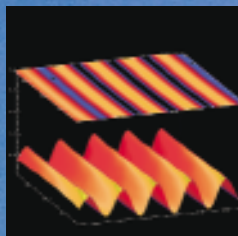
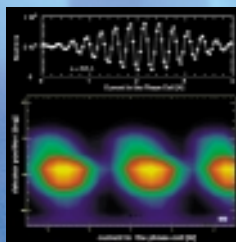
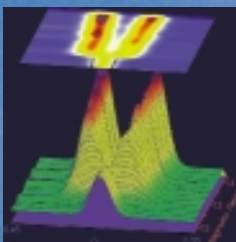
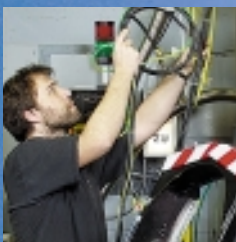
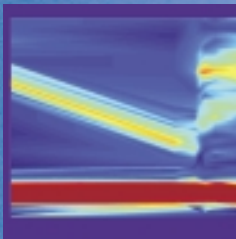


Neutron-Scattering Instrumentation at the Research Reactor BER II

Berlin Neutron Scattering Center – BENSC, March 2001



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Editorial

The Berlin Neutron Scattering Center (BENSCH) makes a great variety of new or upgraded neutron scattering instruments available to the national and international scientific community. BENSCH is hosted by the Hahn-Meitner-Institut, which in the main focusses on structural and solar energy research and is financed by the Federal Republic of Germany and the City of Berlin.

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Prof. Ferenc Mezei

Neutrons have now been used for about 50 years to probe the microscopic structure and processes in complex matter. They continue to play a key role in the exploration of topics ranging from catalysts to magnetism, from so called 'soft matter' to superconductivity.

For their pioneering work in neutron scattering in the late 1940s and 50s Bertrand Brockhouse (Canada) and Clifford Shull (USA) received the 1994 Nobel Prize in Physics.

Nowadays a still growing community of some 7000 scientists uses neutrons: in physics and chemistry, in materials science, engineering, biology and earth science.

Why Neutrons?

The basic understanding of materials (metals, alloys, ceramics, polymers, liquids, glasses, etc.) and biological matter requires the detailed knowledge of the arrangement and the dynamics of their atoms or molecules. The special features make neutron radiation in synergy with other microscopic probes a unique tool in exploring matter:

- The interaction of the neutrons with a nucleus is exactly known, which facilitates the direct, unambiguous theoretical interpretation of experimental data.
- The energy of neutrons is particularly well suited to study not only atomic structures but also atomic motions in matter.
- Neutrons can easily penetrate thick materials. This offers unique possibilities for material testing and for the development of sophisticated sample environments to observe materials under extreme conditions (temperature, pressure, magnetism and combinations of these conditions).
- Via its magnetic moment the neutron interacts particularly strongly with magnetic atoms. This makes neutron scattering play a central role in the study of magnetism.

- Neutrons interact differently with the various isotopes of the same atomic species. Thus the scientist can mark selected atoms or molecules by isotope replacement to study their specific behaviour. Furthermore neutrons interact very strongly with hydrogen atoms which makes them the first choice tool for the investigation of organic and especially biological matter.
- Neutrons can activate materials. Applications range from non-destructive chemical analysis to medical diagnosis and therapy.

Neutron diffraction will continue to be a basic technique for the exploration of the structure of matter and will remain of eminent importance for the study of an ever widening field of subjects.

BENSC

The Berlin Neutron Scattering Center (BENSC) at the upgraded research reactor BERII is Germany's most modern facility for neutron scattering research and one of the best and most widely used neutron sources in Europe. BENSC is open to the international community of all kinds of disciplines.

BENSC offers access to a great variety of new or upgraded neutron scattering instruments, suited for research in many fields of science. A large range of sample environment equipment is available to carry out experiments under extreme sample conditions.

This brochure gives a broad view on the instruments and the sample environment available at BENSC. It will also explain briefly how to apply for beamtime. BENSC puts special emphasis on providing expert support to scientists with no previous experience in neutron scattering and on service for the special needs of young scientists and students.

Ferenc Mezei
(BENSC Director)

Research Reactor BER II, Cold Source and Neutron Guides

The research reactor BER II at the Hahn-Meitner-Institut Berlin is a light water cooled and moderated swimming pool type reactor to be operated at 10 MW thermal power. Fuel and control elements are MTR type mounted on a grid plate with 42 positions. The BERII was converted from HEU (High Enriched Uranium) to LEU (Low Enriched Uranium) core and is now in operation with LEU-core since January 2000. The core configuration operates with 24 fuel elements and uses six additional control elements. The remaining grid positions are filled with reflector elements and irradiation tubes. The core is surrounded by a beryllium reflector wherefrom nine cylindrical beam tubes deliver thermal neutrons to the experiment hall.

In addition there is a conical beam tube with a horizontally inserted cold source. The cold source is operated at temperatures of 25-35 K with hypercritical hydrogen in the pressure range of 14-17 bar.

Six neutron guides deliver cold neutrons from the cold moderator cell to a neutron guide hall adjacent to the experiment hall. A summary of the characteristic neutron guide data is given in the table below.

The undisturbed thermal neutron flux density in the beryllium reflector amounts to $1.2 \cdot 10^{14} \text{ n/cm}^2\text{s}$. The disturbed thermal neutron flux density was measured at $7 \cdot 10^{13} \text{ n/cm}^2\text{s}$ in a tangential beam tube and $8.6 \cdot 10^{13} \text{ n/cm}^2\text{s}$ in a radial beam tube.

The capture flux density was measured at the end of a ^{58}Ni coated neutron guide at $1.10 \cdot 10^9 \text{ n/cm}^2\text{s}$.



Characteristic neutron guide data

	coating	radius of curvature (m)	character wavelength (nm)	width (mm)	height (mm)	Instrument	
NL 1A	^{58}Ni	1 300	0.33	30	125	V1 B8	PG monochr. end position
NL 1B	^{58}Ni	3 000	0.22	30	125	V2-FLEX	PG monochr.
					50 upper	V14	PG monochr.
					50 lower	V11 B7	end position end position
NL 2	^{58}Ni	3 300	0.21	30	125	---	---
				30	55 upper	V3-NEAT	end position
				30	55 lower	V9 V10	PG monochr. PG monochr.
NL 3A	^{58}Ni	1300	0.38	30	50	V4-SANS	end position
NL 3B	^{58}Ni	500	0.53	30	50	V12a,V12b V13	PG monochr. end position
NL 4	^{58}Ni	straight	--	60	100	V6	PG monochr.
						V5	end position

The BENS User Service

BENS User Service would like to welcome the national and international scientific community and encourage especially young scientists to use its facilities.

The user service was established in 1993. Besides short-term beam time access BENS User Service offers the possibility for long-term cooperation. This includes access for Ph.D.-students as well as for research groups who operate their own instrument and assist in instrument development and user service.

Besides academic research BENS User Service is always open to industrial related projects.

How do I get a proposal form?

To apply for beam time please complete the online proposal submission form which can be found on our webpages. Interested parties from the industry are requested to contact the Scientific Secretary directly.

Are there any deadlines for proposal reception?

Short-term beam time is allocated semi-annually. The User Committee assesses proposals and decides on beam time allocation. The decision is based on the information given in the proposal and – in case of continued research – on presented experimental reports.

The deadlines for handing in your proposal are March 15th and September 15th for allocations in the periods of July to December and January to June, respectively.

I have a very urgent experiment.

Can I get beam time right away?

Users with particularly urgent experiments or ideas which promote new techniques or feasibility experiments should contact the BENS User Service Director directly.

Do I need a local contact person?

All external users need a local contact who helps to prepare and to perform the experiment. Your proposal should be prepared carefully and in close collaboration with your local contact. Therefore it is advisable

to get in touch with the eligible instrument scientists well in advance. In order to find the respective person you may consult this brochure or our instrument webpages.

The experiment is done.

What happens next?

The results of all experiments carried out at BENS User Service have to be reported to the User Committee and are published annually as "Annual Scientific Reports". These reports are only interim summaries and do not release the user from the obligation to publish the results in an appropriate international journal.

Your report should record the results of your experiment and a representative data set but does not necessarily need to contain the final conclusion or data analysis. Please present your report using the preformatted form available at the BENS User Service webpage and use the internet for upload.

Do I have to refer to BENS User Service in my publications?

BENS User Service local contacts, operators of complex sample environment facilities and scientists responsible for building recent instruments and equipment are – as a rule – to be credited by co-authorship of user experiment publications. For this purpose the respective scientist(s) should be contacted before the publication is submitted.

This condition might be dropped with explicit agreement of BENS User Service in individual cases for frequent users of instruments in long-term routine operation.

Do I have to pay a fee?

Our service is free of charge for members of universities and other public institutions assuming that the experiment results will be published in internationally accepted scientific journals. Industrial applicants please contact the Scientific Secretary.

Is there any support available?

Limited BENS User Service funds are available to assist with travel costs and related expenses of external users. Customarily two scientists per experiment are supported.

In addition, members of research teams based in the EU Member States  (except Germany) and Associated States may qualify for a travel grant provided by the European Commission (Access to Research Infrastructures action of the Improving Human Potential program). Priority will be given to new user groups (for more detailed information see <http://www.cordis.lu/improving>).

Please note: Arrangements for travel support have to be made with the BENS User Service Scientific Secretary well in advance.

Where can I stay whilst carrying out my experiment?

For accommodation a 30-bedroom on-site guest house is at your disposal. The BENS User Service Guest Office will gladly assist you with arrangements.

Further information

For further information please contact the BENS User Service Scientific Secretary (Rainer Michaelsen, e-mail: rainer.michaelsen@hmi.de, direct call -3043) or look at the continuously updated BENS User Service webpages.

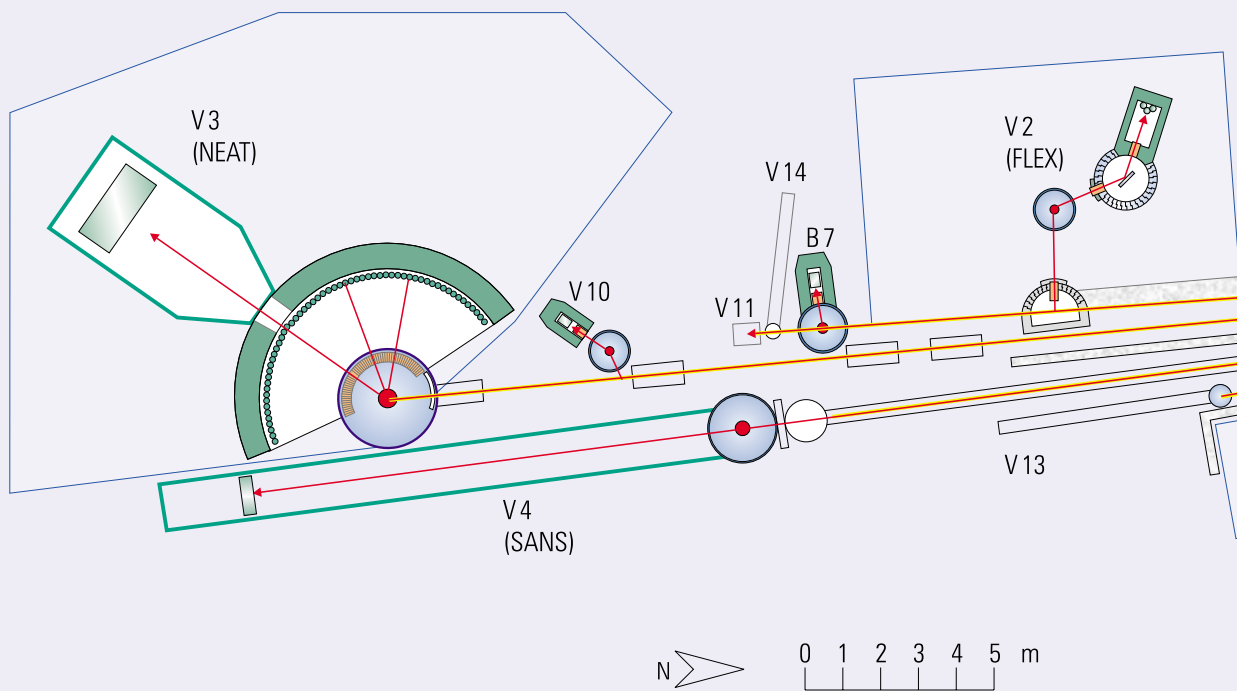
Office of the Scientific Secretary
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email: bensc@hmi.de
Web: <http://www.hmi.de/bensc>

Arrangement of the Instruments



Neutron Guide Hall (Cold Neutrons)

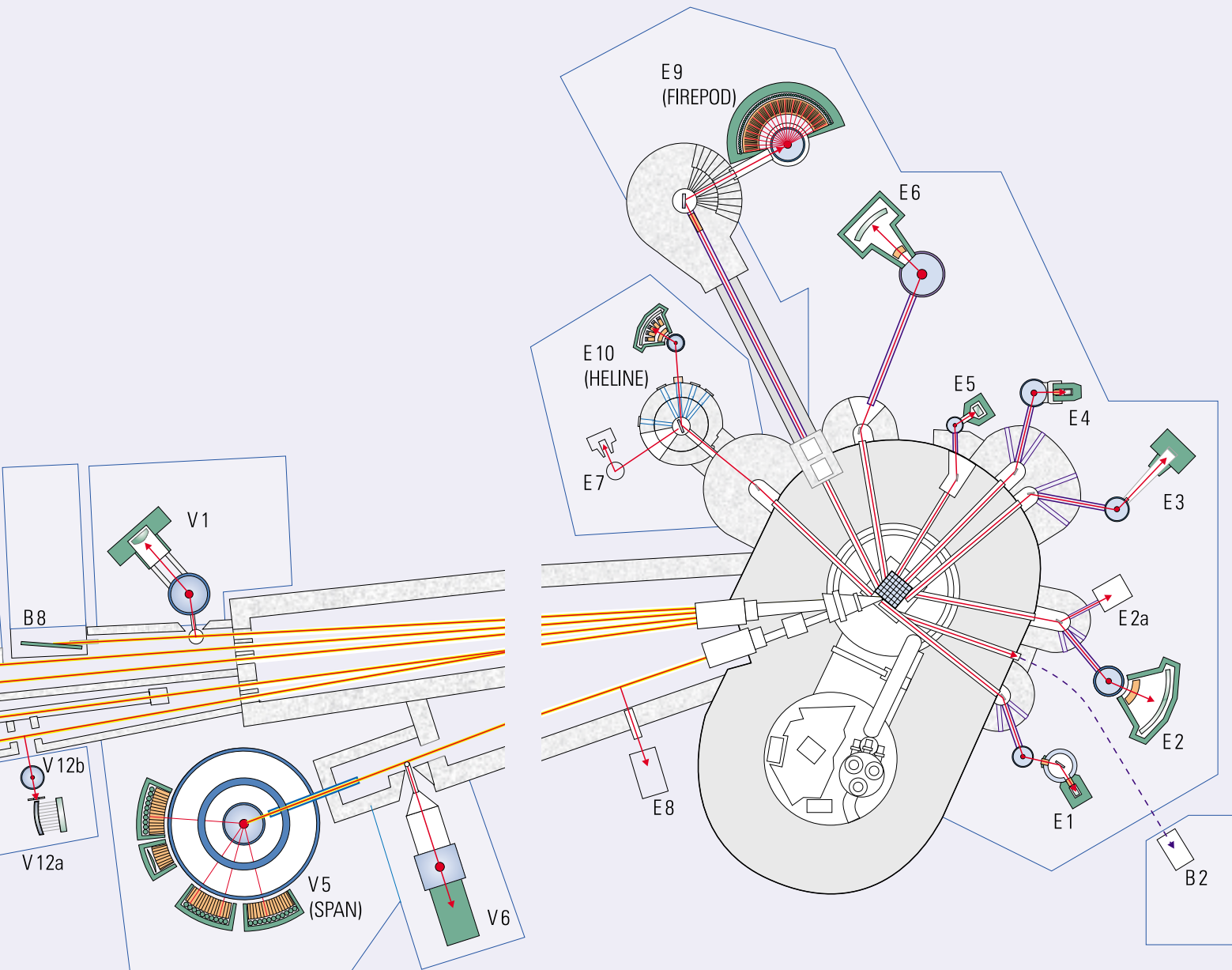
View from the south end of the hall
looking parallel to the neutron
guides





**Experiment Hall
(Thermal Neutrons)**

View from the west corner of the hall looking at several neutron scattering experiments



E1

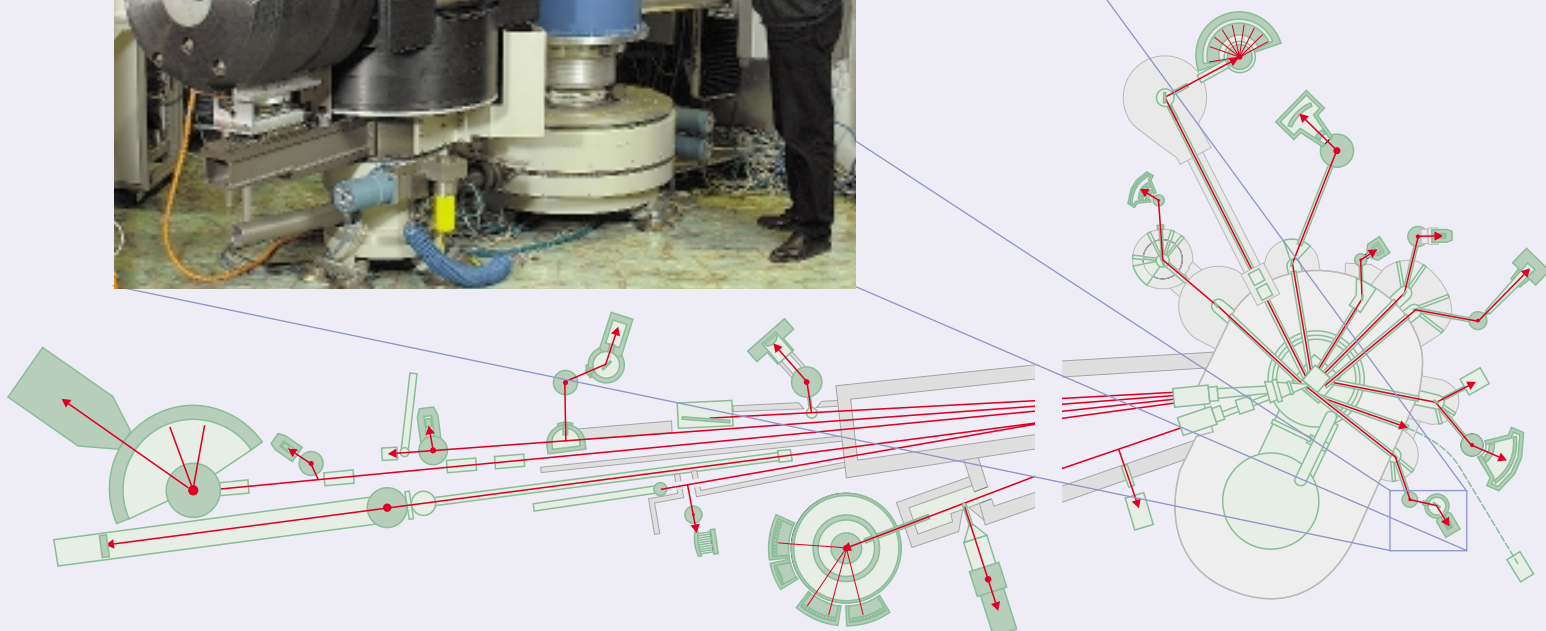
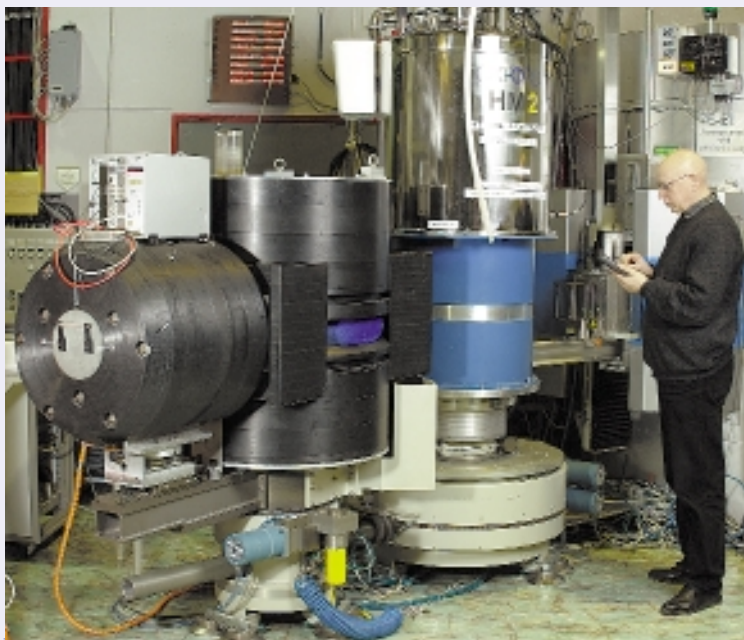
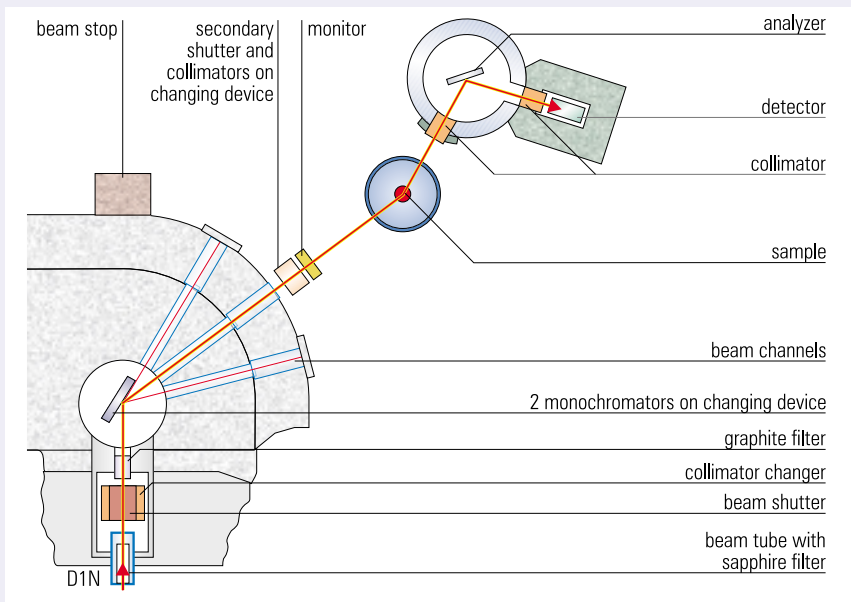
Triple-Axis Spectrometer with Polarization Analysis

The triple-axis spectrometer E1 with polarization analysis is installed at the beam tube D1N. The monochromator shielding has three channels for fixed take-off angles at $2\theta_M = 20^\circ, 42.5^\circ$ and 65° . At present it is not possible to change the incoming energy continuously.

