

# **INELASTIC SCATTERING**

## **I**

### **Triple-axis instruments**

## **“TRIPLE AXIS EQUIPMENT POOL”**

*The triple axis group has a pool of sample environments available for use on  
1T1, 2T1, 4F1, 4F2 and G 4-3.*

*Request for their use are made to the local contact.*

- ❁ *Graphite filter*
  
- ❁ *Furnace → 200 - 1800°C*  
*Furnace → 20 - 400°C*
  
- ❁ *Nitrogen flow cryofurnace → 80 - 600 K*  
*He Cryogenerators → 10 - 300 K*  
*Top loading He cryogenerators → 10 - 300 K*  
*<sup>4</sup>He cryostats → 1.5 - 300 K*  
*Dilution insert → 100 mK - 6 K*
  
- ❁ *Electromagnet horizontal or vertical field      0 - 1.1 Tesla*  
*Helmoltz coils vertical field → 0 - 0.17 T*  
*Cryomagnet vertical field      → 0 - 6 T*
  
- ❁ *Pressure cryostat → 0 - 300 K with :*
  - ♦ *He hydrostatic pressure cell (isotropic)      → 0 - 5 Kbar*
  - ♦ *Clamp hydrostatic pressure cell (isotropic) → 0 - 16 Kbar*
  - ♦ *Clamp hydrostatic pressure cell (windows) → 0 - 25 Kbar*
  
- ❁ *Electric field insert (0 - 4 kV) for top loading cryogenerator*

Beam tube : .....	Tangential 40 x 80 mm <sup>2</sup>
Monochromator : .....	PG 002, Cu 111, Cu 220
Incident wavelength : .....	$0.6 < \lambda$
Incident energy resolution : .....	Variable, typical 5 %
Analyzer : .....	PG 002
Collimations - In pile : .....	40', 25', 15'
Collimations - Mon-sample : .....	66', 49', 31', 14'
Collimations - Sample-an.: .....	75', 49', 30', 23', 20', 12'
Collimations -An.-det. : .....	75', 49', 30', 23', 20', 12'
Range of monochromator	
take-off angle : .....	$15^\circ < 2\theta_m < 80^\circ$
Range of scattering angles : .....	$-50^\circ < \varphi < 125^\circ$
Range of detector angle : .....	$-100^\circ < 2\theta < 100^\circ$
Range of goniometer arcs : .....	$\pm 20^\circ$
Distance goniometer-center of beam : .....	$170 \pm 30$ mm
Flux at specimen : .....	Strongly dependent on collimation and energy
Beam size at specimen : .....	Defined by diaphragm (30 x 40 mm <sup>2</sup> )
Momentum transfer : .....	$0.3 - 10 \text{ \AA}^{-1}$
Energy transfer : .....	0.8 - 100 meV
Detector : .....	<sup>3</sup> He (upright, area : 50 x 100 mm <sup>2</sup> )

#### Ancillary equipment

★ "Triple Axis Equipment Pool"  
(see on front of this chapter)

This triple-axis spectrometer is installed on the thermal neutron beamline and is dedicated to the study of inelastic neutron scattering due to collective excitations in condensed matter. The triple-axis geometry allows measurements of the scattering function  $S(\mathbf{Q}, \omega)$  in single crystals at well defined values of the reciprocal lattice vector  $\mathbf{Q}$  and the energy,  $\omega$ . In the past the spectrometer has been successfully utilized for investigations of lattice dynamics (phonons) and magnetic excitations (magnons and more exotic excitations in strongly correlated electron systems) in a wide variety of materials. The spectrometer has vertical and horizontal focusing of both the monochromator and analyzer, which optimizes the observed intensity at the expense of wavevector resolution. This feature allows one to obtain useful results even with relatively small samples.

