamics are accessible. Atomic vibrations in compounds with disparate masses can be effectively probed. Element-specific dynamics can be extracted using isotope contrast in the scattering.

In special cases, however, the use of other probes may be preferable. To overcome restrictions from scattering kinematics when working at small momentum transfer as imposed by disordered systems such as liquids and glasses or if very small samples volumes are available, X-ray inelastic scattering might be beneficial. At small momentum transfer, Brillouin and Raman light scattering might be used to investigate acoustic and optic phonons.

Even for neutron inelastic scattering itself other experimental approaches are available. In particular, for mapping  $S(\mathbf{Q},\omega)$  over large areas of reciprocal space or for the investigation of systems, in which the vector property of momentum transfer is less important (as in the case of low-dimensional systems), the neutron Time-of-Flight techniques may prove more efficient than the  $\mathbf{Q}$ - and  $\omega$ -selective Three-Axis Spectroscopy.

#### **Further considerations**

Three-Axis Spectrometers can host a wide range of sample environments such as cryomagnets for high vertical and horizontal fields, high-temperature furnaces, very low-temperature cryostats or a vacuum box for small-angle scattering in addition to conventional closed-cycle refrigerators and cryostats. Their low instrumental background may be advantageous for diffraction experiments with small samples and weak signals. Three-axis spectrometers are also used in conjunction with the inelastic spin-echo technique, and further instrumental options such as one- or three-dimensional polarisation analysis are available. Further details are indicated on the instrument pages and are available on request from the instrument scientists.

#### Three-Axis Spectrometer at ILL

ILL supports four scheduled instruments - INI, IN8, IN14 and IN20. Limited beamtime for users is available on the two CRG instruments IN12 and IN22, as well as on one test instrument IN3, which is otherwise used for instrumental developments. For user-friendliness, the instruments offer similar flexible control software and equipment such as analysers, collimators and filters. Details for each instrument, including its instrumental options and specificities are indicated on the corresponding Yellow-Book pages.

**IN I**, the Three-Axis Spectrometer on the hot-source beam tube H8, is used for measuring scattering with high energy transfer, ultimately up to I eV, at variable momentum transfer. The high incident energies overcome limitations due to scattering kinematics as required in studies of magnetic excitations and atomic dynamics in liquids.

**IN3** is a classical Three-Axis Spectrometer installed on the thermal guide H24. It is set-up for tests in the thermal energy range, up to 30 meV, with resonant spin echo option as well as a multiplexed secondary spectrometer.

**IN8** is a high-flux thermal-neutron spectrometer installed on the thermal beam H10 in the reactor hall. It is designed for inelastic scattering experiments on single crystals over a wide range of energy (up to about 100 meV) and momentum transfer.

### Three-Axis Spectrometers

**IN12** is a CRG instrument installed on the cold neutron (curved) guide H142 used mainly with incident energies smaller than 6.5 meV for high-resolution studies on samples requiring a low instrumental background. IN12 may be used with polarisation analysis.

**IN14** is a spectrometer installed on the cold neutron guide H53. Due to its proximity to the source, it has sufficient flux to extend the range of cold Three-Axis Spectroscopy to incident energies of about 15 meV. For polarised neutron work, a supermirror bender on the primary spectrometer is used in combination with a Heusler analyser. **IN20** is a Three-Axis Spectrometer installed on the thermal beamtube H13 in the reactor hall, covering a similar range of energy and momentum transfer to IN8. It is equipped with focusing Heusler monochromator and analyser, which offer high count-rates in experiments with ID- and 3D-polarisation analysis. It can host neutron spin-echo equipment for high-resolution quasi-elastic and inelastic experiments.

**IN22** is a CRG instrument installed on the super-mirror thermal guide H25. It covers the energy range up to about 50 meV combined with a low instrumental background. It can be set up for experiments with ID- and 3D-polarisation analysis.



#### **Nuclear and Particle Physics Instruments**

The Nuclear and Particle Physics Group operates 4 scheduled instruments: Two instruments (PN1- fission spectrometer "LOHENGRIN" and PN3- high resolution gamma facility "GAMS") deal mainly with nuclear physics and applied nuclear physics aspects. Two other ones (PF1- intense cold neutron beam facility and PF2 - ultracold neutron facility) are covering mainly neutron particle physics aspects. Additionally to the scheduled instruments there exists a thermal neutron interferometer (S18) which is operated as a CRG C instrument. The former cold neutron position at H53 (previously called PF1A) is now operated as a CRG C instrument, devoted to a new generation of neutron EDM measurements.

The recoil mass separator for unslowed fission products **LOHENGRIN** uses fission products originating from a source of fissile isotopes placed in a beam tube (H9) near the core of the reactor. Specific fission products are selected by a combination of a magnetic and an electric sector field whose deflections are perpendicular to each other. The freely recoiling fission products are analyzed according to the energy over ionic charge (E/q) and mass over ionic charge (A/q). The main directions of research on PNI were in the past centered around studies of the fission process but are now more and more concentrated on spectroscopy of very neutron-rich nuclei. To this purpose the spectrometer was equipped with a clover-detector array.

The high resolution gamma ray facility, **GAMS**, makes use of the fact that at the ILL reactor one can obtain extremely high specific activities when exploiting thermal neutron capture at an in-pile target facility. This allows to aim for the application of gamma spectroscopy with the highest possible energy resolution. Gamma rays emerging from the in-pile targets are successively diffracted by two crystals (either flat or bent). The diffraction angles are controlled by high resolution interferometers. The technique allows to obtain a resolution of  $\Delta E \gamma / E \gamma$  which approaches the 1 ppm level. Many studies on this facility have aimed to contribute to our understanding of the structure of nuclei. Others are devoted to the determination of standards and fundamental constants. The measurement

of Doppler profiles induced by the recoil, which nuclei experience when they emit gamma rays allows to i) deduce information about short lifetimes of excited nuclear states and gives ii) insight into the low-energy slowing down process of atoms in matter.

The intense cold polarised neutron beam facility **PF1** is installed at the end position of the new cold guide H113. The guide cross section is  $6x20 \text{ cm}^2$  and the neutron flux density is  $1.4\times10^{10}$  neutrons cm<sup>2</sup>s<sup>-1</sup>. Neutron particle physics experiments which have recently been carried out with cold polarised neutrons concerned mainly neutron lifetime determination by using proton trapping, diverse measurements of neutron decay asymmetry coefficients and studies of parity and time reversal violation effects on polarised neutron induced fission.

The ultracold neutron facility **PF2** was built by TU Munich in collaboration with ILL.At the experimental positions it provides a density of 50 cm<sup>3</sup> of ultracold neutrons (UCN) with speeds less than 5m/s. UCN are produced at the top end of a vertical guide where neutrons with speeds of 50m/s are converted by the so-called Steyerl turbine into UCN with about 5m/s. The UCN are then led by horizontal guides to several experiments in parallel. There is also an output for very cold neutrons (VCN) with a wavelength of 100Å. As the neutron is electrically neutral this offers specific experimental advantages such as (for UCN) the option for storage in traps. Consequently the majority of measurements carried out a PF2 use this feature. Experiments carried out recently on this facility concerned - amongst others - the measurement of the neutron lifetime, the measurement of the neutrons.

The CRG C instrument **S18** is a perfect crystal neutron interferometer which can also be configurated as a high resolution Bonse Hart camera. This instrument can be used for precise measurement of neutron scattering lengths and for basic neutron quantum optics studies and related phenomena. For this latter, please refer to the ILL web-site.