Instrument Description

The whole spectrometer is made of non-magnetic materials. A second turntable below the sample table with its axis collinear to the sample axis can be used for mounting and orienting ancillary equipment, such as Helmholtz coils used to produce a horizontal magnetic field.

The analyzer and detector are constructed into a single „Tanzboden“ unit. The detector is mounted on a cantilever arm which can be rotated freely around the analyzer axis after decoupling it from a beam tube device leading through the analyzer shielding. By rotating both the cantilever arm and the detector by 180° it is possible to quickly change to a two-axis mode of operation. The analyzer shielding has an unconventional design: a horizontal segment of the polyethylene shielding is replaced by a rubber tire filled with water, over which a specially formed polyethylene block containing the beam channel can be moved. This beam tube device is coupled to – and automatically rotates with – the detector arm.



Applications

The spectrometer with polarization analysis was designed to separate the magnetic scattering unambiguously from non-magnetic scattering processes. It is particularly useful for

- distinguishing between spin waves and phonons, when both excitations have similar energies
- analyzing the paramagnetic scattering in q, ω -space
- determining spin densities.

Utilizing the polarization option it is also possible to apply neutron depolarization techniques on the investigation of magnetic structures on a mesoscopic scale.

Without polarization analysis the instrument can be used as a conventional triple-axis spectrometer with fixed incoming energy, e.g. for

- measuring phonons
- separating quasielastic from inelastic scattering.

Selected example

The incommensurate-commensurate phase transition in the frustrated quantum system CsCuCl_3 at about 16 T and 1.8 K observed using the high field magnet VM-1 equipped with the Dy-booster.

Instrument Data – E1

Beam tube	D 1N in-pile cross section: 60 x 90 mm ²
Monochromators (can be changed remotely)	PG 002 with variable horizontal and vertical curvature Heusler 111 with variable vertical curvature
Monochromator take-off angles	$2\theta_M = 20^\circ, 42.5^\circ$ and 65°
Range of scattering angle at sample table	$-20^\circ < 2\theta_S < 114^\circ$ with configurational restriction
Analyzers	PG 002 with variable curvature, which can be used horizontally or vertically; Heusler 111
Range of scattering angle at analyzer	$-140^\circ < 2\theta_A < 140^\circ$
Collimators	$\alpha_1 = 70'$ (= open), $40', 20'$ (can be changed remotely) $\alpha_2 = 80'$ (= open), $40', 20'$ (can be changed remotely) $\alpha_3, \alpha_4 = 60', 40', 20'$ (can be changed manually)
Polarization Analysis	
- Monochromator	Heusler 111 with variable vertical curvature
- Analyzer	Heusler 111 (curvature not yet implemented)
- Guide fields	vertical, various lengths, permanent magnets
- Spin flipper	Mezei type with correction coils
- Polarization	$> 93\%$, $R > 30$ with 20 mm circular diaphragm Collimation: open - $20'$ - open - open x,y,z - spinturners for 3dim analysis
Flux at sample position	$4 \cdot 10^6$ n/cm ² s (PG 002, vert. bent, open collimation) $4 \cdot 10^5$ n/cm ² s (Heusler 111, flat, open collimation)
Instrument responsible	J. Klenke, jens.klenke@hmi.de, direct dialing -3167

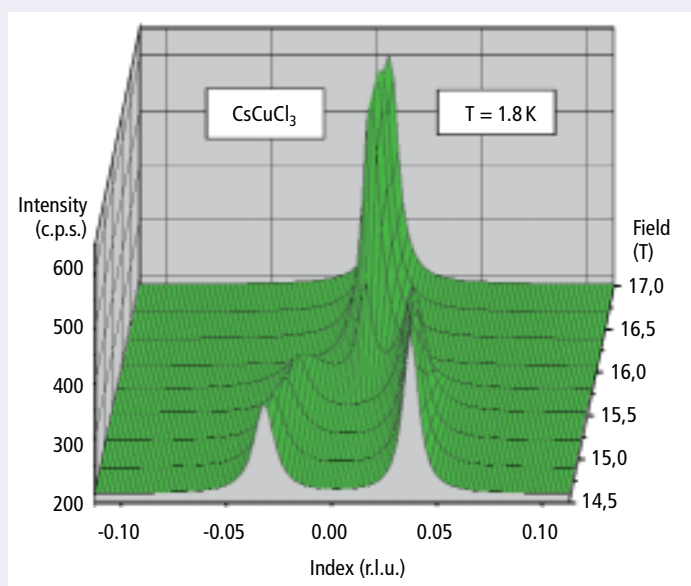


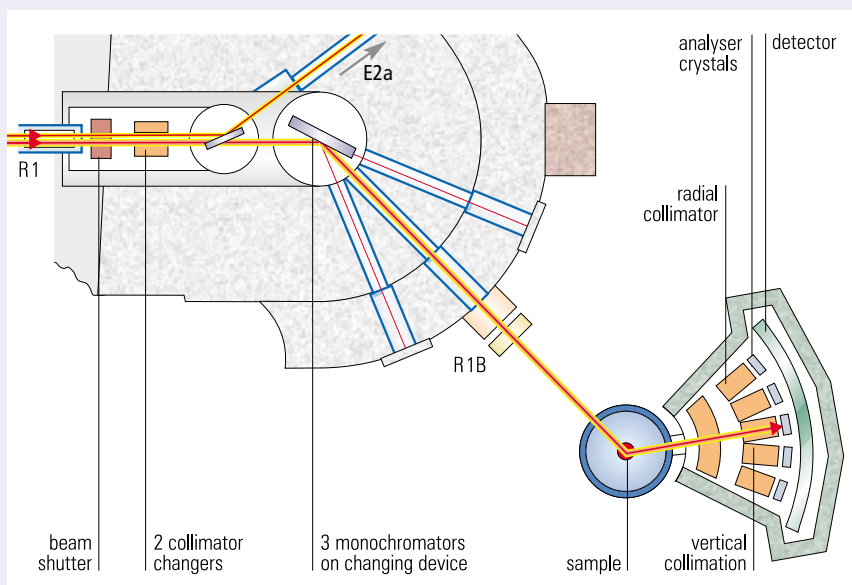
Fig. 1: Magnetic diffraction patterns clearly indicating the IC-C phase transition of CsCuCl_3 at about 16 T

E2

Flat-Cone and Powder Diffractometer

Institut für Kristallographie der Universität Tübingen

The instrument can be used for both powder and single crystal investigations. A large position sensitive detector, low background even at small scattering angles and good resolution enable the experimentalist to investigate magnetic and crystal structures, phase transitions and also diffuse scattering arising from magnetic or structural disorder. In the case of single crystal applications the detector can be tilted to determine scattering distributions in three dimensions of reciprocal space (flat-cone) with the possibility of energy analysis.



Instrument description

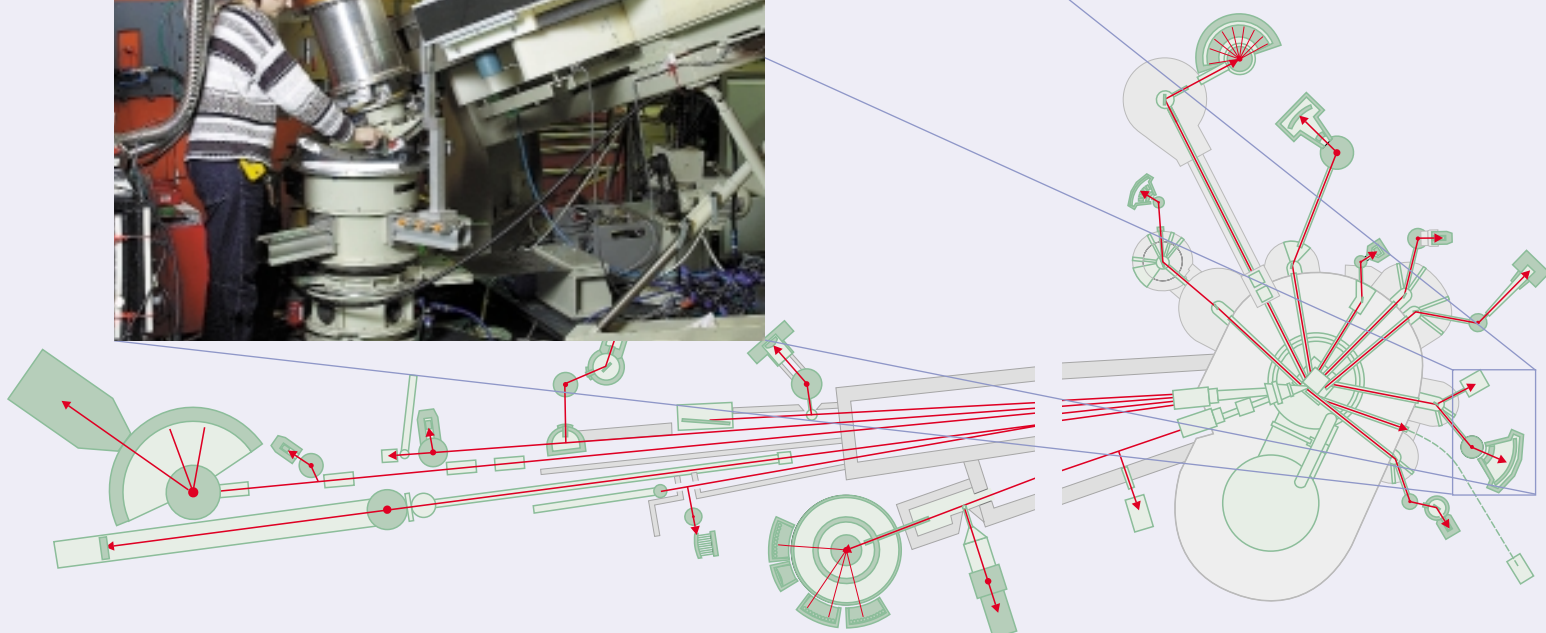
The diffractometer E2 is equipped with a position sensitive detector covering 80° of 2θ , which can be tilted out of the scattering plane (flat-cone technique). Three primary collimations and three wavelengths can be chosen automatically in some minutes time. Parasitic scattering from cryostat or furnace walls is reduced by an oscillating "radial" collimator.

For single crystal work the multidetector and the sample table can be tilted around an axis perpendicular to the monochromatic beam to investigate upper layers in reciprocal space. For the investigation of elastic and inelastic diffuse scattering distributions, five analyzer crystals and collimators can be mounted in front of the multidetector. The crystals cover 40° 2θ of the sample simultaneously and diffract in vertical planes. Three-dimensional data in reciprocal space can be collected systematically for a given energy transfer.

Powder applications

For powder studies, the multidetector measures 400 data points simultaneously. The measurement of intermediate points in the profile can be done by an automatic rotation of the multidetector, providing more information for Rietveld refinements. With medium resolution and high intensity, the instrument can be used for the study of:

- magnetic and crystal structures
- phase transitions
- in-situ kinetic of phase transitions and chemical reactions



Single crystal applications

As single crystal diffractometer the instrument can be used for the study of:

- complicated distributions of Bragg and superstructure reflections in three dimensions of reciprocal space (Flat-Cone)
- diffuse scattering arising from structural and magnetic disorder

The Flat-Cone method is a special Weissenberg-Technique by which three-dimensional diffraction data are measured layer by layer in reciprocal space. One specific layer or plane can be adjusted by tilting the multidetector and the sample table by an angle μ . All scattering events of this layer than can be obtained by rotating around the axis of the sample table.

Energy analysis of diffuse scattering can also be done to some extent, especially to record the elastic contribution.

TVtueb – a Data Analysis Tool

TVtueb is a platform developed for WindowsNT to view and analyze one- or two-dimensional data sets. The single-crystal tools include automatic indexing, determination of intensity and position of peaks, transformation into reciprocal space, background analysis, intersections, three-dimensional peak fitting algorithms, correction of PSD-efficiency and comfortable parameter plotting. An extended version is available for modelling diffuse scattering distributions arising from paramagnetic short-range order and structural disorder. Via the Windows clipboard data can be exchanged with commercial software. The program is developed by Jens-Uwe Hoffmann and Rainer Schneider and can be downloaded from www.flat-cone.de.

Selected examples

RKKY-like interactions in the paramagnetic phase of holmium: Spin correlation in holmium result from a competition of a temperature dependent oscillating exchange interaction, a hexagonal crystal field anisotropy and strong magnetostrictive effects. Below the Néel-point $T_N \approx 133\text{K}$ the favoured magnetic structure is of helical character producing satellite reflections along the reciprocal c^* -axis. Within the paramagnetic regime only diffuse scattering distributions are observable. These data are fitted by an extended

molecular field theory (fig. 1). The resulting interaction parameters show an oscillating behaviour, which is expected if the magnetic exchange is mainly mediated by conduction electrons, RKKY-interaction (fig. 2). The corresponding predominant Fermi-vector is determined to be $k_f = 0.54 \text{ \AA}^{-1}$.

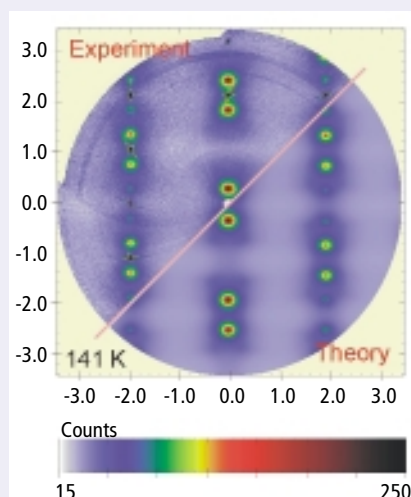


Fig. 1: Paramagnetic diffuse scattering distribution: experiment versus theory

E2a Crystal-Test Diffractometer

The set-up consists of a two-circle diffractometer with a ^3He single detector and a xz -translation stage for the sample. The instrument operates with a special software to determine the mosaic widths of monochromator crystals for many volume elements. The resolution of rocking curves is up to $0.5'$ (FWHM) due to a perfect crystal monochromator.

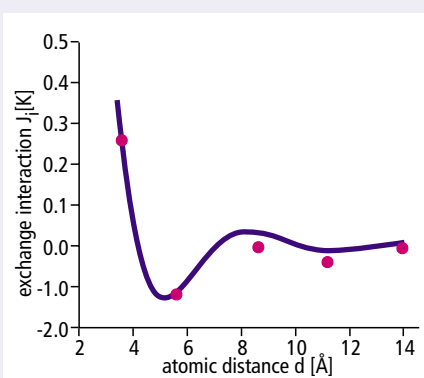


Fig. 2: Resulting exchange interactions as a function of the atomic distance in c^* -direction

Instrument Data – E2

Beam tube	R 1B
Collimators	15', 30', 60' (open)
Monochromator crystals	Cu 220 ($\lambda=0,091 \text{ nm}$) Ge 311 ($\lambda=0,121 \text{ nm}$) PG 002 ($\lambda=0,240 \text{ nm}$)
Range of scattering angle	$-10^\circ < 2\theta < 107^\circ$
2θ -resolution	$0.3^\circ\text{-}1^\circ$
Tilting angle	$0^\circ < \mu < 18^\circ$
Multidetector	- Radius 1500 mm - Angular range 80° (400 wires, or data points) - Distance between wires 5.3 mm (0.2°) - Effective height 90 mm - Pressure 1 bar - Efficiency at 0,12 nm 30% 0,18 nm 40% 0,24 nm 55%
Analyzer crystals	5 crystals, PG 002, covering a 2θ -sample range of 40° simultaneously - Energy resolution 1 meV ($E_i=14.1 \text{ meV}$) - Energy transfer $-13 \text{ meV to } +4 \text{ meV}$ (E_i-E_f)
Flux at sample position	$2 \cdot 10^6 \text{ n/cm}^2\text{s}$ (flat PG monochromator without collimation)
Instrument responsible	R. Schneider, r.schneider@hmi.de , direct dialing -2185 D. Hohlwein, hohlwein@hmi.de direct dialing -2708

E3

Dedicated Residual Stress Diffractometer

The dedicated residual stress diffractometer E3 is equipped with a two-dimensional position sensitive detector. It is installed at the beam tube T2.

Instrument description

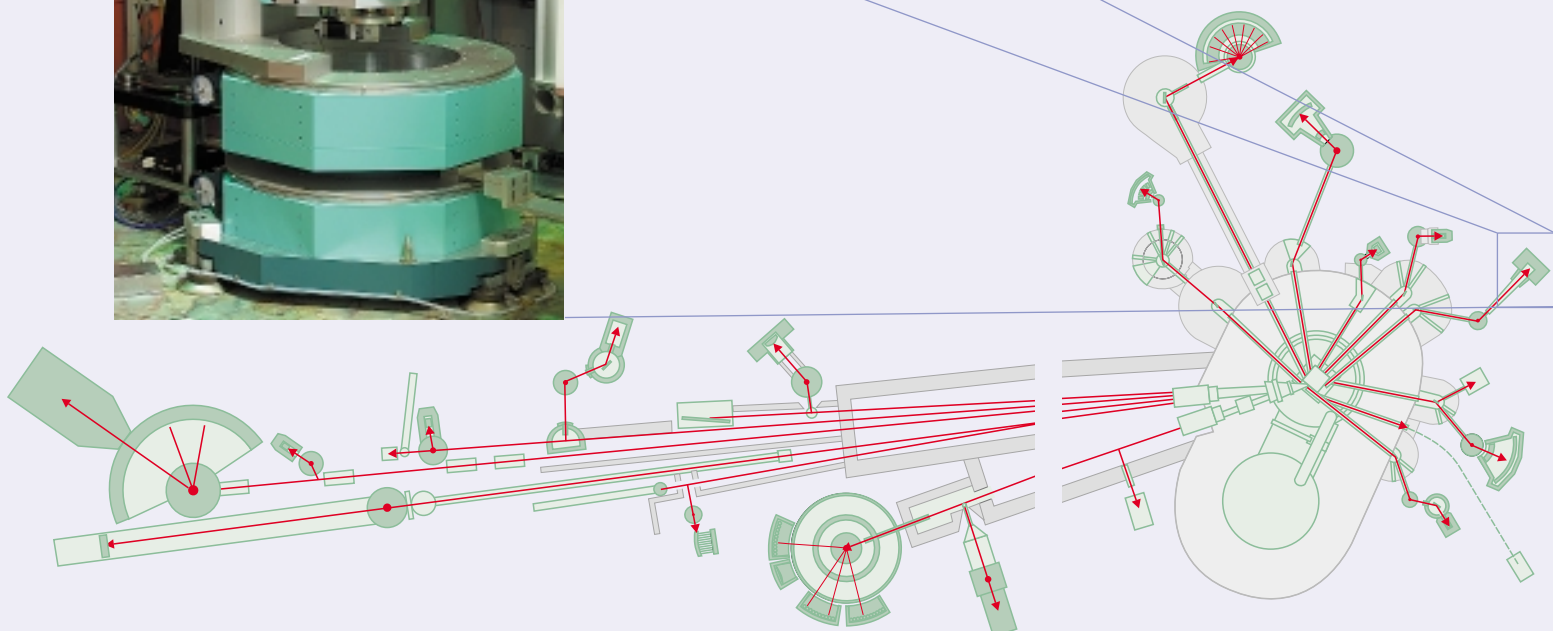
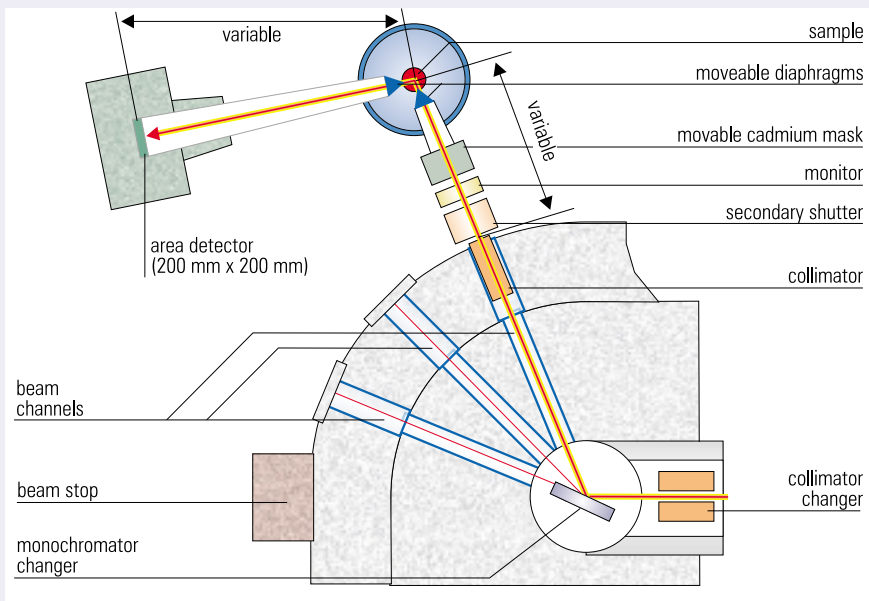
The monochromator take-off angle is at $2\theta_M = 65^\circ$ fixed. Monochromators available are Cu (220), flat, $\lambda = 0,137$ nm, Ge (311) vertically focusing, $\lambda = 0,184$ nm

and HOPG (002), flat, $\lambda = 0,36$ nm. As collimation in front the monochromator 10' collimation, 30' collimation and open collimation are available. After the monochromator 10' collimation, 15' collimation, 30' collimation and open collimation can be used.