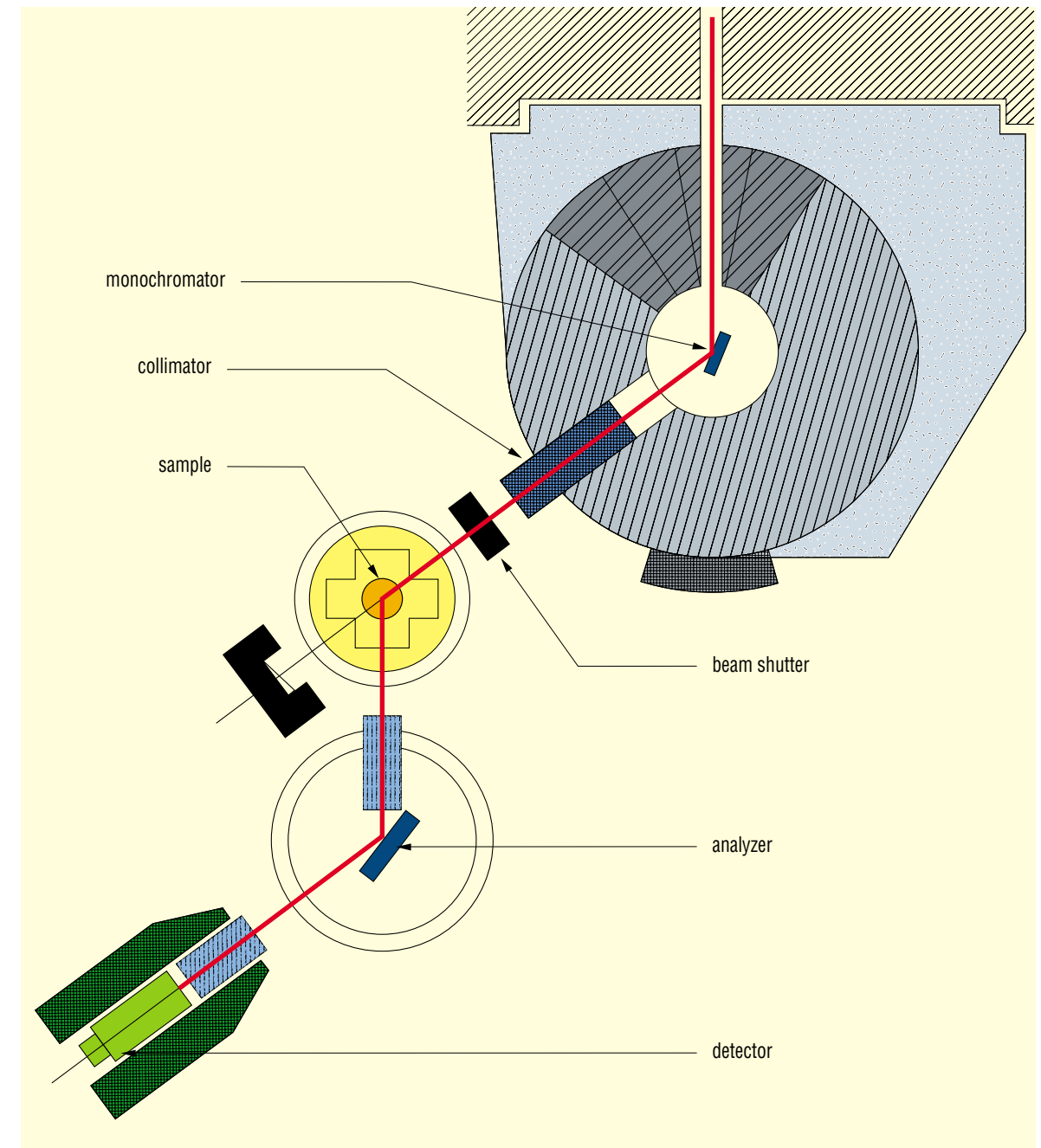
The main components of the instrument are the monochromator stage, the sample stage, and the analyzer stage. Neutron trajectories are defined by Soller collimators. Rutherford collimators with replaceable blades are available as well. The instrument is fully computer-controlled, with the software allowing scans in and out of the scattering plane.

The monochromator stage allows the use of three

different monochromators (PG002, Cu111, and Cu220). All are vertically and horizontally focusing in order to increase the neutron flux at the sample position. The horizontal curvature for all monochromators, and the vertical curvature for the PG002 and Cu220 monochromators are fixed. The Cu111 monochromator has a variable vertical curvature, to achieve optimal focusing for a wide range of incident neutron energies. The monochromators, which are mounted inside a mobile concrete drum, can be interchanged by remote control.

The rotating sample stage is equipped with a double goniometer as well as translation stages, which allow one to tilt the sample in any direction as well as to adjust the horizontal and vertical positions of the sample.

The analyzer stage can be used with three different analyzers (flat PG002, focusing PG002). They are mounted on small individual modules that one can install in reproducible orientations. The focusing PG002 monochromator has fixed vertical curvature and variable horizontal curvature. It contains two remote-controlled slits, a vertical one before the analyzer crystal and a horizontal one before the detector. These can be used to optimize the signal to background ratio as well as the analyzer resolution.



General layout of the spectrometer 1 T1.

*This spectrometer has been built by German scientists and is operated in collaboration between the INFP Karlsruhe and the L.L.B*

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Beam tube .....	Tangential on thermal source channel 2 T : 5 x 12 cm <sup>2</sup>
Monochromator .....	Option unpolarized neutrons : 1) PG 002, $\eta \sim 0.6^\circ$ 15 x 13 cm <sup>2</sup> 2) Cu 111, $\eta \sim 0.8^\circ$ 15 x 13 cm <sup>2</sup>
Monochromator .....	Option polarized neutrons : Heusler, $\eta \sim 0.5^\circ$ 14 x 13 cm <sup>2</sup> All monochromators have a vertical curvature automatically adapted to the incident neutron energy
Analyzer .....	Option unpolarized neutrons PG 002, $\eta \sim 0.6^\circ$ 11 x 9 cm <sup>2</sup>
Analyzer .....	Option polarized neutrons Heusler, $\eta \sim 0.5^\circ$ 11 x 10 cm <sup>2</sup> Both analyzers have an horizontal curvature automatically adapted to the final neutron energy. The PG 002 has additionally a vertical curvature which can be manually changed
Beam size at specimen .....	3 x 4 cm <sup>2</sup>
Incident energy .....	8 - 140 meV (unpolarized neutrons) 8 - 70 meV (polarized neutrons)
Momentum transfer .....	0 - 8 Å <sup>-1</sup>
Energy transfer .....	0 - 100 meV (unpolarized neutrons) 0 - 55 meV (polarized neutrons)
Detector .....	<sup>3</sup> He
Typical energy resolution : .....	$\delta\omega \approx 0.8$ meV at $k_f = 2.662$ Å <sup>-1</sup> ( $E_f = 14.7$ meV) $\delta\omega \approx 3.5$ meV at $k_f = 4.1$ Å <sup>-1</sup> ( $E_f = 35$ meV)
Collimation : .....	10' to 60'
Range of scattering angle : .....	0° ≤ 2θ <sub>s</sub> ≤ 360° (± 20° double goniometer)
Ancillary equipment	★ "Triple Axis Equipment Pool" (see on front of this chapter)