For sample positioning an Eulerian cradle with integrated xyz-translation table (maximum weight of the sample 10 kg), a translation table (maximum weight of the sample 200 kg) with 300 mm movement in vertical direction (z-direction) and 300 mm in horizontal direction (x- and y-direction) can be employed. The sample size can be as large as 800 mm diameter.

For defining the gauge volume slits with different sizes varying between minimum 0.5×0.5 mm² and maximum 4×20 mm² are accessible. A laser system for sample positioning and various sample holders e.g. for cylindrical sample are available.

The instrument is equipped with a two-dimensional detector with a grid distance of 1 mm. The usable 2θ -range is 3° to 120° . The distance between sample and detector can be varied between 500 mm and 1500 mm.



Auxiliary equipment for in-situ measurements are a bending device and a focusing mirror furnace ($T_{\max} = 2000\text{ K}$). Other furnaces as well as cryostats or cryomagnets also may be mounted on request.

Applications

- residual stress analysis in monocrystalline and polycrystalline materials
- residual stress analysis on machine components
- in-situ residual stress during mechanical loading (bending) or thermal loading
- elastic and plastic deformation behaviour of polycrystalline materials

Selected examples

In co-operation with Volkswagen AG and BMW AG residual stresses in deep-rolled and induction hardened crankshafts were investigated. The results of the experiment serve for an optimization of the process parameter as well as for testing FEM models (fig. 1,2).

The largest sample so far investigated for residual stress with neutrons is an aluminium alloy compressor impeller of 800 mm diameter. Further investigations include residual stress analysis at different stages of the manufacturing process of Ni-base turbine disks, in composites at elevated temperatures, on friction stir welds, in brake disks as well as on cold and hot extruded tubes and profiles.

Instrument Data – E3

Beam tube	T 2
Monochromators vertically focusing	Wavelength at $2\theta = 65^\circ$ Cu (220) 0.137 nm Ge (311) 0.184 nm HOPG (002) 0.360 nm
Neutron flux	$2.3 \cdot 10^6\text{ n/cm}^2\text{s}$ ($\lambda = 0.24\text{ nm}$, no collimation)
Collimations	$\alpha_1 = 10', 30'$ $\alpha_2 = 10', 15', 30'$
Maximal beam section at sample position	$60 \times 30\text{ mm}^2$
Minimal beam section at sample position	$0.5 \times 0.5 \times 1\text{ mm}^3$
Detector	^3He (128 x 128 pixels)
Radius	variable
Channels	128
Angular Range (2θ)	$3^\circ - 115^\circ$
Auxiliary Equipment	Eulerian cradle with integrated xyz-translation device; high-T-furnace (1000 K); focusing mirror heating device (2000 K);
Instrument responsible	A. Pyzalla, pyzalla@hmi.de, direct dialing -3042

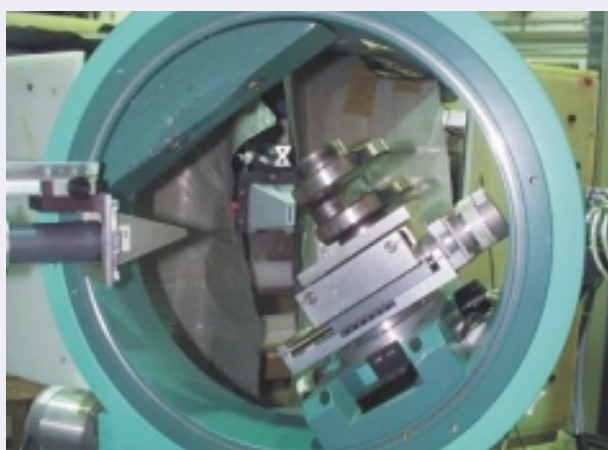


Fig. 1: Induction hardened crankshaft in the neutron diffractometer E3

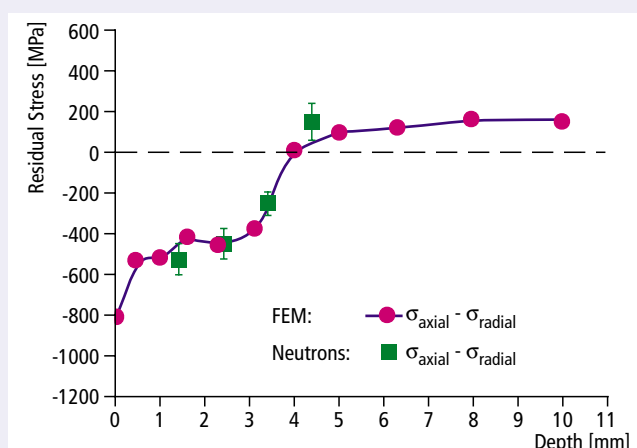


Fig. 2: Results of the residual stress analyses in the induction hardened zone, comparison to FEM

C. Hackmair, T. Georges, H.M. Mayer, A.Pyzalla 1999

E4 and E4b

Two-Axis

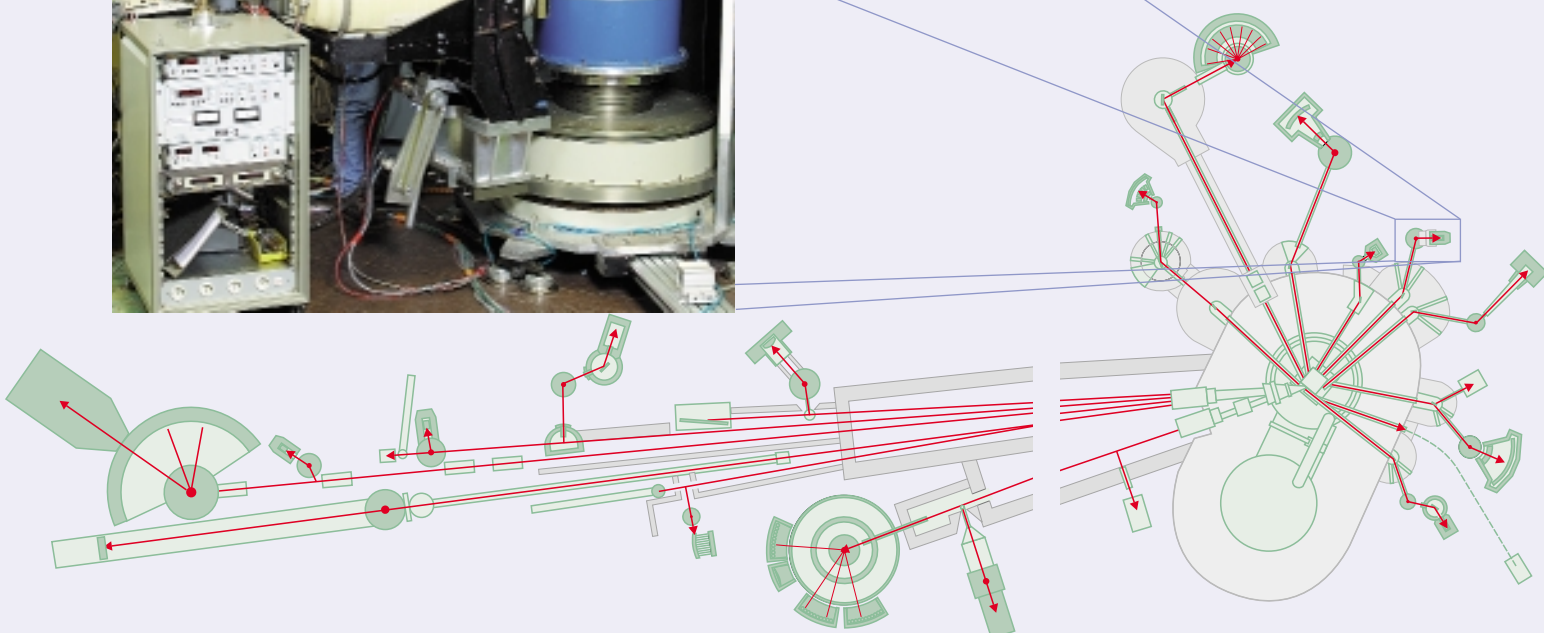
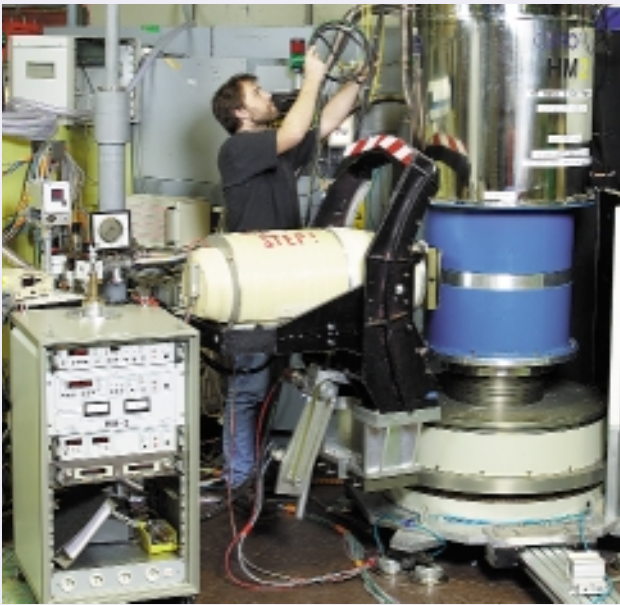
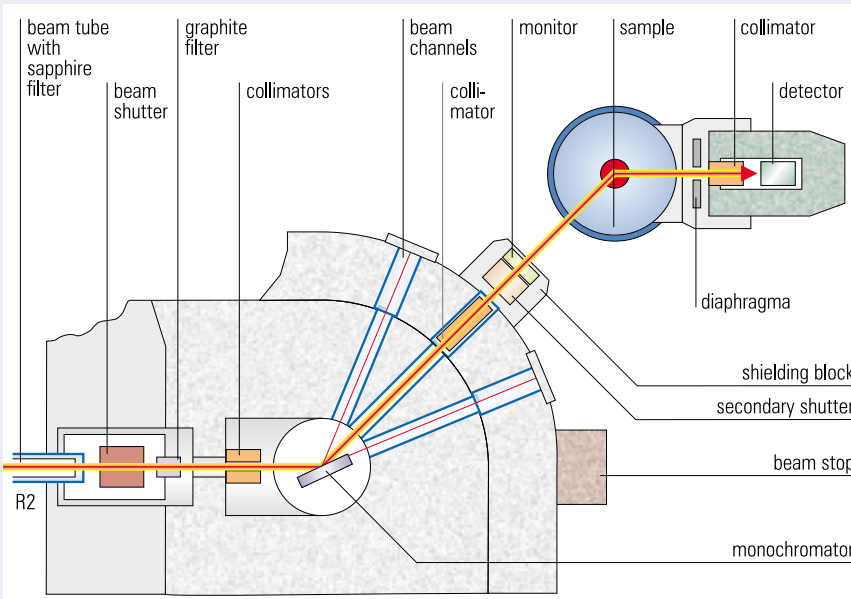
Diffractionmeter

The two-axis diffractometer E4 is installed at the beam tube R2. The instrument is primarily suited for magnetic structure determination under various conditions, which includes magnetic fields up to 17 T, temperatures down to 30 mK and pressures up to 10 kbar. The most common application is to reveal spatial arrangement ordered spin structures. The polarized neutrons option facilitates the separation of magnetic

contributions from nuclear scattering. The measurement of flipping ratios allows registration of very weak magnetic scattering and the mapping of spin density distributions.

Instrument Description E4

Pyrolytic graphite crystals (002) that can bend vertically act as focusing monochromator. The monochromator shielding contains three beam channels at $2\theta_M = 20^\circ, 42.5^\circ$ and 65° with the instrument installed at $2\theta_M = 42.5^\circ$ most of the time. This position corresponds to the incident wavelength of 0.244 nm. The in-pile collimation can be changed remotely ($\alpha_1 = 20', 40'$, geometrical divergence = $60'$). The detector is a single tube filled with ^3He gas. Saturation occurs at 40 000 counts/s. In view of typical experiments with superconducting magnets that have small split opening the detector is confined mostly in the horizontal scattering plane. However, it is possible to lift the detector out of the plane (inclination ν). This is useful in order to access reflections from another crystallographic layer (if the sample environment permits). However, at the moment this option is not fully implemented yet. The additional option of polarized neutrons uses a super mirror bender



and π -flipper. The instrument operates under the system CARESS; automatic control of temperature and magnetic field is provided.

Applications

- Magnetic structure determination
- Study of magnetic and structural phase transitions
- Determination of magnetic phase diagrams
- Study of critical points as a function of magnetic field and temperature
- Measurement of correlation functions above the ordering temperature

Selected examples

- Delafossite-type compound CuFeO_2 has distinct triangular lattice layered structure with rhombohedral stacking along the c -axis and has been extensively studied as one of model materials of triangular lattice antiferromagnet (Fig. 1).

E4b Two-Axis Diffractometer

This additional and new two-axis spectrometer is mounted at R2 behind the E4 experiment and uses the transmitted beam from the E4 sample.

Instrument Description

The E4b is equipped with a Huber cradle (Model 5201.3) and controlled by PC-Lab. To enable simple application Huber goniometerheads (Model 1001,1004) are useful.

Applications

The instrument support single crystal orientation for all BENS users while their main experiments are running. In combination with E4 polarization quality of the transmitted beam is controllable.

Fig. 1: H-T magnetic phase diagram of CuFeO_2 . Magnetic field is applied along the c -axis. Open and closed symbols are used for the anomalies that appear in increasing and decreasing either H or T , respectively. Shades are put to denote the spread of first-order phase boundaries due to hysteresis.

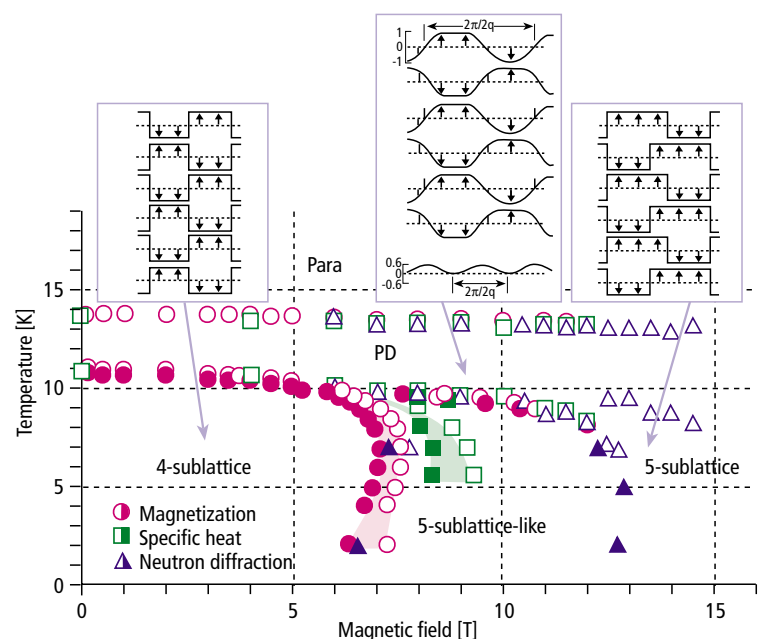
Reference: S. Mitsuda et al.
BENS Experimental Reports (1999), p. 58

Instrument Data – E4

Beam tube	R 2
Monochromator angles	$2\theta_M = 20^\circ, 42.5^\circ, 65^\circ$
Monochromators	PG (002) with variable vertical curvature
Wavelength	$\lambda = 0.244 \text{ nm}$
Range of scattering angle	$0^\circ \leq 2\theta \leq 120^\circ$
Collimation	automatic change of $\alpha_1 = 20', 40'$ geometrical divergence: $\alpha_1 = 60'$ manual variation of α_2, α_3
Flux at sample position	$2.6 \cdot 10^6 \text{ n/cm}^2\text{s}$
Detector	single ^3He tube
Options	polarized neutrons (super mirror bender) measurement of flipping ratios lifting detector polarization analysis (super mirror analysis)
Sample environment	horizontal magnetic field < 6 T vertical magnetic field < 17 T temperature range 0.03 - 600 K hydrostatic pressure 0 - 10 kbar 4-circle mode
Instrument responsible	K. Prokes, prokes@hmi.de, direct dialing -2804

Instrument Data – E4b

Beam tube	R 2
Monochromator	Depending on the E4 setup
Range of scattering angle	$-170^\circ < 2\theta < 170^\circ$
Collimation	none
Flux at sample position	not available yet
Options	goniometerhead coils for analyzer crystals super mirror setup for $\lambda = 0,24 \text{ nm}$



E5

Four-Circle Diffractometer

E5 is a conventional four-circle diffractometer. It is located at the beam tube R 3. The wavelength of 0.09 nm allows the investigation of single crystals with unit cell volumes of up to 2 nm³; the maximum value for a cell length is limited to 2.5 nm.

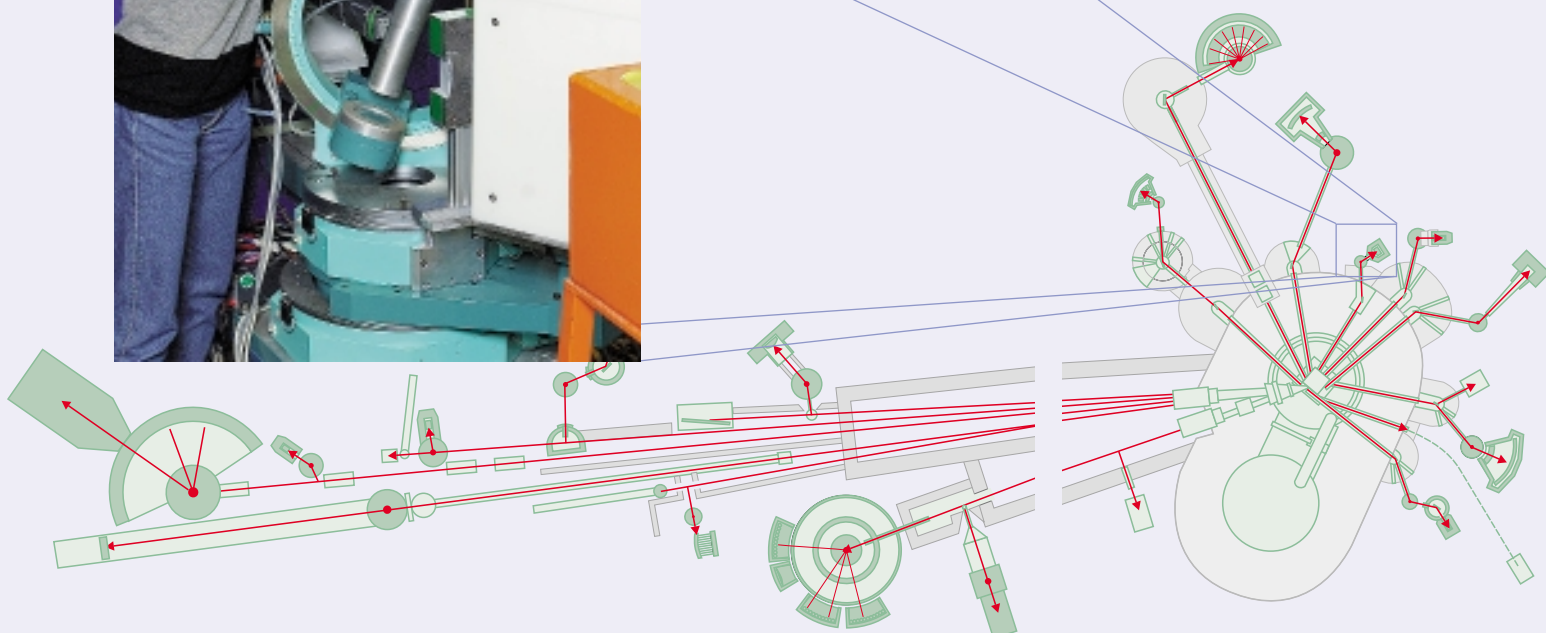
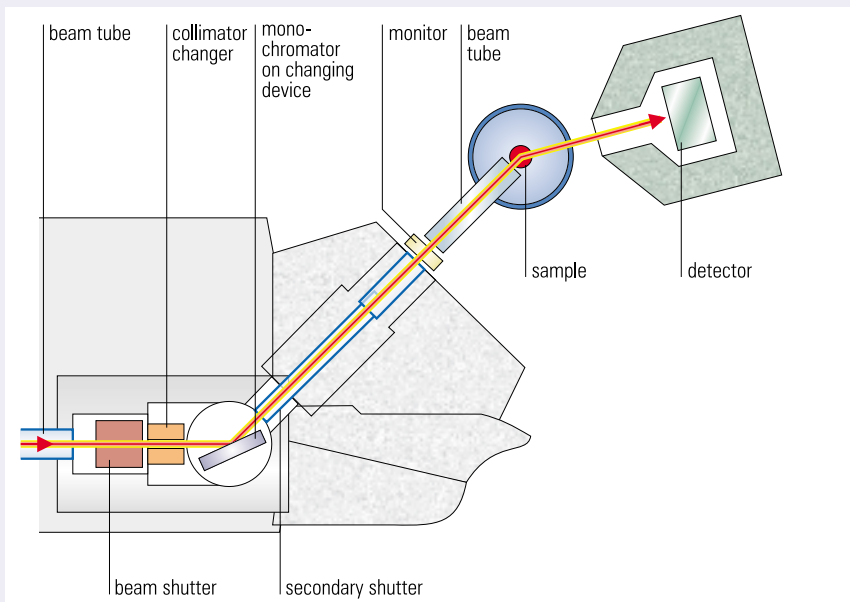
Instrument Description

The instrument is equipped with a two-dimensional position sensitive ³He-detector, 90 x 90 mm² in area (32 x 32 pixels), which is used in single reflection mode. The efficiency of detection is 85% at 0.1 nm.

The monochromator take-off angle is fixed at 42°, which causes a rather coarse resolution at the larger scattering angles, where generally the bulk of the data is recorded.

A resonance filter (erbium) is available in order to suppress $\lambda/2$ contributions. For magnetic structure determination the wavelength of 0.24 nm is accessible.

The MAD software package from the ILL has been installed to control the instrument.



Applications

The instrument is commonly used for standard crystallographic work, especially for the determination of the positional and thermal parameters of hydrogen atoms in crystal structures of molecular, ionic or intermetallic systems. The dynamic orientational disorder and the long-range order of NH_4^+ -ions in ammonium halides has been investigated (Paasch, M. et al., *Z. Physik B 99* (1996), 339), as well as the mechanism of proton conductors (Melzer, R. et al., *Sol. State Ionics 92* (1996), 119), the hydrogen bond system and the hydrogen atom disordering in mixed-anion salts (Trojanov, S.I. et al., *Z. Kristallogr.* 215 (2000), 377).

Further, E5 experiments can support magnetic studies especially in the case when the magnetic moments of the atoms are relatively weak.

Selected examples

A typical example for a crystallographical structure determination is given by the purely organic free radical compound 4,5-dimethyl-1,2,4-triazole-nitronyl-nitroxide ($\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_2$). This compound belongs to the relatively new class of "molecular magnetic materials" and shows an interesting magnetic behaviour at low temperatures.

In this case, special emphasis was placed on the determination of the low temperature crystal structure and on the localization of hydrogen bonds. Atomic coordinates and thermal displacement parameters (including those of the hydrogen atoms) at 11 K have been determined as input for a spin density distribution experiment.

Instrument Data – E5

Beam tube	R 3
Monochromator	Cu 220 in reflection ($\lambda = 0.09 \text{ nm}$) PG 002 ($\lambda = 0.24 \text{ nm}$)
Neutron flux at sample position	$1.2 \cdot 10^6 \text{ n/cm}^2\text{s}$ (Cu 220 without filter) $3 \cdot 10^6 \text{ n/cm}^2\text{s}$ (PG 002 with graphite filter)
Scattering angle:	
monochromator	$2\theta_M = 42^\circ$ (fixed)
sample	$10^\circ < 2\theta < 110^\circ$
Maximum sample size	7 mm diameter
Sample environment	12 - 350 K (closed cycle refrigerator) 300 - 600 K (air flow furnace) 600 - 1200 K (closed shell furnace)
Instrument responsible	M. Reehuis, reehuis@hmi.de, direct dialing -2692 A. Loose, loose@hmi.de, direct dialing -2793

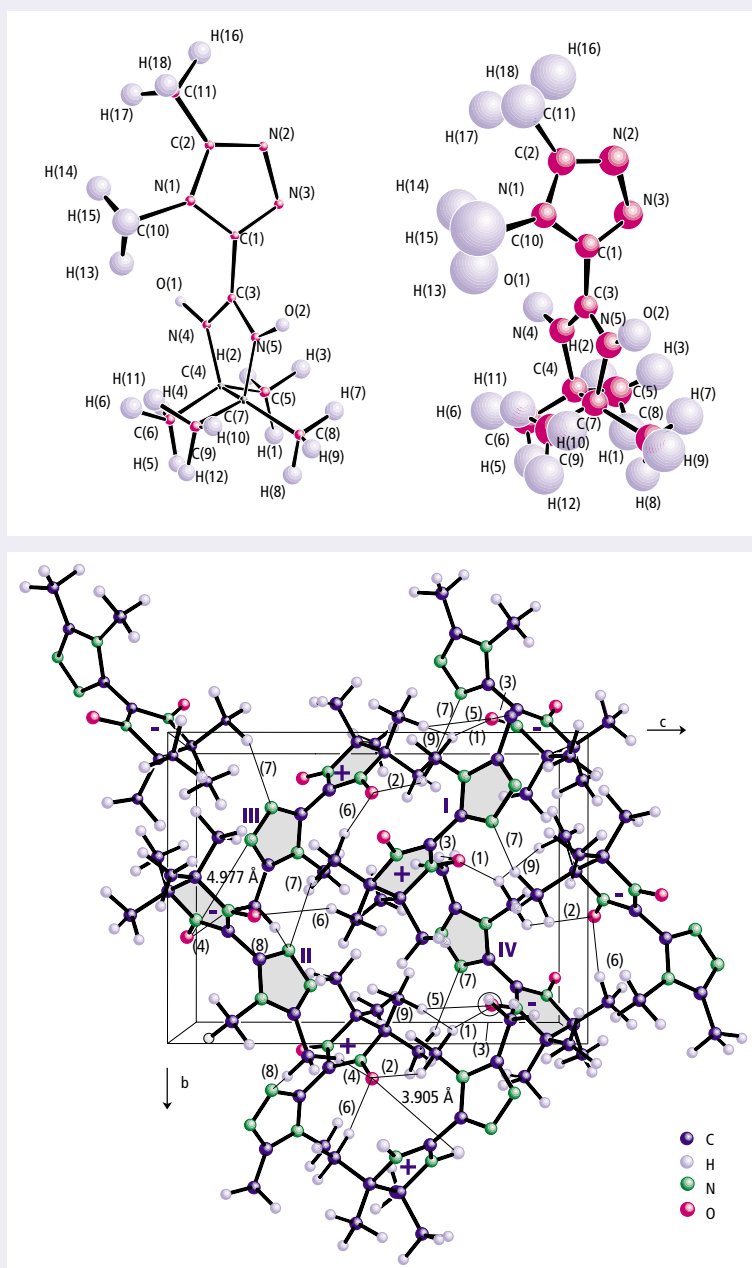


Fig. 1: Crystal structure of the 4,5-dimethyl-1,2,4-triazole-nitronyl-nitroxide molecule at 11 K (left) and at 300 K (right)

Fig. 2: Projection of the crystal structure at 11 K on the bc-plane with possible magnetic exchange pathways [II: $1/2 - x, y, 1/2 + z$; III: $1/2 + x, 1/2 - y, -z$; IV: $-x, 1/2 + y, 1/2 - z$]
A. Loose, R. Feyrerherm, M. Reehuis, J.-P. Sutter (2000)

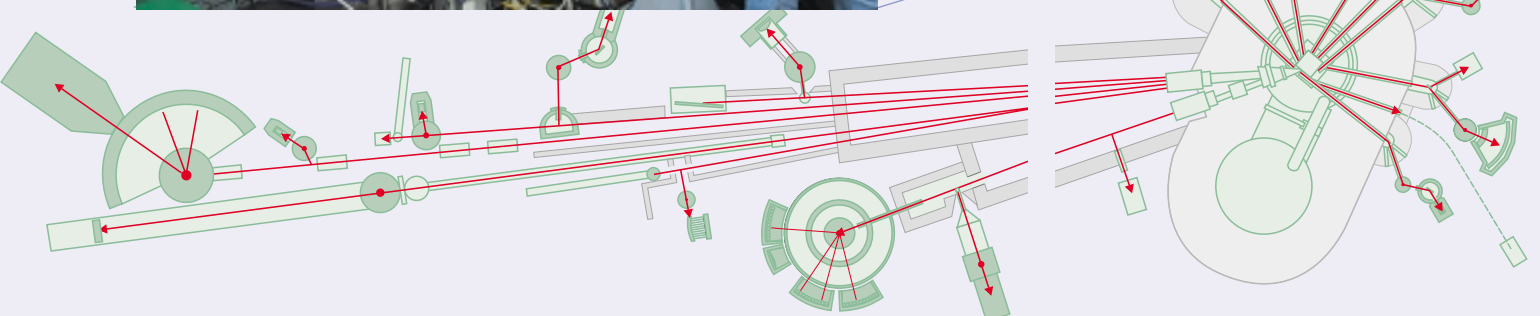
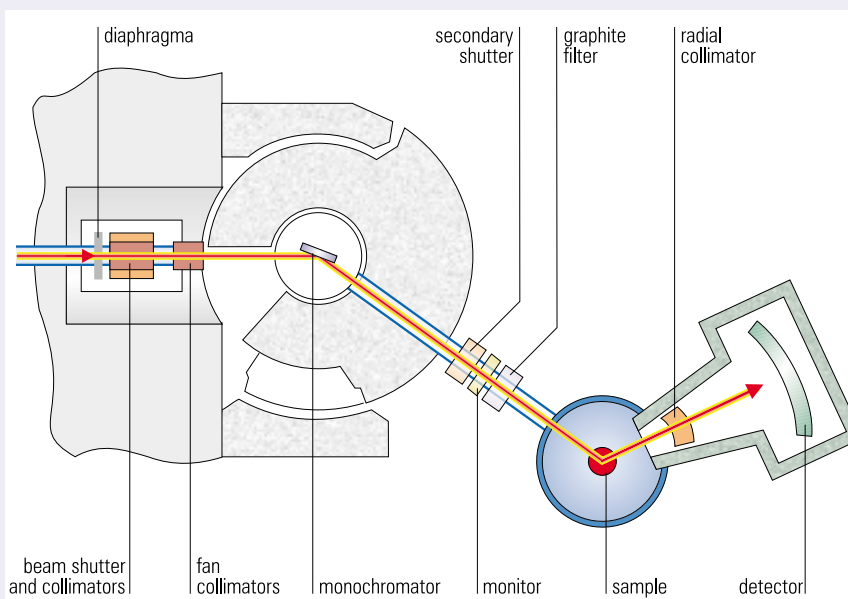
E6

Focusing Diffractometer

The diffractometer E6 is installed at the beam tube T 4. It is equipped with a horizontally and vertically bent monochromator consisting of 105 pyrolytic graphite crystals ($20 \times 20 \times 2 \text{ mm}^3$) mounted on a 15×7 matrix leading to a relatively high flux of $5 \times 10^6 \text{ n/cm}^2\text{s}$ at the sample position using $\lambda = 0.24 \text{ nm}$. In combination with a position sensitive detector and variable in-pile collimation it is mainly used to study magnetic materials. Measurements can be carried out on both powder samples and single crystals.

Instrument description

As opposed to a conventional diffractometer (small divergence, large beam cross section, flat monochromator) the focusing diffractometer uses a horizontally and vertically bent monochromator in combination with an adjustable fan collimator imitating a vertical slit with varying distance from the monochromator. By varying the horizontal bending of the monochromator and the fan opening of the in-pile collimator a correlation between the direction of the incoming neutron and its wavelength can be achieved. Thus the orientation of the resolution ellipsoid can be changed with respect to the scattering vector Q (H. Dachs, A. Axmann, Proc. of the Neutron Diffraction Conference Petten 1975, RCN 234, p 508). In the focusing configuration the resolution ellipsoid is oriented with its long axis perpendicular to Q , so the resolution parallel to Q is maximized. This mode yields an increase in neutron flux at the sample position of a factor 2 maintaining the resolution. The diffractometer can also be used in a standard configuration with in-pile collimators.



Applications

- measurement of Bragg reflections of powder samples and single crystals
- measurement of critical scattering close to a phase transition
- separation of diffuse scattering from Bragg reflections
- studies of specimen with weak scattering intensities such as adsorbed molecular layers on graphite substrates
(*B. Leinböck et al., Phys. Rev. Lett. 84 (2000) 1954*)

Selected examples

Study of the magnetic and critical behaviour of a PrCo_2Si_2 single crystal (*A.M. Mulders, HMI/BENSC Experimental Reports 1997*): the compound shows three different transitions characterized by propagation vectors $(0,0,1)$, $(0,0,25/27)$, and $(0,0,7/9)$, respectively. Figure 1 shows magnetic reflections around the (100) peak of the intermediate phase.

As a second example studies of hysteresis effects across an incommensurate-commensurate phase transition in $\text{Mn}_{0.87}\text{Fe}_{0.13}\text{WO}_4$ demonstrate the capabilities of E6 in magnetic structure determinations from powders. A selected part of typical diffraction patterns of this system is shown in figure 2 (*Y. Ding, PhD thesis 1999*).

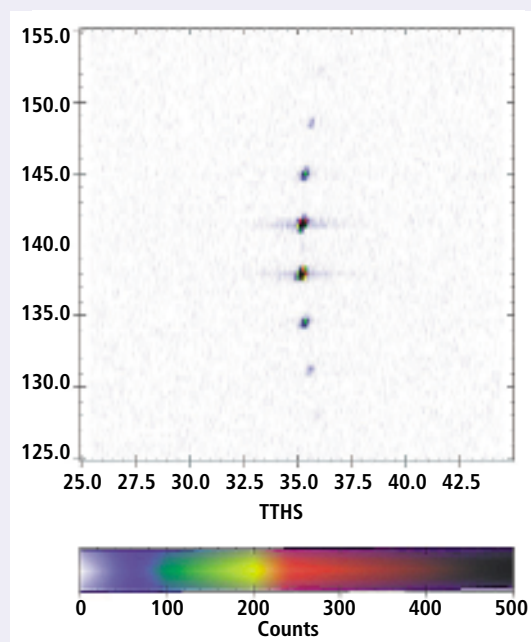


Fig. 1: Diffraction pattern around the (100) reflection of PrCo_2Si_2 at $T = 11.8$ K indicating a magnetic propagation vector $k = 0,0,25/27$

(*A.M. Mulders, HMI/BENSC Experimental Reports 1997*).

Instrument Data – E6

Beam tube	T4
PG Monochromator (002)	$27^\circ < 2\theta_M < 42^\circ$, $0.16 \text{ nm} < \lambda < 0.25 \text{ nm}$ standard operation at 0.24 nm because of 2 nd order contamination at other wavelengths
Neutron flux at sample	$5 \cdot 10^6 \text{ n/cm}^2\text{s}$ (0.24 nm double focusing at sample position and with open collimation)
Range of Scattering angle	$5^\circ < 2\theta_S < 110^\circ$
Detector	BF3 (1.5 bar) banana type with 200 channels of 0.1° width, oscillating radial collimator for background reduction
Inpile collimation	10', 20' and adjustable radial collimator
Software	Fully automated instrument control by CARESS software on a DEC Alpha workstation under VMS and DecWindows
Sample environment	available temperature range: 25 mK - 2000 K magnetic fields up to 7 Tesla
Instrument responsible	N. Stüßer, stuesser@hmi.de, direct dialing -3171

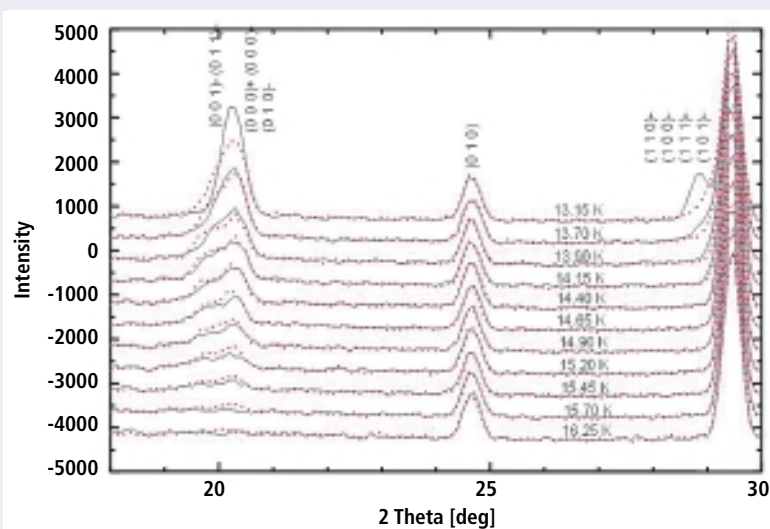


Fig. 2: Temperature behaviour of powder diffraction at $\text{Mn}_{0.87}\text{Fe}_{0.13}\text{WO}_4$. The straight and dotted lines show measurements at increasing and decreasing temperatures, respectively
(*Y. Ding, PhD thesis 1999*).

E9

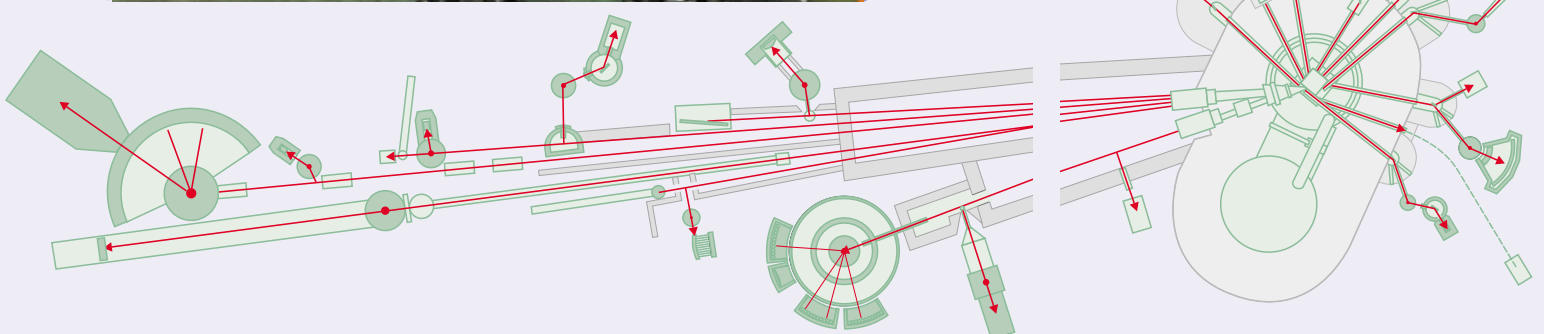
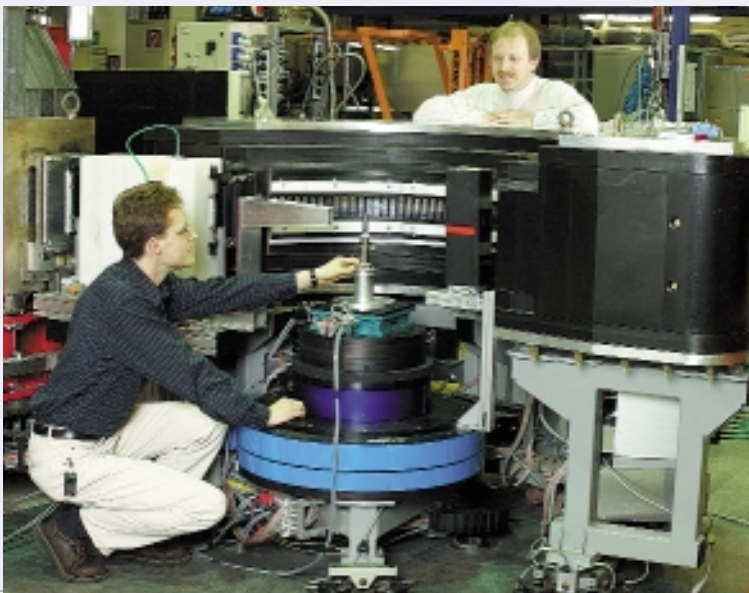
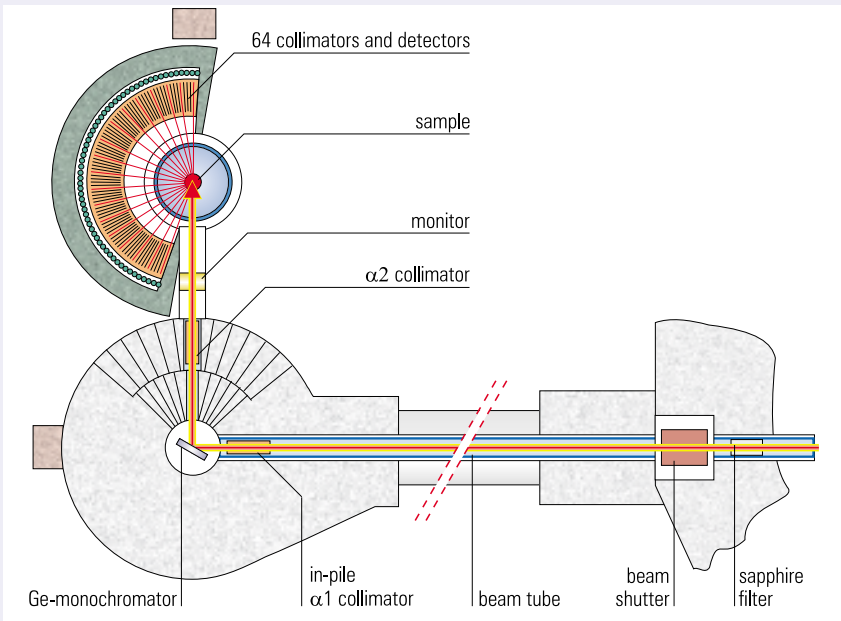
Neutron Powder Diffractometer (FIREPOD)

The instrument is dedicated to the determination and refinement of crystal structures with unit cell volumes up to 1000 Å³. In order to apply the Rietveld method successfully data sets of sufficient resolution and statistics depending on the complexity of the structure are needed. To fulfill these demands it was decided to design and build an instrument based on a classical angular dispersive diffractometer. Beside

the standard setting with a take-off angle at the monochromator above 90° the instrument allows to vary the take-off angle in a large angular range. In combination with the optional use of different reflecting planes of the Ge-monochromator crystal the diffractometer offers a great flexibility in the choice of wavelength and resolution.