This spectrometer has been built to study inelastic scattering from condensed matter. This corresponds to collective excitations either from the lattice (phonons) or from magnetically ordered systems (magnons). The triple axis spectrometer can be also used to study the dynamics in more disordered samples such as amorphous systems and spin-glass as it fully measures the scattering function  $S(Q, \omega)$  over a wide energy range and at any position in the reciprocal space. For instance, in strongly correlated electron systems such as high- $T_c$  superconductors, one can fully determine the generalized spin susceptibility. By selecting the neutron polarization one can further separate magnetic scattering from lattice contributions. A polarized option can be used on 2 T.

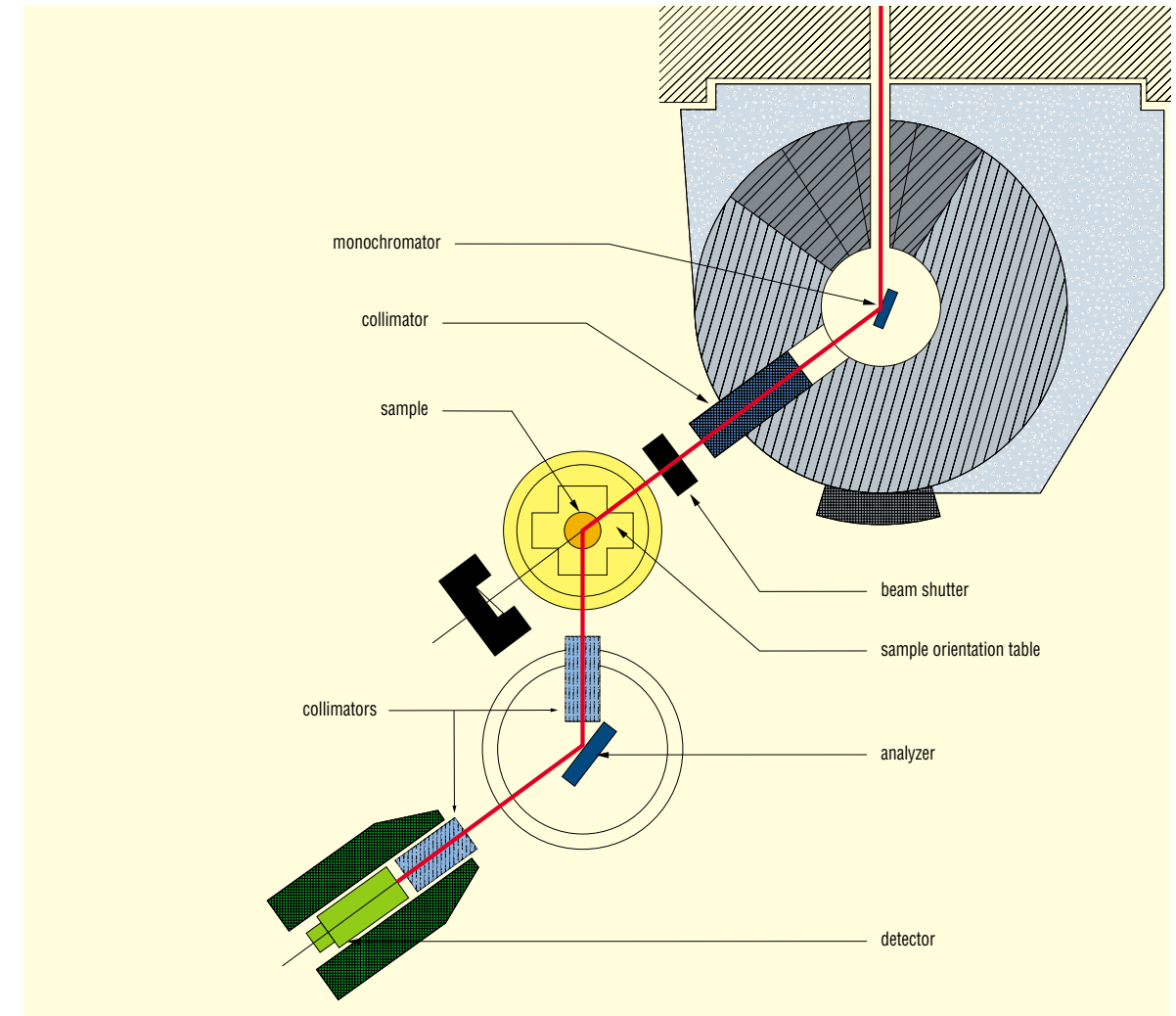
The spectrometer is composed of 3 elements, each rocking around an axis :

- 1) The first axis is a monochromator to select neutrons with specific incident energy. This part is inside a mobile concrete block (called drum).
- 2) The second axis is related to the sample to be studied which can be oriented in any direction.

- 3) The third axis is an analyzer allowing to determine the final neutron energy. After being selected by the analyzer, the neutrons are finally measured by a <sup>3</sup>He detector located in a closed block in order to reduce the background level.

With the polarized option, the neutron polarization is selected by a monochromator and an analyzer, both made of an Heusler alloy which allows to select only neutrons with a specific spin state. A coil flipper is used to reverse the neutron spin state and select each component of the neutron cross-section.

Horizontal guide fields are installed in the monochromator drum up to the sample position and vertical guide fields between sample to the analyzer. A small field (~ 15 Oe) of arbitrary orientation can be applied at the sample position using an Helmholtz coils system consisting of three coils on a cylinder surface and two circular coils.



General layout of the spectrometer 2 T1.

On different segments of the neutron path (reactor-monochromator, sample-analyzer, analyzer-detector), Soller collimations can be placed to choose the angular divergence and improve the spectrometer resolution. All equipment of the triple axis pool can be installed at the sample position on the goniometers system (Cryostat (with dilution insert), Close-cycle refrigerator, Vertical Magnetic coil, Furnaces, Pressure cell...).

Due to its implementation on a thermal neutron beam, this spectrometer is well adapted for studying excitations over a wide energy range 1.5 to 100 meV (0.3 to 25 THz) which covers the typical range of phonon and magnon branches in single crystals.

All triple-axis measurements can be fitted on line by an homemade fitting programme. This programme performs a convolution product of all standard neutron cross-sections by the spectrometer resolution function.

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Areas are given.....Width x height  
 Beam tube.....Left beam of tangential channel 4F,  
 aimed to cold source SF2  
 Radiant surface : 8 x 15 cm<sup>2</sup>  
 Output of the channel : 4 x 7 cm<sup>2</sup>  
 Monochromator.....Double monochromator set-up  
 M 1 : Pyrolytic graphite  $\eta = 0.4^\circ$  11 x 8.5 cm<sup>2</sup>  
 allows controlled vertical focussing  
 M2 : Pyrolytic graphite  $\eta = 0.8^\circ$  11 x 8.5 cm<sup>2</sup>  
 Analyzer.....Pyrolytic graphite  $\eta = 0.4^\circ$  6 x 6 cm<sup>2</sup>  
 Horizontally bent pyrolytic graphite 6 x 6 cm<sup>2</sup>  
 Incident wavelength.....1.8 <  $\lambda$  < 6 Å  
 Incident energy resolution.....300 >  $\delta E$  > 3 GHz  
 Collimation (horizontal).....in pile : 50', 30', 15'  
 between monochrom.(optional) : 50'  
 others : 60', 40', 20', 10'  
 Range of monochromator angle (M2).....31° < 2 $\theta$  < 149°  
 Range of scattering angle.....-5° ≤  $\phi$  ≤ 140°  
 Range of analyzer angle.....0 < 2 $\theta_A$  ≤ 150°  
 Range of crystal orientation.....0 ≤  $\psi$  ≤ 360°  
 ± 20° double goniometer  
 Detector.....<sup>3</sup>He  
 Beam size at specimen.....4 x 8 cm<sup>2</sup>  
 Background.....~0.5 count/minute