Instrument description and applications

Since the main objective of the instrument is the determination and refinement of crystal structures high diffraction angles of $2\theta \approx 105^\circ$ at the monochromator are normally used. This standard setting results in a flat resolution function with a minimum width of the reflections at the 2θ -region with the highest density of reflections. A sapphire single crystal filter of total thickness of 110 mm in the primary beam is used to reduce the number of epithermal neutrons. In order to increase the neutron flux at the sample a vertically focusing Risø design Ge-monochromator is used. The detector bank consists of 64 x 10'-collimators in front of 64 ³He single detector tubes. The angular distance between two detectors is nominally 2.5° 2θ. By step



scanning this interval a diffraction pattern is obtained covering a total range of $160^\circ 2\theta$. The effective height of each of the detector tubes is 150 mm. The resulting vertical detector aperture is about 7° .

With collimations $\alpha_1 = 10'$ and $\alpha_2 = 20'$ (high-resolution mode) the highest possible resolution is achieved with FWHM of about $0.28^\circ 2\theta$ for the sharpest reflections. With α_1 removed (high-intensity mode) the in-pile collimation is about $18'$ and the lowest FWHM is about $0.33^\circ 2\theta$. With a maximum neutron flux at the sample of about $10^5 \text{ n}/(\text{cm}^2\text{s})$ in the high intensity mode the collection of a complete diffraction pattern usually takes about 7 h. In the high-resolution mode the intensity is decreased by about 50%. However, the design of the detector bank allows to use big sample container with a diameter of up to 15 mm (standard container: 8 mm) and thus a sample volume of about 5 cm^3 . Thereby the scattered intensity of low absorbing samples is increased by a factor of about three without reducing the instrumental resolution.

Selected examples

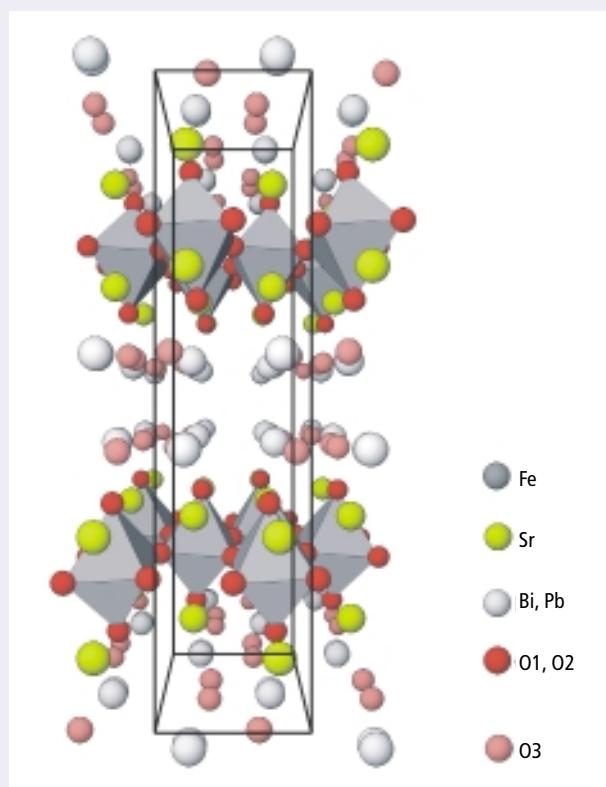
Taking advantage of the abilities of the E9 the structure of superconducting $\text{BiPbSr}_2\text{FeO}_{6.25}$ was refined from neutron powder diffraction data (3g sample amount, 15h measuring time in high-intensity setting). The neutron diffraction pattern allowed the refinement of isotropic displacement parameters and site occupation factors simultaneously. The strong anisotropic displacement of the iron atom could be refined. The data are in very good agreement with those given in the literature (N. Stüßer et al., *Z. Phys. B* 83 (1991), 165).

The structure of the superconductor $\text{BiPbSr}_2\text{FeO}_{6.25}$ refined by neutron powder diffraction data

Többens, D.M., et al., *Mat. Sci. Forum* (2000),
N. Stüßer et al., *Z. Phys. B* 83 (1991), 165

Instrument Data – E9

Beam tube	T 5, thermal flux about $10^{14} \text{ n}/\text{cm}^2\text{s}$ at the Be reflector
Monochromator	Focusing composite Ge with reflecting planes (311), (511) and (711), take-off angle $50^\circ \leq 2\theta \leq 130^\circ$, (511) normal to crystal surface, mosaicity FWHM = $17'$
Wavelength	0.12 - 0.28 nm (continuously adjustable)
Collimation	α_1 : $10'$ or $18'$ α_2 : $20'$ or $40'$
Detector bank	64 x ($10'$ -collimator and ^3He single detector with $\varnothing = 1.5''$ and 8 atm fill pressure) arranged on a radius of 1050 mm, precision of positioning $\leq 0.002^\circ$ in 2θ
Accessible 2θ range	$4^\circ - 158^\circ$
Vertical detector aperture	7°
Max. resolution $\Delta d/d$	$\approx 2 \cdot 10^{-3}$
Max. neutron flux at sample	$\approx 10^5 \text{ n}/\text{cm}^2\text{s}$
Sample environment	Cryostats and furnaces covering $200 \text{ mK} \leq T \leq 1800 \text{ K}$, pressure cells up to 2 GPa, magnets with $B \leq 6 \text{ T}$
Sample volume	Up to 5 cm^3 depending on sample environment
Instrument responsible	D. Többens, toebbens@hmi.de, direct dialing -2793 M. Tovar, tovar@hmi.de, direct dialing -2768



E10

HELINE

(³He Neutron experiment)

The instrument E10 is a two axis diffractometer located at the beam tube D15. It shares this beam tube, the primary shielding and the monochromator mechanics with the material research spectrometer E7. The beam for both spectrometers is separated by 1°. At the monochromator position 6 m away from the reactor core

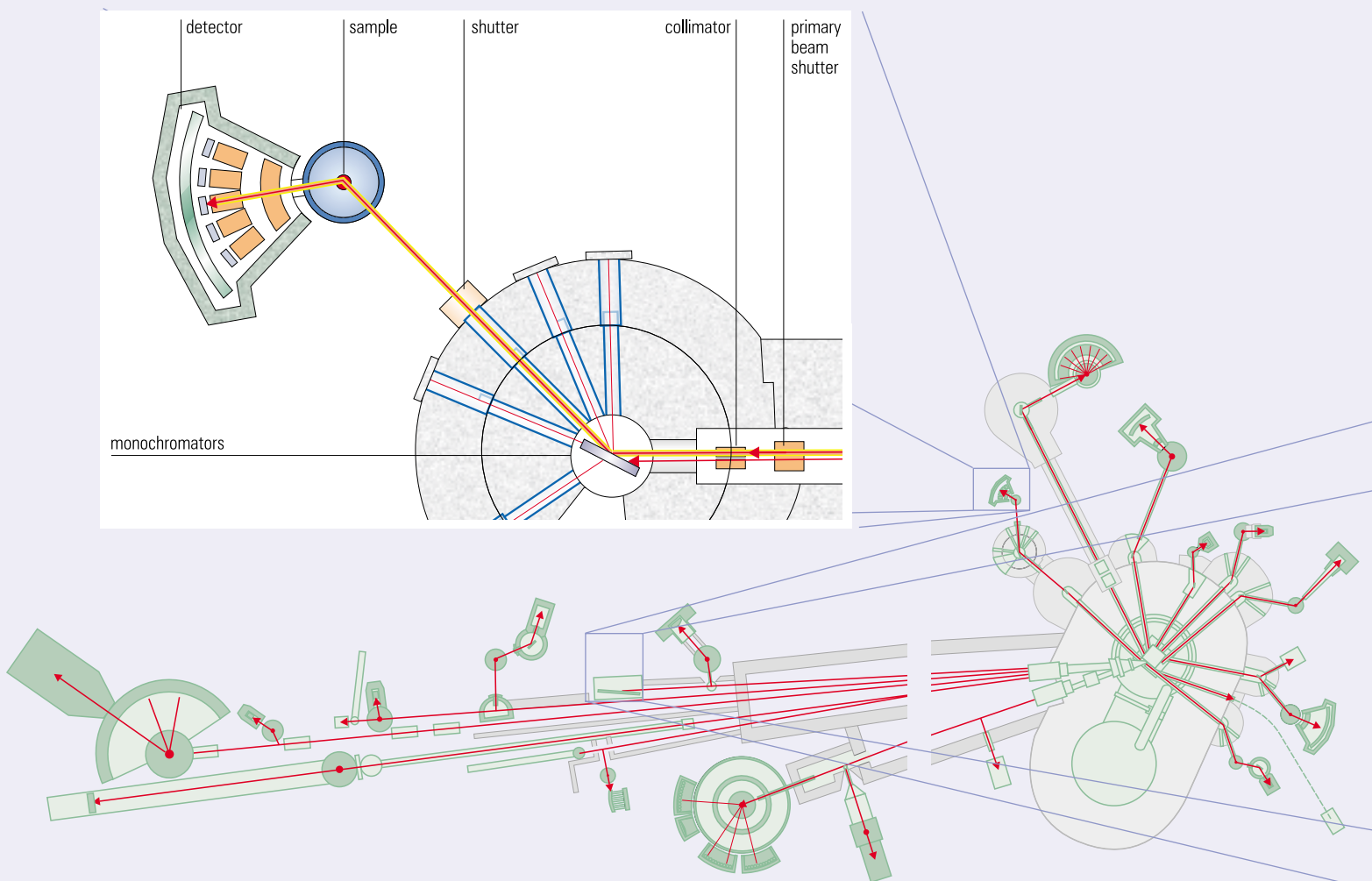
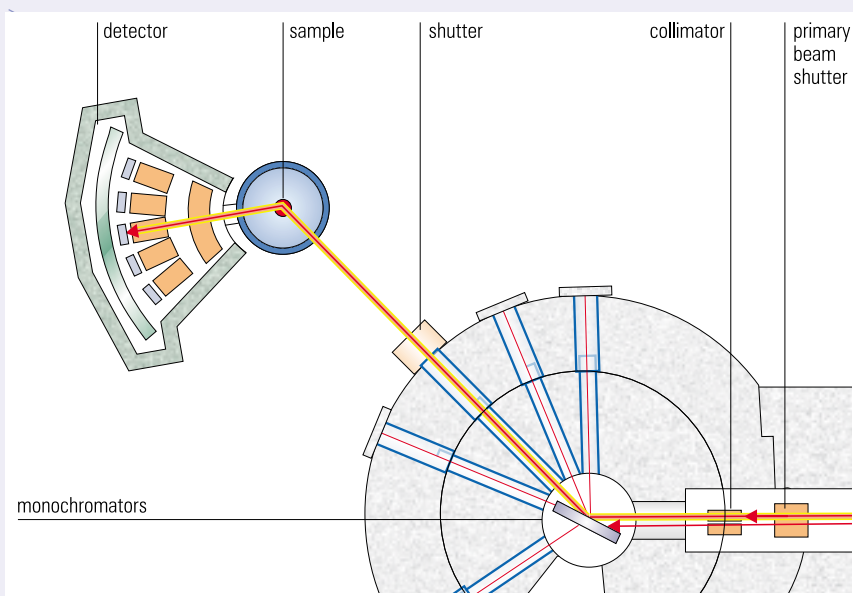
this results in a distance of 120 mm between the monochromators of both instruments. Two focusing monochromators with a height of 180 mm can be mounted on E10. Presently a pyrolytic graphite monochromator is installed, the second position will be used for a polarizing monochromator.

Instrument Data – E10

Primary beam tube	D15
Monochromator	PG (002), (vertically focusing) Fe ₃ Si (002) (Option)
Filter	in pile sapphire filter PG filter
Flux	at 0.15 nm expected: 1·10 ⁶ n/cm ² sec
Monochromator angles	2θ _M = 60°, 42°, 23° - 27°
Collimation	α ₁ = 0.25° (0.5° in pile, remote control of α ₁) α ₂ = 0.8°
Options	Thermal neutron guide with beam splitter Polarized neutrons with Fe ₃ Si-monochromator Lifting counter
Instrument responsible	K. Siemensmeyer, siemensmeyer@hmi.de, direct dialing -2757

The instrument E10 is designed for studies of nuclear magnetic order in solid ³He at ultralow temperature. As the absorption coefficient of ³He is very high an operating wavelength of 1.5 Å was chosen. The diffractometer is optimized for use with large cryostats and magnets. It has a vibration damping system and the spectrometer as well as the monochromator shielding is non magnetic.

To detect relatively small signals, it is equipped with 5 single counters which provide high detection efficiency. A second linear detector covers a scattering angle of 20° and can be used in parallel with the single counter system. Background reduction is achieved with a radial collimator in front of the single counter assembly and an 0.8° collimator in front of the sample.



B8

Irradiation Device for Neutron-Autoradiography

The instrument B8 allows to irradiate and activate artistic, technical, or geological items (foils, stones etc.) and other materials with cold neutrons and to investigate it afterwards with imaging plate technique and/or to analyse it with gamma-spectroscopy. It is mostly used for paintings but also usable for other purposes (neutron activation analysis).

The main utilisation of the irradiation facility will be within the common research project of the Hahn-Meitner-Institut Berlin and the Painting Gallery of the Berlin State Museum (Gemäldegalerie Berlin, Staatliche Museen Preussischer Kulturbesitz).

Advantages of the method

- Activation cross-section (n, β) depending on the isotope
- Different pictures depending on the half-lifetimes of the isotopes
- Low γ -radiation (cold source)
- non-destructive

Application Autoradiography of paintings

After neutron activation of a painting the induced β -decay is used to blacken highly

sensitive films or imaging plates to get the distribution of the pigments. The gamma-spectroscopy with a Ge-detector delivers information about the composition of the pigments. The image-plate technique allows direct digital processing.

With this method conceptual changes and corrections ("pentimenti") during the creation of the painting become visible. In some cases decisions about the authenticity can be made. The art historian or restorer receives valuable information about the brush of the artist and the actual condition of the painting.

Experimental principle

The painting is fixed on a support in front of a neutron guide end with the open area $3.5 \times 12.5 \text{ cm}^2$. The surface of the painting is adjusted under a small angle ($< 5^\circ$) with respect to the axis of

the guide. Thus a 12.5 cm wide strip of the painting is illuminated by the neutrons. The main free path of the neutrons within the paint layer is much longer than in the case of perpendicular transmission.

The support will be moved up and down with a velocity of a few cm/s in order to receive a uniform activation of the total area of the panel.

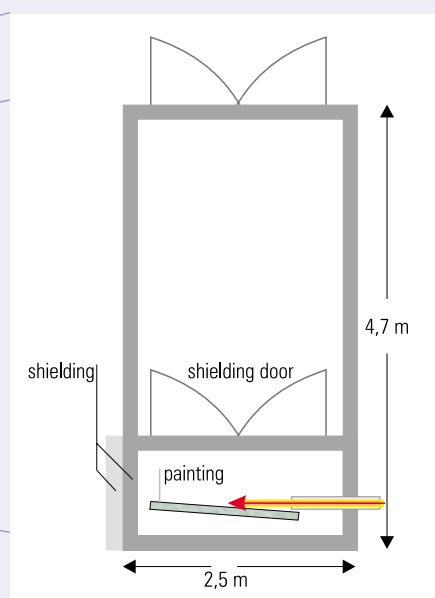
Set-up

The facility is installed in a secure closed container. The basic area of the container is $250 \times 450 \text{ cm}^2$.

On a special table in a shielded room in the basement the film exposure and the gamma-spectroscopy can be performed for the suitable times (up to more than four weeks) depending on the half-lifetimes of the isotopes.

Instrument Data – B8

Neutron guide	NL1A
Neutron guide cross section	$35 \times 125 \text{ mm}^2$
Wave length	white beam (cold spectrum)
Typical flux	$1 \cdot 10^9 \text{ n/cm}^2\text{s}$
Instrument responsible	B. Schröder-Smeibidl, schroeder-smeibidl@hmi.de, direct dialing -2337



V1

Diffractionmeter for Cold Neutrons with Area Detector

(Membrane Diffractionmeter)

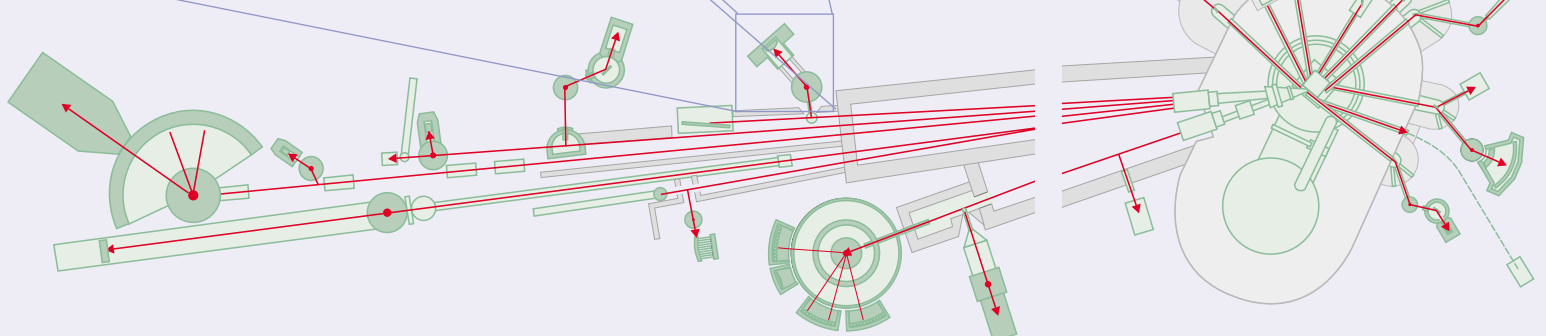
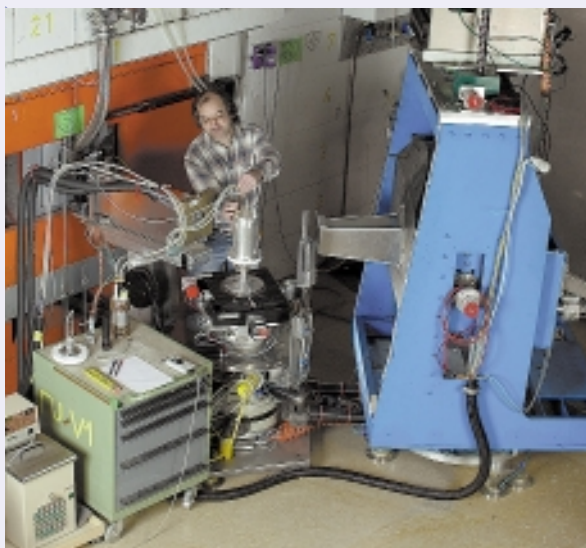
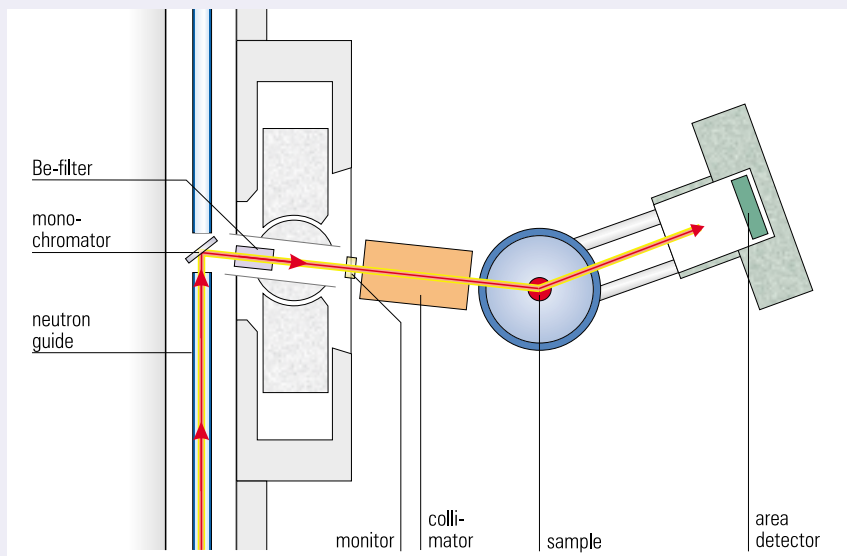
(Cooperative project with the Institut für Biochemie, TU-Darmstadt and the Institut für physikalische Biologie, Heinrich-Heine-Universität Düsseldorf)

The diffractometer V1 with variable incident wavelength is installed at the curved neutron guide NL 1A. It is equipped with a high-resolution area detector. The design of the instrument is dedicated for biological samples or other samples with large unit cells (5-10 nm in cell length).

Instrument Description

The diffractometer is located at the curved neutron guide NL 1A. The vertically focusing graphite monochromator provides adjustable wavelengths between 0.3 nm and 0.6 nm, making use of the full cross section of the neutron guide (3 cm wide, 12.5 cm high). A movable Be-filter at liquid nitrogen temperature may be used to suppress second order wavelengths below 0.39 nm. If less stringent collimation conditions allow, high flux at short monochromator-sample distances (approx. 80 cm) are made possible by a compact construction of shieldings. Sample and detector supports are movable on aircushions. The maximum Q value in all configurations with Be-Filter is limited to 22 nm^{-1} .

The ^3He -detector provides a sensitive area of $19 \times 19 \text{ cm}^2$ with a spatial resolution of $1.5 \times 1.5 \text{ mm}^2$. The sample-to-detector distance may be varied from 80 to 200 cm; the detector position is adjustable not only by $2\theta_s$ but also in height and inclination.



The sample support conforms with HMI standards, thus cryostates etc. may be mounted. For biological samples, special sample containers with humidity and temperature control are available. Sample preparation can be done in the biochemical laboratories.

Instrument control and data acquisition is implemented by CAMAC interfaced to a Compaq Alpha Workstation.

Applications

The instrument is designed for experiments with biological membranes, polymers, microemulsions, micelles and other partly oriented systems. The high spatial resolution of the detector is appropriate for studying reflections from biological single crystals and magnetic satellite reflections.

Selected examples

The possible interaction of the β -amyloid with lipid membranes was investigated with specifically deuterated peptides (Figures 1-3).

Instrument Data – V1

Beam tube	NL 1A
Type	Basic design: 2-axes diffractometer with χ - ϕ cradle ($\pm 10^\circ$) Options: 4-axes diffractometer, realized by additional χ - ϕ Eulerian cradle
Monochromator	pyrolytic graphite (002), vertically focusing
Wavelength	selectable between 0.3-0.6 nm (cold neutrons), corresponding to monochromator angles $2\theta_M = 60^\circ$ - 120° (not alterable during experiment)
angular range	-10° to 120° 2θ
Collimation	$\alpha_0 = 1^\circ$ at 0.45 nm (resulting from the ^{58}Ni -neutron guide) α_1 : defined by two slit systems
Monochromator-to-sample distance	0.8 m - 1.5 m (extendable)
Sample-to-detector distance	0.8 m - 2.0 m
Detector	^3He , 19 x 19 cm; pixel size 1.5 x 1.5 mm ² ; height and inclination adjustable
Software	HMI standard CARESS, with special features for area detector. Powder diffraction data evaluation
Instrument responsible	T. Hauß, hauss@hmi.de, S. Dante, sylvia.dante@hmi.de direct dialing -2071

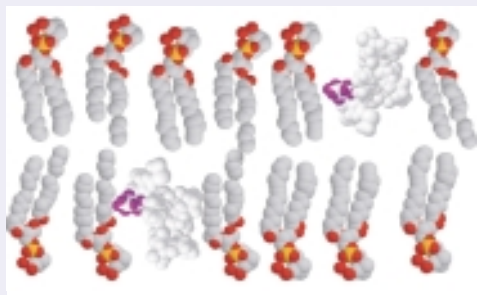


Fig. 1: A lipid membrane structure with a small β -amyloid peptide. The purple balls indicate the deuterium label in one specific amino acid.

Fig. 2: Lamellar diffraction pattern of a membrane sample.

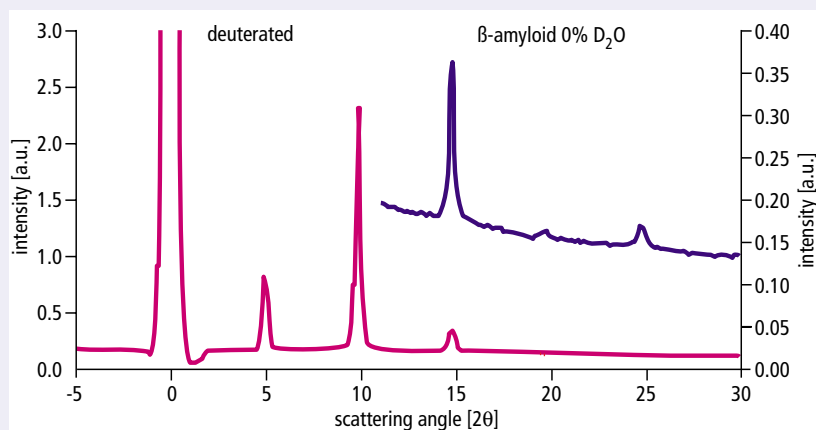
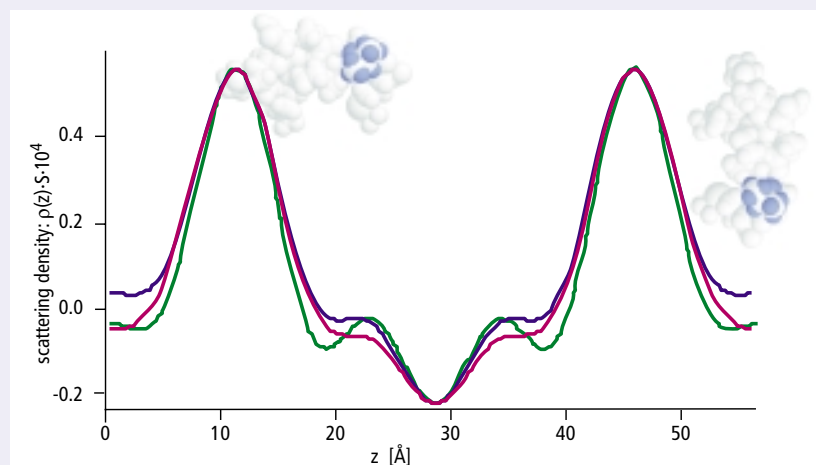


Fig. 3: Scattering density profiles of a lipid membrane (green) with protonated (red) and deuterated (blue) peptide. The positive difference of the latter profiles gives the location of the deuterium label.



Triple-Axis Spectrometer for Cold Neutrons (FLEX)

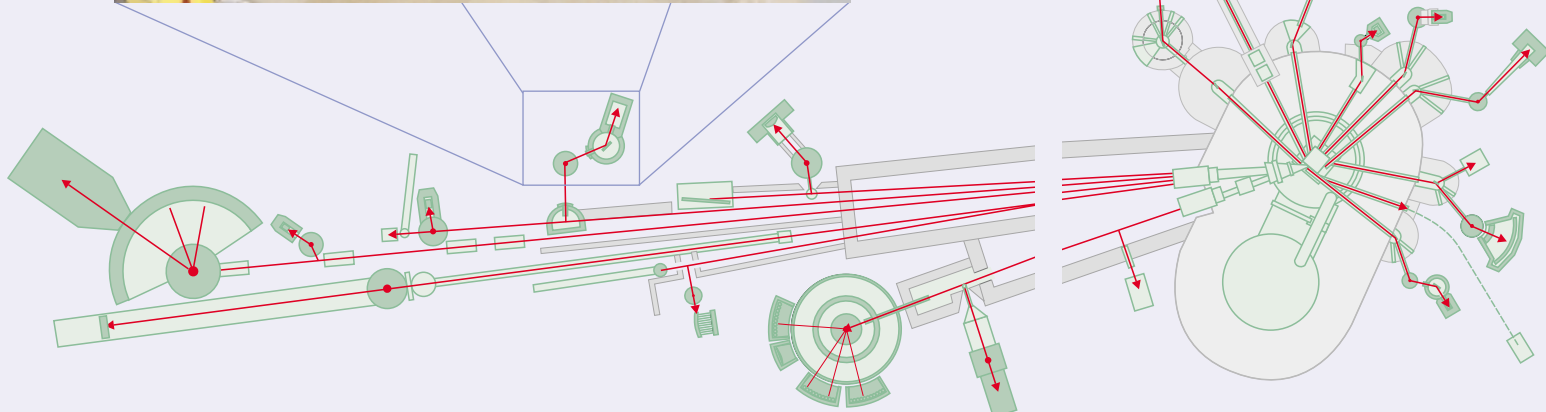
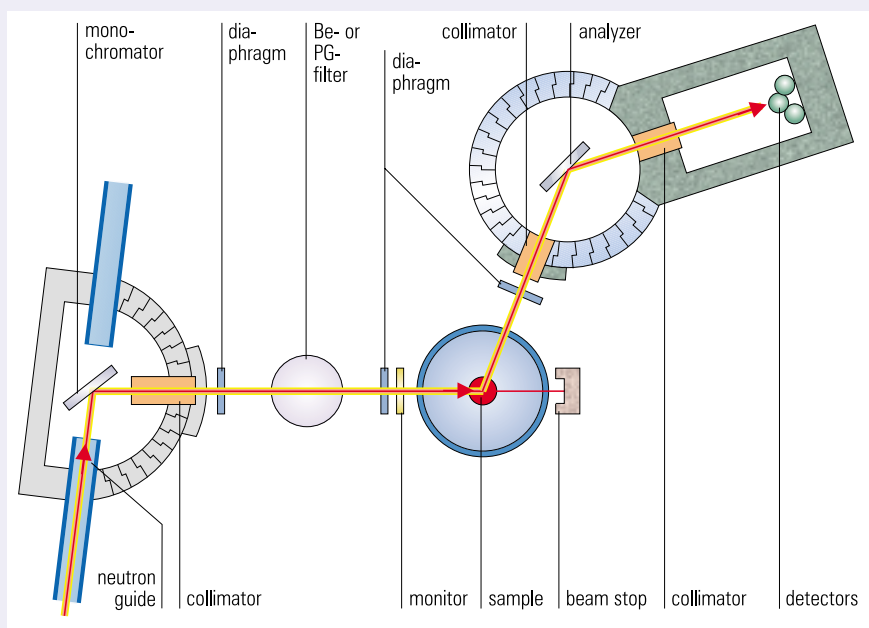
FLEX is a triple-axis spectrometer installed at the cold neutron guide NL 1B. The use of small incident neutron energies inherently gives good resolution properties. The instrument name is derived from the flexibility of the spectrometer parameters which permit non-standard experiments and methodical development.

Instrument description

The distances between monochromator and sample, between sample and analyzer and between analyzer and detectors can be varied in order to choose optimal scattering geometry for best intensity at the required angular and energy resolutions. For the same purpose a tunable curved monochromator and analyzer are used, and the detector solid angle can optionally be extended for diffuse scattering experiments.

In addition it is possible to insert collimators, second order filters and polarizing devices. The spectrometer is built using non-magnetic materials where possible, to allow the use of polarized neutrons in the same setup as for unpolarized neutrons.

A sketch of the instrument in the unpolarized set-up is given in the figure. The monochromator (vertically focusing) and the analyzer (horizontally focusing) are pyrolytic graphite (PG 002) strips. The monochromator angle range provides incident neutron wavelengths between 1.7 Å (27 meV) and 6.5 Å (1.9 meV). To eliminate second order ($1/2$) contamination of the



beam, a tunable pyrolytic graphite filter is used for $\lambda \leq 4 \text{ \AA}$ and a cooled Be filter for $\lambda \geq 4 \text{ \AA}$. These filters can also be placed on an optical bench in front of the analyzer. Positioning of the spectrometer modules is performed on air pads moving on a marble "Tanzboden". To allow automatic and continuous variation of monochromator and analyzer settings, the shielding wedges are lifted pneumatically. The position of the three vertical ^3He -detectors is adjustable by a translation table to achieve optimal conditions in the focused analyzer configuration.

The elastic energy resolution of the spectrometer, measured with a Vanadium rod as a function of neutron wavevector k , is shown in the small figure. Data are given for both, the standard set-up with typical collimations and the focused analyzer option.

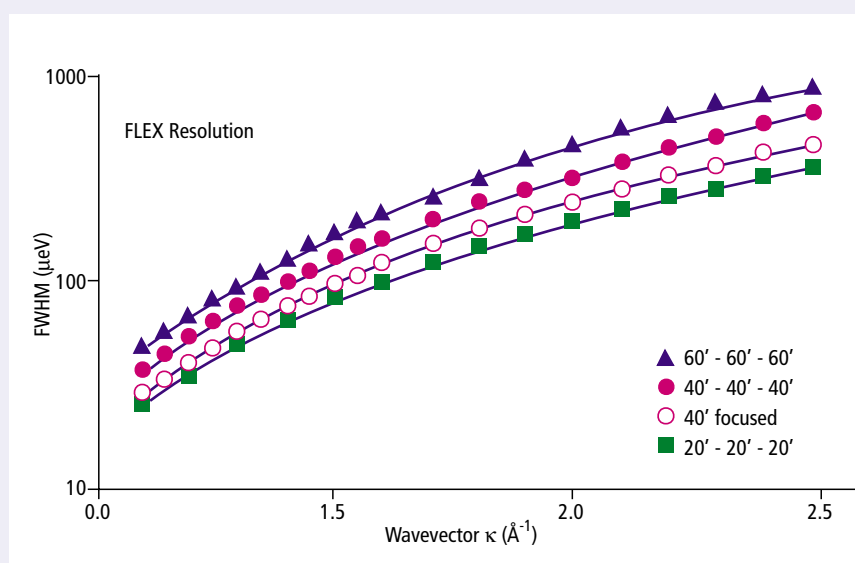
For the polarized beam option a transmission polarizer is available. A Heusler analyzer, mounted on a tunable horizontally focusing device, is expected to be available within the near future.

Applications

- low-energy phonon dispersion
- soft modes
- low-energy spin wave dispersion
- low-energy crystal field excitations
- quasielastic scattering

Instrument Data – V2

Neutron guide	NL 1B with beam cross-section 125 mm (height) x 30 mm (width) and a radius of curvature of 3000 m
Monochromator	Pyrolythic graphite (002), with variable vertical curvature
- angular range	$30^\circ < 2\theta_M < 150^\circ$
- wavelength range	$0.17 \text{ nm} < \lambda_M < 0.65 \text{ nm}$
- energy range	$1.9 \text{ meV} < E_M < 27 \text{ meV}$
Range of scattering angle at sample table	$-155^\circ < 2\theta_S < 155^\circ$ (with configurational restrictions)
Analyzer	Pyrolythic graphite (002), with variable horizontal curvature
Range of scattering angle at analyzer	$-130^\circ < 2\theta_A < 130^\circ$
Collimators	Gadolinium coated Soller collimators before sample, analyzer and detector; divergences 20', 40', 60'
Polarizer	Supermirror on silicon substrate in transmission
Polarization analyzer (foreseen)	Heusler (111), with variable horizontal curvature
Filters (optional)	Pyrolythic graphite (tunable), cooled beryllium
Flux at sample (unpolarized)	$4.5 \cdot 10^6 \text{ n/cm}^2\cdot\text{s}$ at 0.24 nm $2.5 \cdot 10^6 \text{ n/cm}^2\cdot\text{s}$ at 0.44 nm (with focused monochromator and 60' collimation)
Instrument responsible	P. Vorderwisch, vorderwisch@hmi.de, direct dialing -2171



Energy resolution (full width at half maximum) for elastic scattering as a function of the neutron wavevector k , measured for three typical collimations and for a configuration with focused analyzer.

Triple-Axis Spectrometer for Cold Neutrons (FLEX)

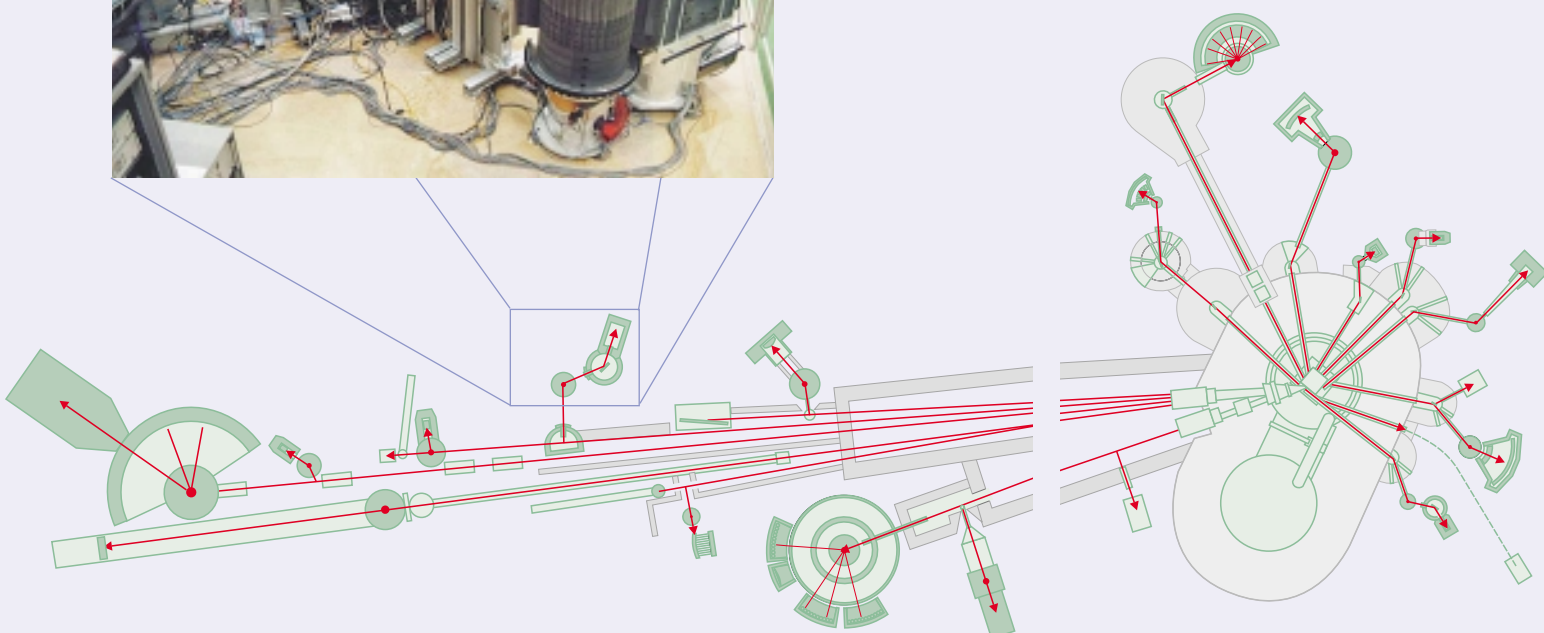
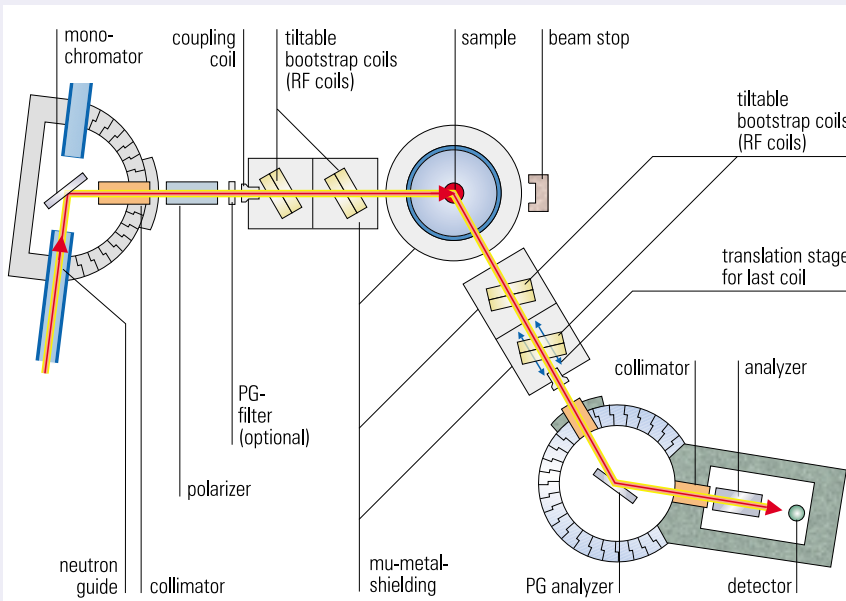
(b) NRSE-Mode

FLEX offers the unique possibility to combine triple-axis spectroscopy with high resolution spin-echo spectroscopy. The Neutron Resonance Spin-Echo technique (NRSE) is based on RF spin flippers replacing the Larmor precession solenoids used in conventional spin-echo spectrometers. This instrument is designed for the application of the 'tilted field' phonon focusing technique, which allows to measure linewidths of dispersive excitations with energy resolution in the order of μeV .

Instrument Description

Using the NRSE option on FLEX a polarizer/analyzer and two sets of RF-coils are inserted between monochromator and sample and between sample and energy-analyzer. The neutron flight paths between the RF-coils are screened by a mu-metal shielding. At the sample position a vertical tube which is divided into two parts to allow for free passage of the incoming and scattered neutrons reduces the residual field to less than 5 mG. The distance between the coils can be varied between 0.5 and 2.5 m (with configurational restrictions) to match specific resolution/intensity demands.

The main components of triple-axis- and spin-echo-instrument combined together can be seen in the photograph. Inside the open boxes (closed during the measurement) the tilted RF coils are also visible. The maximum beam cross section is restricted to $30 \times 30 \text{ mm}^2$ (at 45° tilt angle) by the coils which will be enlarged to $35 \times 50 \text{ mm}^2$ with a set of new coils in the near future. The transmission polarizers restrict the minimum available wavelength with polarized neutrons to 3.7 \AA . As a second order filter the tuneable PG filter can be used.



Applications

- linewidths of low-energy dispersive excitations in non-magnetic and antiferromagnetic samples
- quasi-elastic linewidths
- high-resolution elastic scattering (Larmor diffraction) with single crystal and powder samples

Selected Examples

As an example the experimental results on linewidths measurements of TA phonons in Pb are shown in Fig. 1. For this measurement the "background" triple axis spectrometer was operated in a configuration to minimize curvature effects. Tilt angles $\theta_1 = -32^\circ$ and $\theta_2 = +26^\circ$ were chosen.