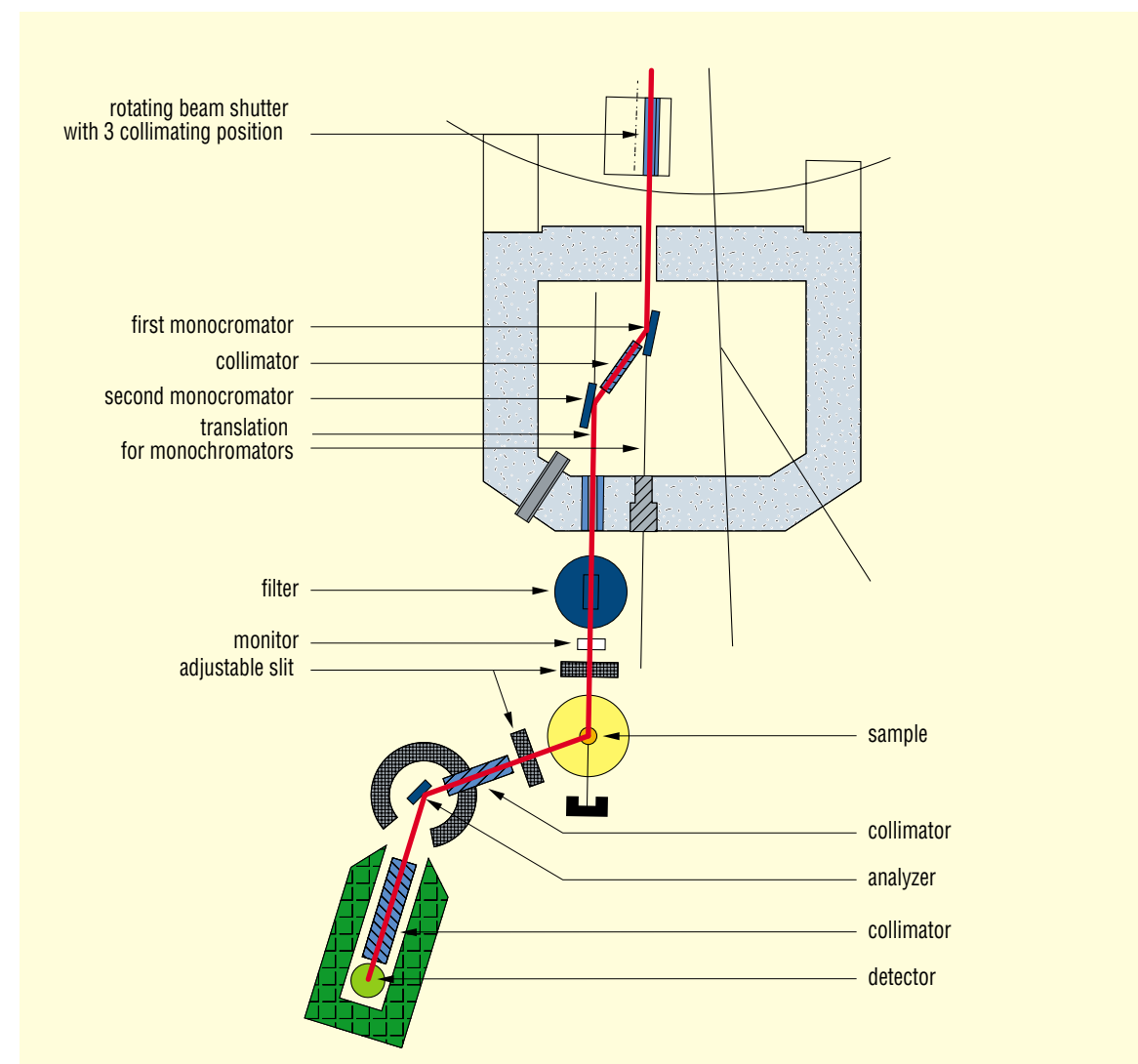
ki (Å <sup>-1</sup> )		1.05	1.55	2.66
Best energy resolution (FWHM at $\omega = 0$ )	(GHz)	3.6	20	120
	(microeV)	15	80	500
Best wave-vector resolution (FWHM)	(Å <sup>-1</sup> )	3.10 <sup>-3</sup>	5.10 <sup>-3</sup>	9.10 <sup>-3</sup>
Flux at sample (n/cm2 sec)		-	3.5x10 <sup>6</sup>	14x10 <sup>6</sup>

Ancillary equipment

- ★ Be filter (77 K)
- ★ Neutron polarization and polarization analysis
- ★ "Triple Axis Equipment Pool" (see on front of this chapter)

4F1 and 4F2 are twin 3-axis spectrometers with very similar characteristics which are fed by a liquid-hydrogen cold neutron source  
 A full description of both spectrometers is given on the 4F2 page.  
 As an option, 4F1 can be equipped for polarized neutrons with polarization analysis.  
 The four intensities I<sup>++</sup>, I<sup>+-</sup>, I<sup>+0</sup>, I<sup>-0</sup> corresponding to neutron spin-flip and non-spin-flip processes can be measured sequentially.  
 This requires the installation of an additional shielded module between the monochromator and the sample, containing a filter, the polarizing supermirror and a Mezei flipper. The supermirror can be rotated to achieve optimal alignment, yielding a polarization efficiency of 98% with a reflectivity of 55% above  $\lambda = 3.5$  Å.

Vertical and horizontal guide fields are available.  
 The sample can be subjected to in a magnetic field:  
 • horizontal field up to 0.7 or 1.4 T (electromagnet), depending on the gap  
 • vertical field up to 0.14 T (Helmoltz coils) or 1.4 T (electromagnet) or 6T (cryomagnet)  
 • 3D-inclined guiding field of 1mT (cubic die magnet with 3 orthogonal windings).  
 The second flipper, made of a superconducting foil and a switched magnetic coil, is placed between the sample and the analyzer.  
 The horizontally curved Heusler analyzer performs both energy and polarization analysis.