The high flexibility in tilt angles without the need of field corrective elements allows high resolution elastic measurements without restricting the divergence of the incoming beam. Depending on the relative orientation of the fields the measurement is sensitive to either a spread in d-spacings or sample mosaic. The resolution does not depend on the scattering angle. Due to the fact that in the Larmor diffraction mode all coil faces have to be parallel to each other not all bragg peaks can be accessed although some flexibility is given by the choice of the incoming wavelength (see table for the restrictions in scattering angle).

Instrument Data – V2 in NRSE-mode

Monochromator	Pyrolythic graphite (002), with variable vertical curvature
- angular range	$67^\circ < 2\theta_M < 150^\circ$
- wavelength range	$0.37 \text{ nm} < \lambda_M < 0.65 \text{ nm}$ ($0.25 \text{ nm} < \lambda_M < 0.65 \text{ nm}$ in near future)
- energy range	$6 \text{ meV} < E_M < 27 \text{ meV}$
Range of scattering angle at sample table	
- inelastic mode	$-110^\circ < 2\theta_S < 110^\circ$
- elastic (Larmor diffraction) mode	$-110^\circ < 2\theta_S < -90^\circ$ or $90^\circ < 2\theta_S < 110^\circ$
Analyzer	Pyrolythic graphite (002), uncurved
Range of scattering angle at analyzer	$-130^\circ < 2\theta_A < 130^\circ$
Effective collimation	40', 40', 40'
Polarizer and analyzer	Supermirror on silicon substrate in transmission
Filter	Tuneable pyrolythic graphite
Flux at sample	$3 \times 10^5 \text{ n/cm}^2 \text{ s}$ at 0.37 nm
Maximum effective spin echo field	1000 Gauß
Spin-echo time range at 0.37 nm	600 ps - 10 ps
$\Delta d/d$ resolution in diffraction mode at 0.37 nm	3×10^{-4} (FWHM)
Instrument responsible	K. Habicht, habicht@hmi.de, direct dialing -2807

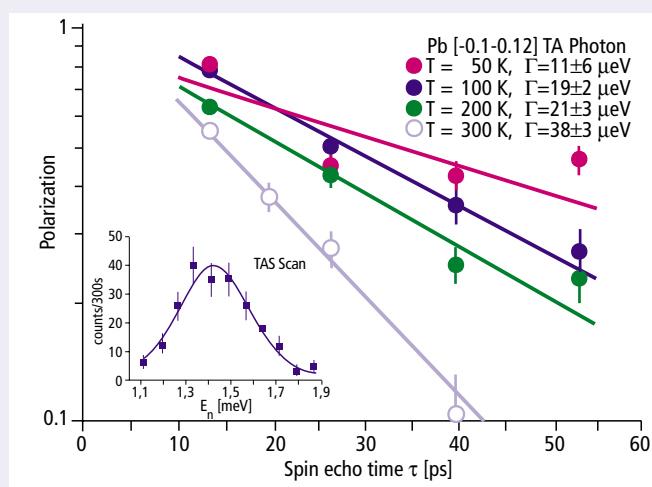


Fig. 1: Linewidths of TA phonons in Pb for different sample temperatures showing the effect of anharmonic forces: The TAS spectrometer is operated in a configuration giving highest Q resolution with an energy resolution of $365 \mu\text{eV}$ (see insert for TAS-scan). The NRSE data has been fit to a model assuming a linear dispersion relation and a Lorentzian lineshape. Γ is the HWHM Lorentzian linewidth.

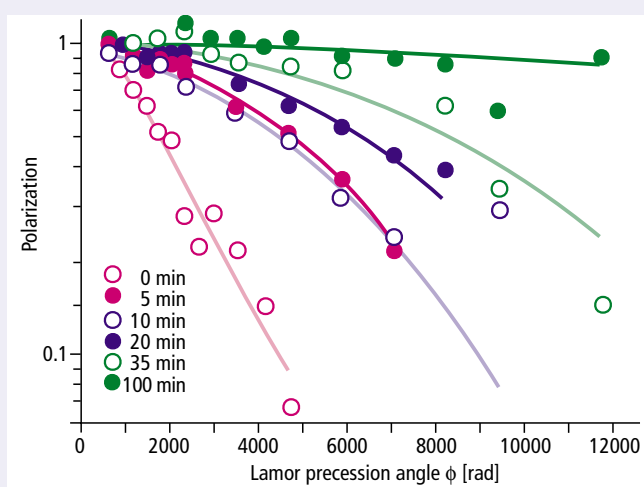


Fig. 2: Polarization as a function of total Larmor precession angle for mechanically deformed and heat treated polycrystalline Al samples with different annealing times (indicated in the figure). Assuming a single Gaussian distribution in $\Delta d/d$ FWHMs ranging from 1.5×10^{-3} to 1.2×10^{-4} can be extracted from the data. However the data of the samples with annealing times 0 - 10 min better fits a model assuming two Gaussian distributions favouring the two component model suggested by material scientists.

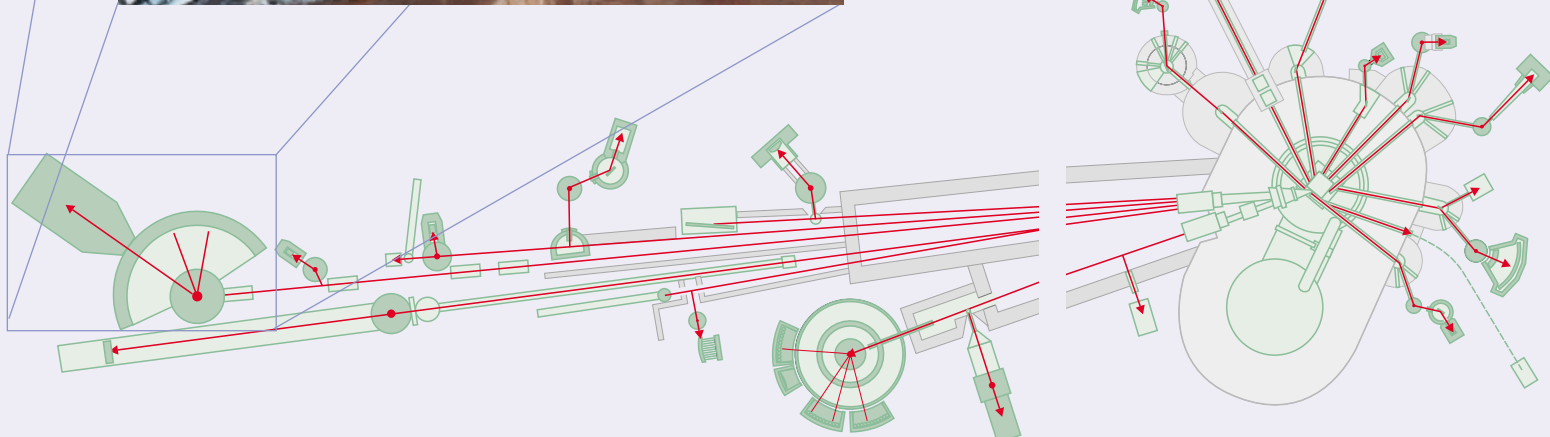
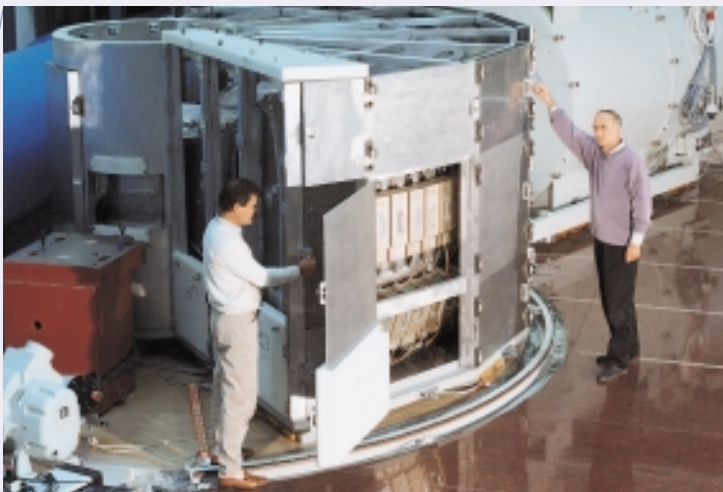
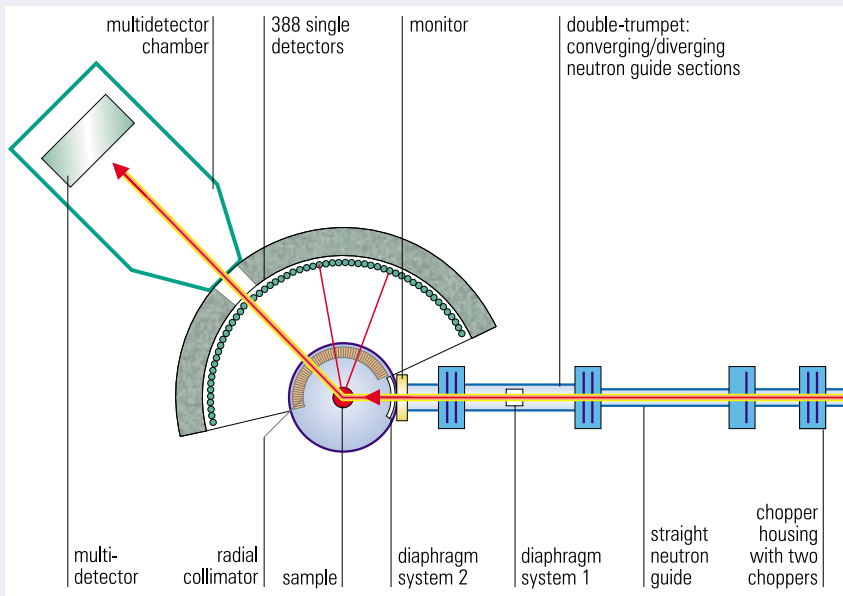
Time-of-Flight-Spectrometer (NEAT)

NEAT is a multichopper spectrometer for inelastic neutron scattering experiments in the region of medium to very small energy and momentum transfers, including inelastic small-angle scattering (e.g. quasi-elastic or Brillouin scattering).

Instrument Description

The primary part of the spectrometer creates a pulsed monochromatic neutron beam with the aid of seven phased disk choppers. The time and energy widths of the neutron pulses are variable in large ranges via the variation of the chopper speed, the chopper windows and the neutron wavelength. Divergence and spatial extension of the incident neutron beam are controlled by the last section of the beam line before the sample. Here the supermirror coated „double-trumpet“ guide section assures reduced pulse width with little intensity loss. Optionally this section can be replaced by a diaphragm system, in order to achieve the beam collimation required for small-angle scattering experiments.

The secondary part of the spectrometer is equipped with a ^3He two-dimensional position-sensitive detector („multidetector“, MD) comprising (64 x 64) detector elements for inelastic small-angle scattering and an array of 388 ^3He single detectors (SD) for large-angle scattering. While the single detectors are mounted at a fixed distance from the sample, the distance from the sample to the multidetector is variable.



Furthermore the multidetector can also be used for large-angle scattering in the same range of distances. This permits an appreciable increase of energy and momentum resolution in regions of the solid angle selected by the user.

Applications

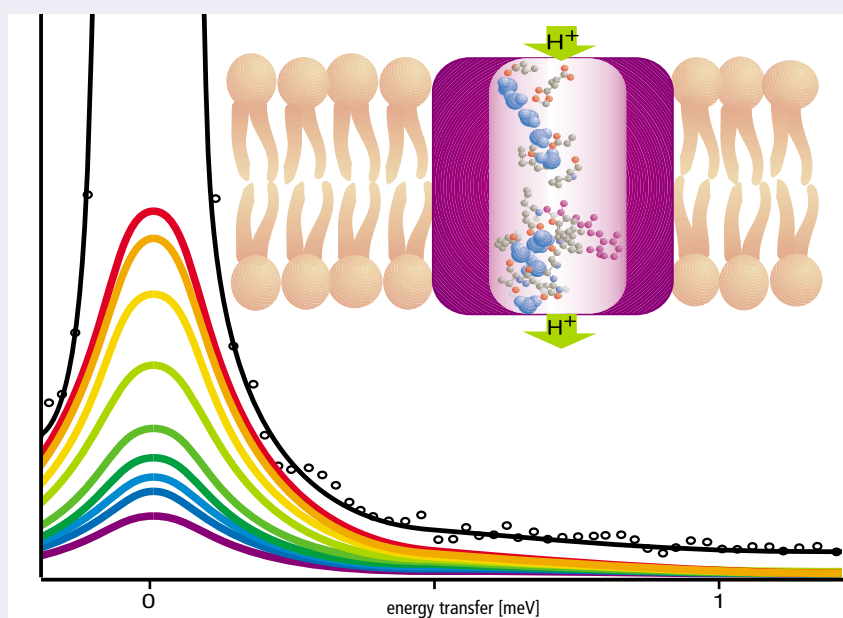
- Dynamics of quantum liquids and rotational tunneling in molecular crystals.
- Crystal field splitting.
- Local and long-range diffusion in disordered systems such as simple classical and molecular liquids, solutions, amorphous solids (superionic, orientational, and spin glasses), polymers, molecular crystals, hydrogen-metal systems, protonic conductors, ionic conducting rotor phases.
- Critical scattering phenomena in dense gases and solids.
- Spin dynamics in high-TC superconductors
- Dynamics of biological systems and soft matter, including proteins, enzymes, biological membranes, hydration water, sugar- and other bio-organic solutions and gels.

Selected example

Investigation of picosecond internal diffusive motions occurring in the light-driven proton pump Bacteriorhodopsin, which is part of the Purple Membrane (see figure).

Instrument Data – V3

Neutron guide	NL 2 (upper part)
Guide cross-section	30 x 55 mm ²
Double-trumpet cross-section at chopper (1,2)	15 x 55 mm ²
Chopper windows	15 x 60 mm ² , 30 x 60 mm ² and 60 x 60 mm ²
Distance chopper (1,2) chopper (6,7)	11970 mm
Chopper speed range	750 rpm, 1000 rpm to 20000 rpm
Incident wavelength range for monochromatic measurements	0.18 nm ≤ λ ₀ ≤ 1.9 nm;
white beam spectrum	0.1 ≤ λ ₀ ≤ 3.4 nm (limits correspond to 1 % level of flux maximum at 0.45 nm in the monitor spectrum of the incident beam)
Elastic energy resolution (FWHM) at SD	6 μeV ≤ ΔE ≤ 5400 μeV
Elastic energy resolution (FWHM) at MD	2 μeV ≤ ΔE ≤ 3800 μeV
Flux at the sample for λ ₀ = 0.6 nm (example)	2 · 10 ⁴ n/cm ² s for the following elastic energy resolutions: ΔE = 250 μeV (FWHM) for SD ΔE = 130 μeV (FWHM) for MD
Range of scattering angles for SD	13.35° ≤ φ ≤ 136.65°
Angular range accessible to MD elements	1.0° ≤ φ ≤ 137°
Distance sample-SD	2500 mm
Distance sample-MD	4080 mm ≤ L ≤ 7300 mm
Sample environment	maxi-cryostat 1.5 K ≤ T ≤ 300 K (100 mm diam.) cryofurnace 1.5 K ≤ T ≤ 570 K (80 mm diam.) HT-furnace 300 K ≤ T ≤ 1270 K (70 mm diam.)
Instrument responsible	R. E. Lechner, lechner@hmi.de direct dialing -2780



The quasielastic incoherent neutron scattering spectra measured with NEAT as a function of temperature in the temperature range from 220K (violet curve) to 300K (red curve). For clarity, only the 300K experimental data (including the elastic component) together with the theoretical curves of the quasielastic components, as obtained from fits to the spectra at 300K and at all other temperatures, are shown.

V4

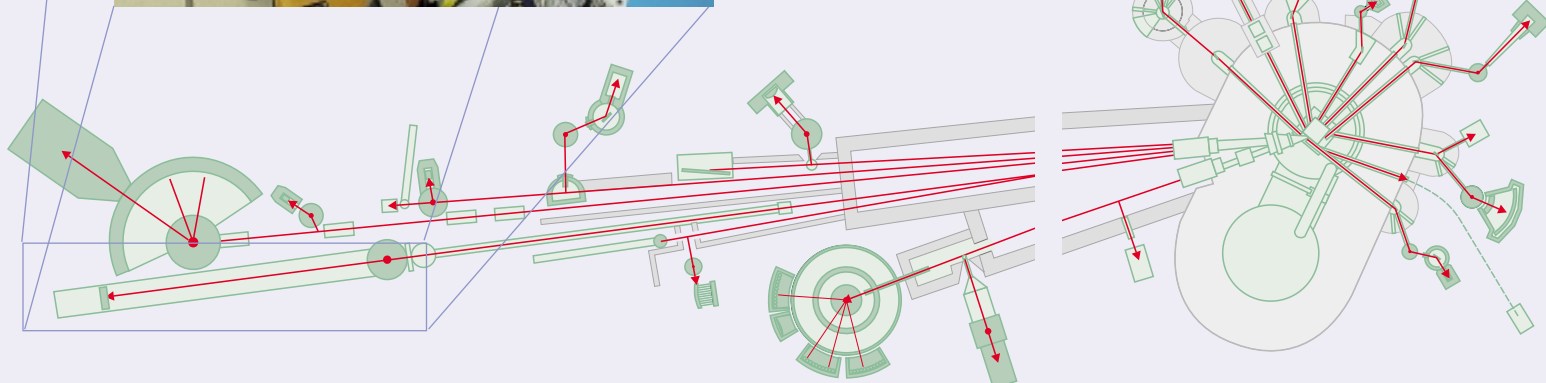
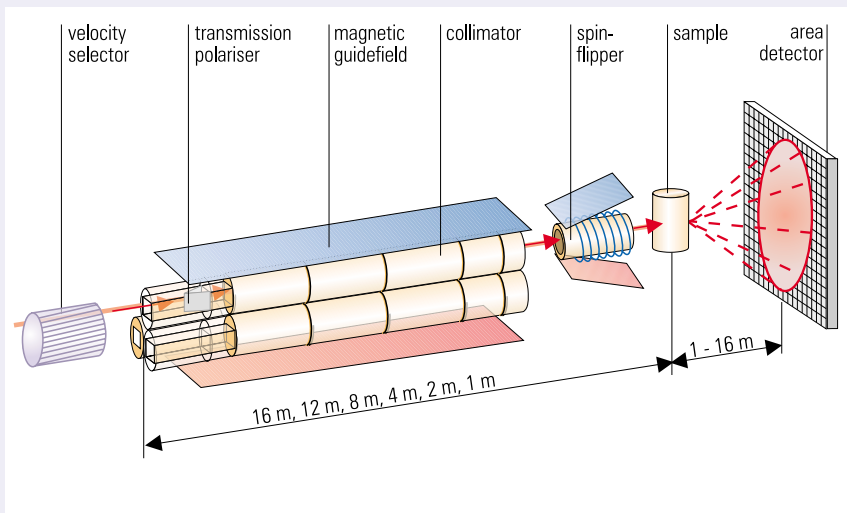
Small Angle Neutron Scattering Instrument (SANS)

The SANS instrument V4 covers a Q-range from 10^{-2} nm^{-1} to 8.5 nm^{-1} allowing density composition and magnetization fluctuations in materials to be measured on a length scale from 0.5 nm to 400 nm.

Instrument Description

The instrument is installed at the curved neutron guide NL 3 A. Incoming neutrons are monochromatized by a mechanical velocity selector with variable wavelength from 0.38 nm to 3 nm.

The two-dimensional ^3He -detector with 64×64 elements of $10 \times 10 \text{ mm}^2$ can be positioned at any distance between 1 m and 16 m from the sample in the horizontal direction. Additionally, at 1 m distance the detector can be moved vertically by 0.3 m extending the Q range to higher values. A large sample chamber is connected to a vacuum system with the detector and collimator tubes. It can be equipped with a temperature controlled sample changer ($5^\circ\text{C} - 80^\circ\text{C}$), electromagnet (2 T) with sample changer or heatable sample stick (600°C), a high temperature furnace (1800°C), an Eulerian cradle, with an *in-situ* adsorption device SANSADSO or with BENS standard sample environments (horizontal and vertical cryomagnets, orange cryostats). Shear cells for high temperatures and magnetic fields are under construction.



The instrument is fully controlled via CAMAC by an ALPHA workstation using the instrument control program CARESS.

Polarized Neutrons: SANSPOL

Polarized neutrons are available at the instrument. A high-transmission supermirror polarizer can be introduced by remote control in front of the 12 m collimation without any modification of the instrument alignment. The polarization direction can be reversed by a RF gradient spin-flipper in front of the sample. The SANSPOL option is characterized by a high neutron flux of more than 30% of the non-polarized beam, a high degree of polarization ($> 90\%$) and high efficiency of the spin-flipper ($> 95\%$) for $\lambda < 1.8$ nm without any additional background.

Applications

- Nanoscaled materials
- Phase separation in alloys and glasses
- Morphologies of superalloys
- Magnetic correlations
- Microporosity in ceramics
- Interfaces and surfaces of catalysts
- Biological macromolecules
- Polymers and membranes
- Flux line lattices in superconductors

Data Reduction Software

The "BerSANS" data reduction software package has been developed by Uwe Keiderling and is constantly being expanded to offer new options and data treatment tools. It contains a set of programs for automated two-dimensional and one-dimensional reduction of large amounts of data files and a set of graphical tools for data analysis, documentation, and publication.