General layout of the spectrometer 4F1

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Areas are given..... Width x height  
 Beam tube..... Right beam of tangential channel 4 F aimed to cold source SF2  
 Monochromator..... Double monochromator set-up  
 M1 : pyrolytic graphite  $h = 0.4^\circ$   
 11x8.5 cm<sup>2</sup> computer controlled vertical focussing  
 M2 : pyrolytic graphite  $h = 0.4^\circ$  11x8.5 cm<sup>2</sup>  
 Analyzer..... Flat pyrolytic graphite  $h = 0.4^\circ$  7.5x5 cm<sup>2</sup>  
 Horizontally curved pyrolytic graphite 6x6 cm<sup>2</sup>  
 Flat Ge (111)  
 Collimations..... In pile : 50', 30', 15'  
 between M1-M2 25' (optional)  
 others : 60', 40', 20', 10'  
 Range of monochromator angle.....  $31^\circ < 2\theta < 149^\circ$   
 Range of scattering angle.....  $-2^\circ < \phi < 150^\circ$   
 Range of analyzer angle.....  $-150^\circ < 2\theta_A < 150^\circ$   
 Range of crystal orientation.....  $0 < \psi < 350^\circ$   
 Beam size at sample..... 2 x 4 cm<sup>2</sup>  
 Detector..... <sup>3</sup>He  $\varnothing = 5$  cm  $h = 15$  cm  
 Incident wavelength (wave-vector).....  $2 < \lambda_i (\text{\AA}) < 6.3$  ( $3.2 > k_i (\text{\AA}^{-1}) > 1$ )  
 Scattered wavelength (wave-vector).....  $1.6 < \lambda_f (\text{\AA}) < 6$  ( $4 > k_f (\text{\AA}^{-1}) > 1.05$ )

$k_i (\text{\AA}^{-1})$	1.05	1.55	2.66
Maximum energy creation (THz)	-	0.75 (3 meV)	3.1 (12 meV)
Best energy resolution (Ghz)	2.3 (9 $\mu$ eV)	13 (50 $\mu$ eV)	80 (320 $\mu$ eV)
Typical energy resolution (Ghz)	7 (30 $\mu$ eV)	56 (220 $\mu$ eV)	300 (1,2 meV)
Maximum wave-vector transfer ( $\text{\AA}^{-1}$ )	1.9	3	5.1
Best wave-vector resolution ( $\text{\AA}^{-1}$ )	$3.10^{-3}$	$5 \cdot 10^{-3}$	$.9 \cdot 10^{-3}$
Flux at sample (n/cm2 sec.)	-	$3.5 \cdot 10^6$	$14 \cdot 10^6$

Ancillary equipment

- ★ Be filter (77 K)
- ★ "Triple Axis Equipment Pool" (see on front of this chapter)

4F1 and 4F2 are twin 3-axis spectrometers with very similar characteristics (see description below), which are fed by a liquid-hydrogen cold neutron source.

Polarized neutrons are only available on 4F1 (see 4F1 page). These spectrometers are designed for measuring dispersive excitations with low energy transfers ( $w < 4$  meV,  $n < 1$  THz) with a good resolution and a high flux (see Table).

They are well suited for measuring acoustic phonon dispersions, soft phonons, spin waves, quasi-elastic scattering, as well as for fine studies of modulated structures.

They are equipped with a double pyrolytic graphite monochromator, providing wavelengths between 6 and 2  $\text{\AA}$  ( $1.05 < k_i < 2.7 \text{\AA}^{-1}$ ). Available collimators are (60', 30', 15') before and (60', 40', 20', 10') after the monochromators. An optional collimator (25', 15') can be added between the two monochromators. The monochromator has a computer-controlled vertical focusing.

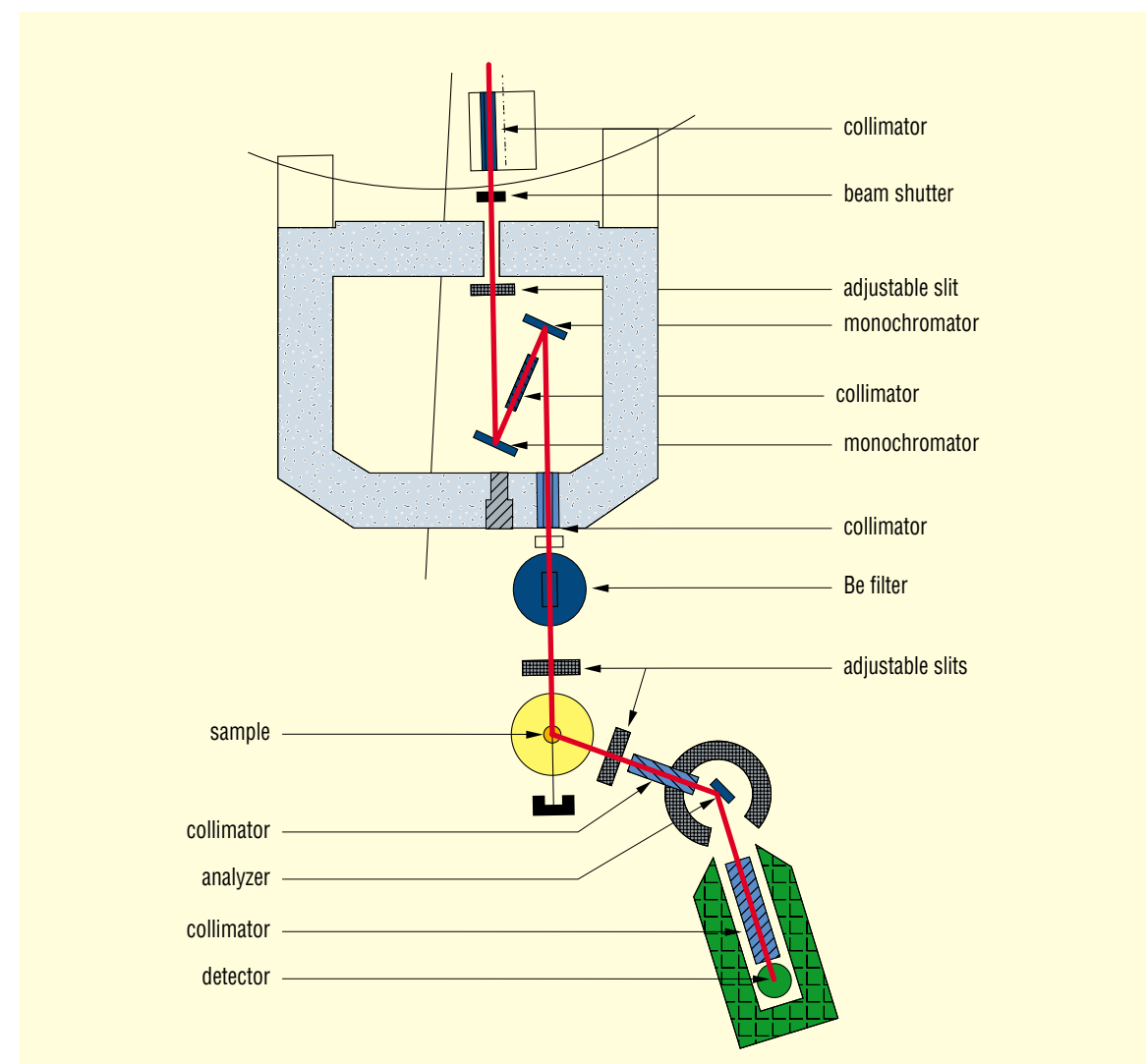
The incident beam can be filtered by a cooled Be or a graphite filter.

The pyrolytic graphite analyzer is normally used in a horizontally focusing geometry. In this mode, the curvature of the analyzer is controlled by the computer, and the collimators (60', 40', 20', 10') are replaced by wedge-shaped tunnels.

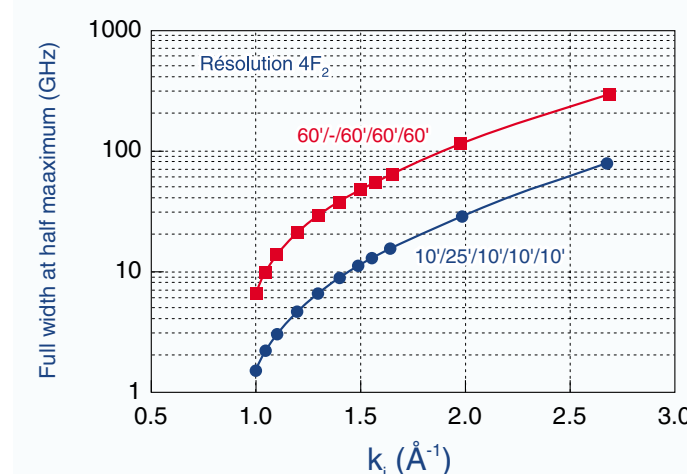
The sample table is equipped with two orthogonal non-magnetic goniometers, allowing tilts of  $\pm 20^\circ$ . Their upper face (serving as a support for the various sample environments) is located 270 mm below the axis of the beam.

The sample-to-monochromator and sample-to-analyzer distances can be adjusted to accommodate various sample environments.

The spectrometer is controlled by a SUN computer running under Unix/Solaris OS. It allows various data processing softwares, including fit and convolution programs, to be run in real time during the measurements.



General layout of the diffractometer 4F2



Energy resolution (GHz) as a function of the incident wave-vector  $k_i$ . Collimations are respectively: in-pile/M1-M2/M2-sample/sample-analyzer/analyzer-counter

Responsibles :

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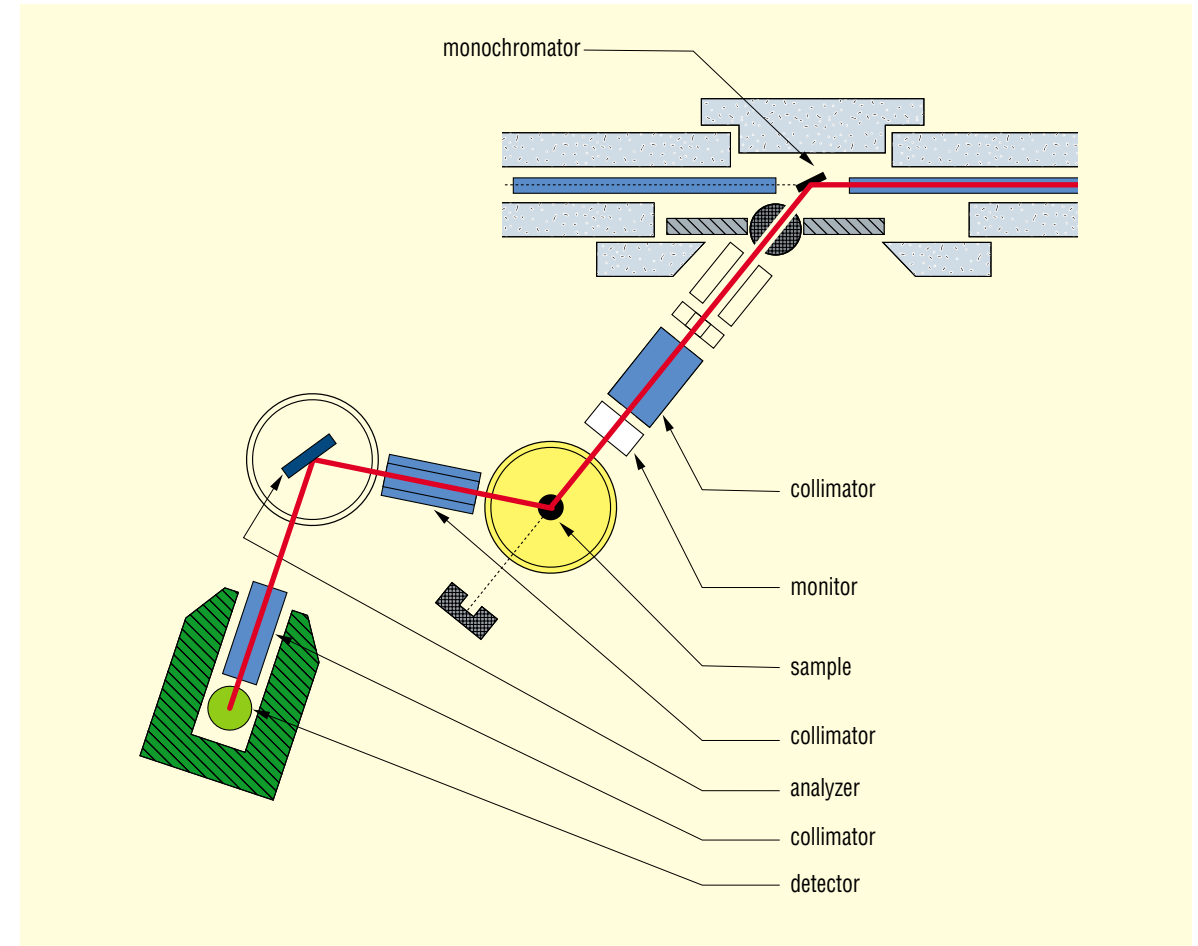
Beam tube .....	Neutron Guide G4 25 x 150 mm <sup>2</sup>
Monochromator .....	Pyrolytic graphite 75 x 150 mm <sup>2</sup>
Analyzer .....	Pyrolytic graphite 75 x 100 mm <sup>2</sup>
	Vertically bent (curvature is adjusted automatically)
Incident wavelength .....	0.235 < $\lambda$ < 0.6 nm
Incident energy resolution .....	0.005 < $\delta\omega$ < 0.2 THz
Collimations .....	Interchangeable, 60', 30', 10'
	on each arm after monochromator
Range of monochromator angle .....	40° < $2\theta$ < 140°
Range of scattering angle .....	-140° < $\phi$ < +140°
Range of analyzer angle .....	-155° < $2\theta$ < +155°
Range of crystal orientation .....	0 < $\psi$ < 360°
	Eulerian cradle or goniometer
Max. flux at specimen .....	5.10 <sup>5</sup> n/cm <sup>2</sup> sec ( $k_i = 18.5 \text{ nm}^{-1}$ )
Beam size at specimen .....	Width : 25 mm ; height 50 mm
→ Momentum transfer .....	0 - 30 nm <sup>-1</sup>
→ Energy transfer .....	0 - 3 THz
Detector .....	<sup>3</sup> He
<b>Ancillary equipment</b>	<ul style="list-style-type: none"> <li>★ Be filter (77 K)</li> <li>★ Furnace (20 - 1200°C)</li> <li>★ Multidetector : only in diffraction mode (without analyzer)</li> <li>★ <b>Triple Axis Equipment Pool</b> (see on front page of this chapter)</li> </ul>

On the one hand this spectrometer is used for the investigation of inelastic scattering at low energies with high resolution like measurements of dispersion curves of phonons and magnons, phonon softening, etc... On the other hand it serves for elastic studies on problems where good peak/background ratio, suppression of inelastic scattering and high resolution of momentum and/or energy transfer are essential.

The neutrons are extracted from the guide by a focusing monochromator of pyrolytic graphite. Wavelengths are available in the range of 0.235 nm to 0.6 nm which allows the use of a pyrolytic graphite ( $k_i = 26.62 \text{ nm}^{-1}$ ) or a beryllium ( $k_i = 15 \text{ nm}^{-1}$ ) filter for suppressing second order contributions from the incident beam.

All modules are set on air cushions. The spectrometer is entirely controlled by a Unix computer system and all elements (mechanical, electrical, software and data treatment) are fully compatible with the other triple axis spectrometers of the LLB. Because of its position at a cold guide, the conditions are particularly favourable for investigations requiring low background and excellent resolution.

The goniometers of this spectrometer permit to mount every equipment available through the triple axis pool such as pressure cells, cooling devices and magnets.



General layout of the spectrometer G 4-3.

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