References:

U. Keiderling, A. Wiedenmann: *New SANS Instrument at the BER II Reactor in Berlin, Germany Physica B 213 and 214 (1995) 895-897*
 T. Keller, T. Krist, A. Danzig, U. Keiderling, F. Mezei, A. Wiedenmann: *Design and Performance of the Polarized Beam at the SANS Instrument at the BER II Reactor. Nucl. Instruments and Meth. A 451 (2000) 474-479*

Instrument Data – V4

Neutron guide	NL 3A, curved, Ni coated, with cut-off $\lambda = 0.38$ nm
Monochromator	mechanical velocity selector
Wavelengths	$0.38 \text{ nm} < \lambda < 3 \text{ nm}$
Wavelength resolution	$8\% < \Delta\lambda / \lambda < 18\%$ (FWHM)
Q-range	$0.01 \text{ nm}^{-1} < Q < 8.5 \text{ nm}^{-1}$
Polarizer	CoFe-Si supermirror with $\theta_{\text{crit}} = 2.2 \theta_{\text{crit}}(\text{Ni})$ transmission geometry: $\alpha = 0.475^\circ$, $\lambda = 1.8$ nm
Detector	2D-position sensitive detector 64 x 64 elements with $10 \times 10 \text{ mm}^2$
Collimation	
Entrance window	$50 \times 30 \text{ mm}^2$
Collimator length	1 m, 2 m, 4 m, 8 m, 12 m (for SANSPOL), and 16 m.
Distances sample-detector	
Horizontal	1 to 16 m continuously
Vertical	0 to 0.3 m only at 1 m position
Option	Polarisation analysis using ^3He transmission analyser and RF spin-flipper
Flux at sample	$2 \times 10^7 \text{ ns}^{-1}\text{sr}^{-1}$ at $\Delta\lambda / \lambda = 10\%$ and collimation 2 m
Instrument responsible	A. Wiedenmann, wiedenmann@hmi.de, direct dialing -2283

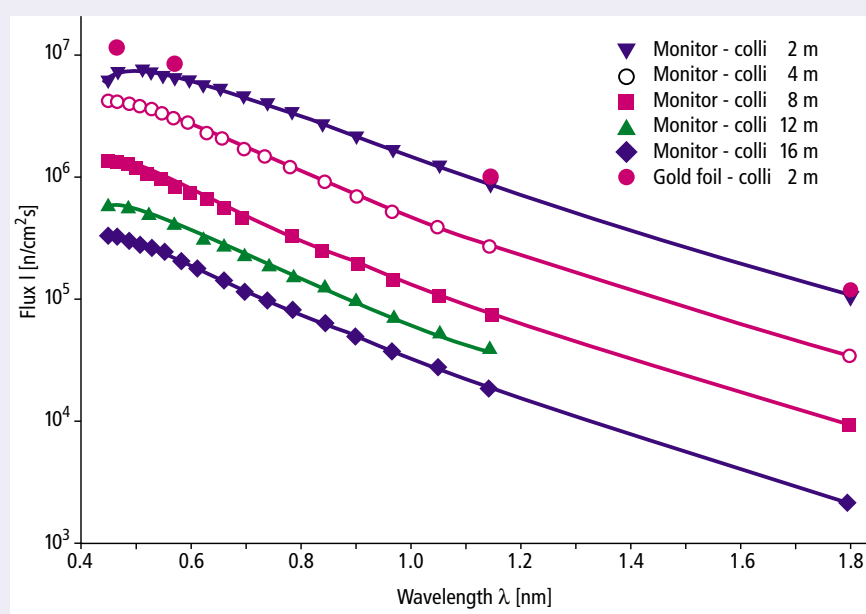


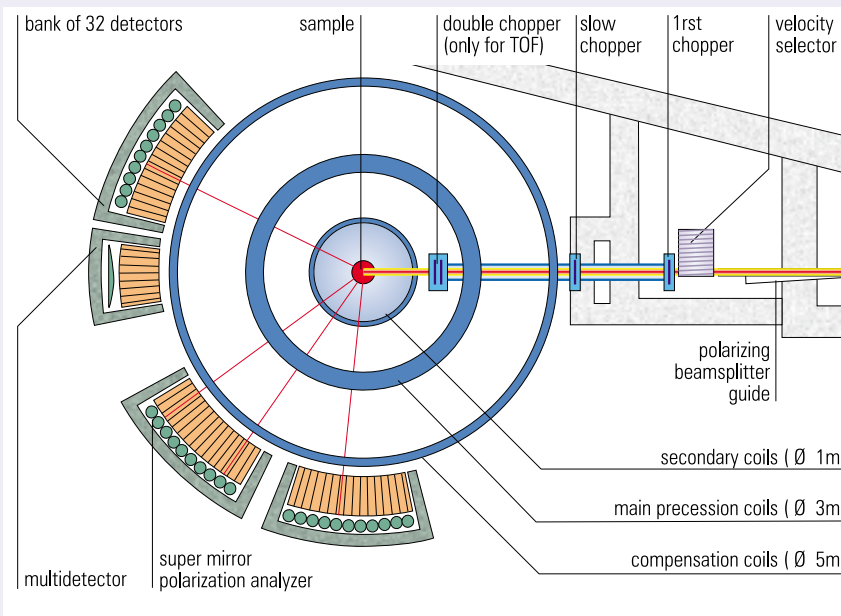
Fig. 1: Total flux at the sample position for resolution $\Delta\lambda / \lambda = 10.5\%$ for different collimation lengths, measured with a calibrated monitor and by gold foil irradiation.

Spin-Echo Spectrometer (SPAN)

Exploring complex systems often requires the combination of spectra covering a broad range both in energy and in momentum transfer (q). The design of SPAN fulfils these requirements and allows for reaching a very wide dynamic range of more than four orders of magnitude by combining the Neutron Spin Echo (NSE) technique with a medium resolution time of flight (TOF) analysis on the same instrument. SPAN also provides optimal intensity conditions for polarization analysis in both diffuse and inelastic scattering.

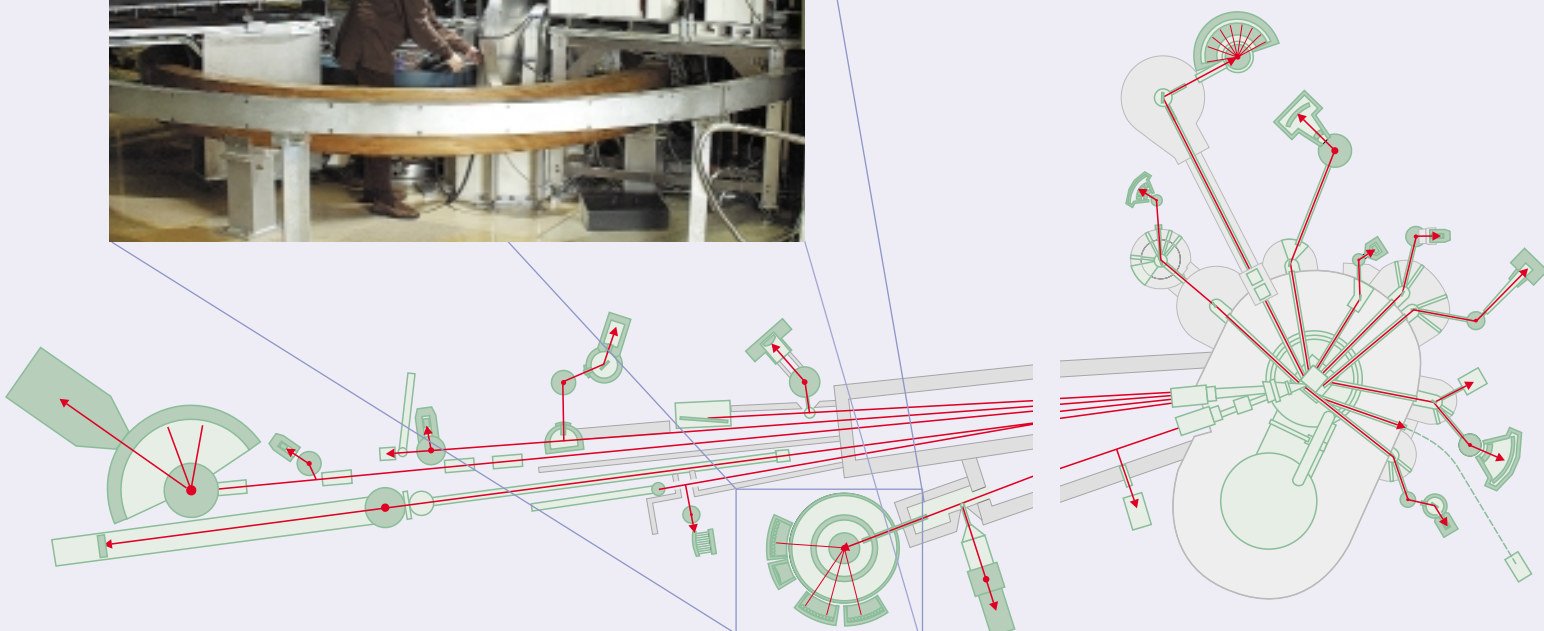
Instrument Description

a) Wide angle neutron spin echo Neutron spin echo (NSE) is the highest energy resolution neutron scattering technique available and allows to examine a large area in time and space in condensed matter physics. Almost thirty years after the discovery of Neutron Spin Echo, however, the large majority of NSE spectrometers are single-detector type. This is due to the tight conditions for the homogeneity of the magnetic field integral (10^{-4} - 10^{-5}) along all neutron trajectories.



The magnetic field configuration realized with the spectrometer SPAN is unique and allows for Wide Angle NSE, i.e. for simultaneous NSE measurements over a wide angular range. The set-up has a symmetry axis, which is vertical and crosses the horizontal scattering plane at the sample position. The resulting magnetic field integral is the same for all scattering angles and NSE can be done simultaneously over the whole angular range accessible to the spectrometer: from -30° up to almost 150° .

The precession field of SPAN is created by the three pairs of coils with diameters of 1 m, 3 m and 4.8 m. Each pair is mounted in a Helmholtz-like fashion, one coil above and one coil below the scattering plane. The main precession magnetic field is created by the coils with a diameter of 3 m, which have antiparallel electric currents. The resulting magnetic field is horizontal with the required axial symmetry in the



scattering plane. The coils with a diameter of 1 m shape the magnetic field around the sample whereas the coils with a diameter of 4.8 m control the axial component of the magnetic field at the position of the $\pi/2$ flippers.

The magnetic field integral of SPAN reaches 0.06 T m, i.e. $\sim 1/3$ of IN11. The present NSE configuration covers an energy range of $300 \mu\text{eV} \geq \omega \geq 1 \mu\text{eV}$ at 3.8 \AA and $24 \mu\text{eV} \geq \omega \geq 80 \text{ neV}$ at 9 \AA respectively. The corresponding Fourier time range ranges from $2.2 \text{ ps} \leq t \leq 0.66 \text{ ns}$ at 3.8 \AA to $0.027 \text{ ns} \leq t \leq 8.2 \text{ ns}$ at 9 \AA respectively.

b) Time-of-flight

In the TOF configuration, the neutrons pass through two single and one double chopper. The choppers have a diameter of 700 mm and rotate at a maximum speed of 10000 rpm. In order to improve the resolution and flexibility of the set-up, the double chopper located just in front of the sample is made of two counter-rotating discs. This design offers the possibility to choose between two different sets of windows. The elastic TOF resolution typically amounts to 0.1 meV FWHM at 7 \AA .

TOF measurements are usually done with all detectors. In that case the analyzers in front of the detectors can be replaced by radial collimators. It is also possible to combine polarization analysis and TOF. In this case only detectors equipped with analyzers can be used.

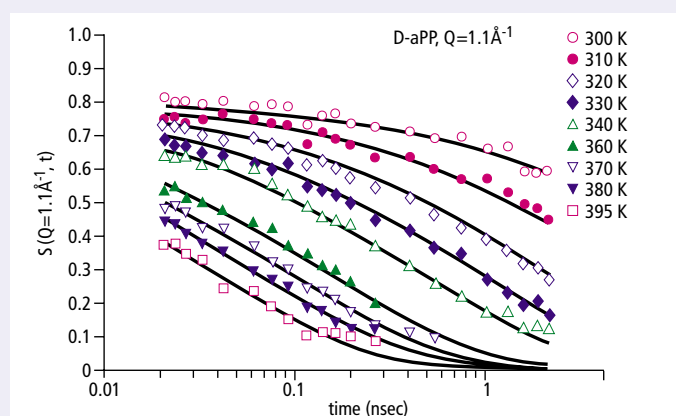


Fig. 1: NSE spectra collected at $\lambda=4.5 \text{ \AA}$ on a deuterated atactic Polypropylen (aPP) sample. The measurements were performed above the glass transition temperature ($T_g = 237 \text{ K}$) at $Q = 1.1 \text{ \AA}^{-1}$, the first interference peak of the static structure factor $S(Q)$, which corresponds to intermolecular correlations. The relaxation becomes slower as the temperature approaches the glass transition temperature. The temperature dependence of the relaxation scales with the macroscopic viscosity. The continuous lines represent a fit of the data to the Kohlrausch-Williams-Watts (KWW) function. All data were fitted simultaneously by keeping the amplitude and the stretched exponent independent of temperature.

(after V. Arrighi, A. Triolo, C. Pappas, *Proceedings of QENS'2000, Edinburgh, UK, 31st August - 1st September 2000, Physica B*).

Instrument Data V5 Spin-Echo Spectrometer SPAN

Neutron guide	Polarizing cavity NL4 with FeCo-Si Supermirrors produced in HMI
Neutron guide cross section	100 x 58 mm
Beam monochromatization	-15% FWHM (velocity selector)
Incident wavelength	between 0.25 nm and 1 nm
Distance sample - detectors	3.5 m
Angular range	between -30° and 150°
Range of momentum transfer	at 0.38 nm : $0.006 - 0.32 \text{ nm}^{-1}$ at 0.9 nm : $0.0025 - 0.135 \text{ nm}^{-1}$
Maximum sample area	$4 \times 4 \text{ cm}^2$
Maximum magnetic field integral	$6 \cdot 10^4 \text{ Oe cm}$
Fourier time range	at 0.38 nm : $0.005 - 0.6 \text{ ns}$ at 0.9 nm : $0.066 - 8 \text{ ns}$
Energy range (NSE)	at 0.38 nm : $120 \mu\text{eV}^{-1} \mu\text{eV}$ at 0.9 nm : $10 \mu\text{eV} - 82 \text{ neV}$
TOF resolution at $\lambda=7 \text{ \AA}$	$100 \mu\text{eV}$
Instrument responsible	C. Pappas, pappas@hmi.de, direct dialing – 2046

Applications

- Phase transitions
- Disordered magnetic Systems (e.g. spin glasses)
- Dynamics of the glass transition
- Lifetime of elementary excitations
- Transport phenomena in porous materials
- Quantum diffusion

Selected Examples

- NSE spectra of atactic Polypropylene (aPP) above the glass transition temperature (Fig. 1)
- NSE spectra of the frustrated disordered magnetic system $\text{CdCr}_{1.8}\text{In}_{0.2}\text{S}_4$ (Fig. 2)

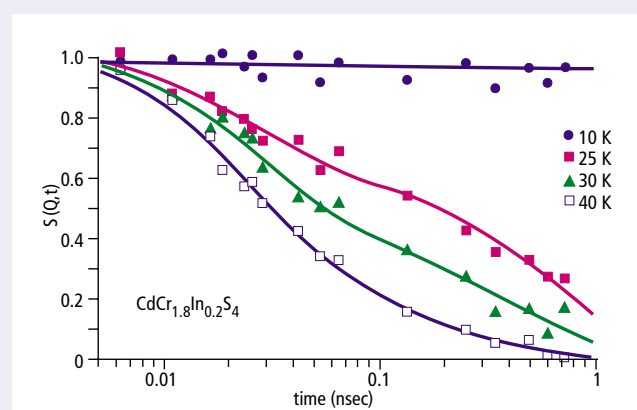


Fig. 2: Paramagnetic spin echo spectra obtained at 4.5 \AA and $Q=0.082 \text{ \AA}^{-1}$ in the 3D-Heisenberg frustrated disordered magnetic compound $\text{CdCr}_{1.8}\text{In}_{0.2}\text{S}_4$, the behaviour of which is at the cross-over between ferromagnetism and spin glass state. The spectra show a double exponential relaxation with two characteristic times t_1 and t_2 corresponding to a fast and slow component respectively.

After S. Pouget, M. Alba, C. Pappas (2000)

V6 Reflectometer

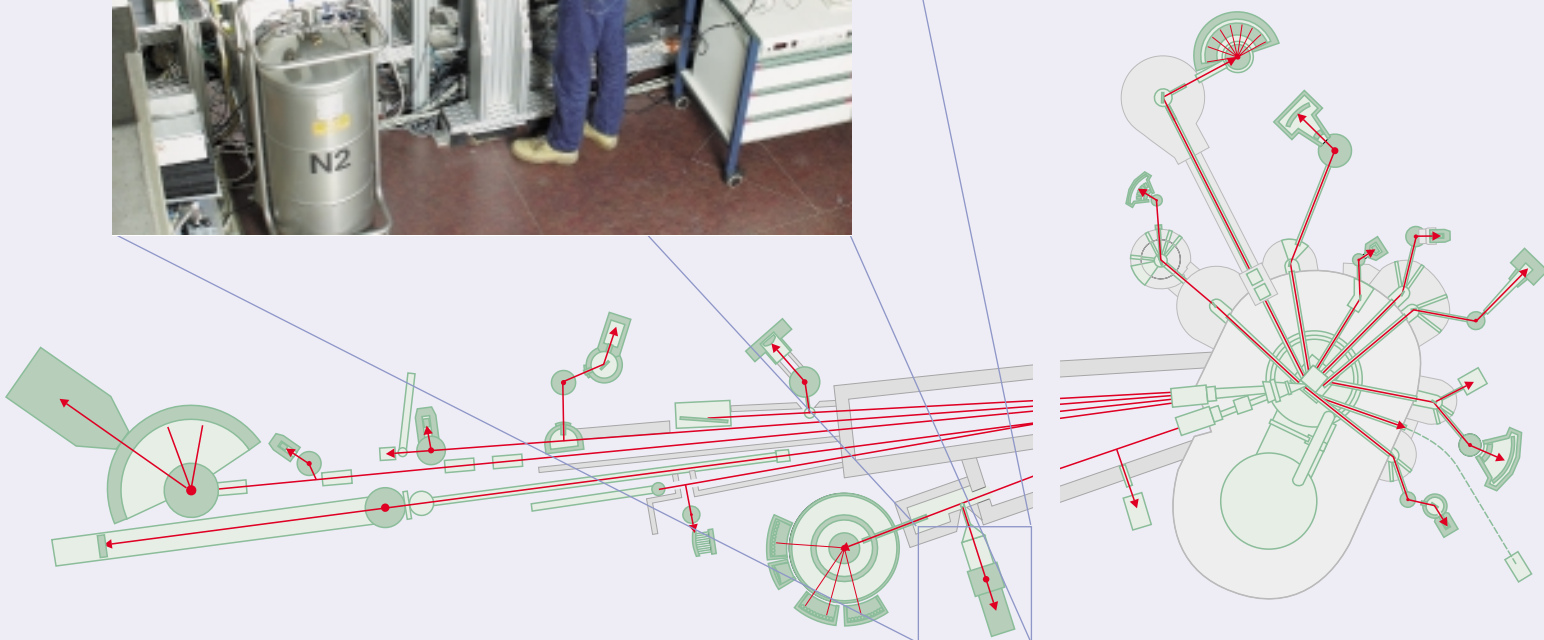
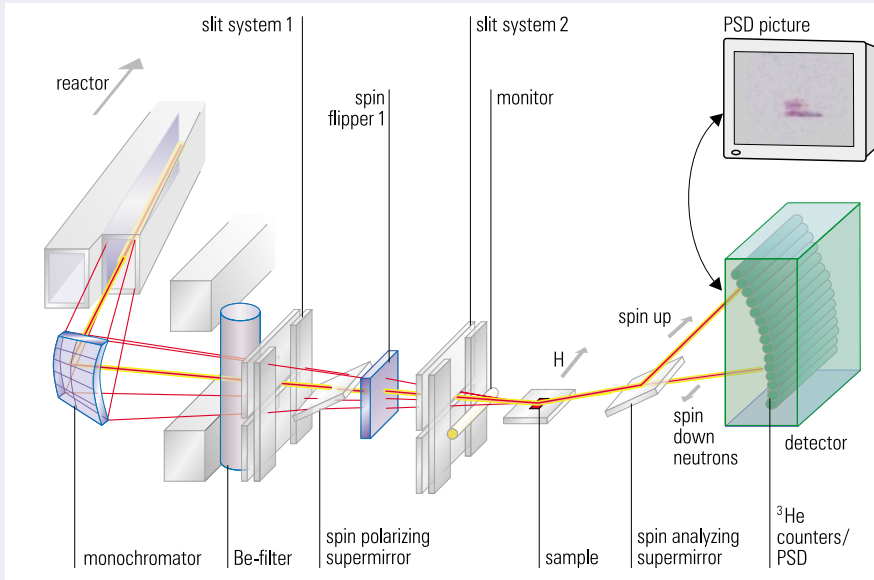
The reflectometer V6 allows to measure the neutron optical reflectivities on flat surfaces at grazing angles. The reflectivity is related to the variation of the refractive index within a depth of about 100 nm, thus structural depth profiles can be studied. The use of polarized neutrons allows in a unique way also the reconstruction of magnetic properties and depth profiles near surfaces.

Instrument Description

The reflectometer is installed at neutron guide NL 4, which supplies the instrument with cold neutrons. Pyrolytic graphite crystals act as monochromators. The used wavelength is 0.466 nm. The beam is collimated by two sets of computer controlled cadmium slits. For solid samples the angle of incidence is usually varied by a precise tilting of the sample surface relative to the (fixed) collimated neutron beam. Liquid samples can be measured using the vertically focusing monochromator. In this mode the sample surface is kept horizontal and the angle of incidence is varied by a precise movement of the slit system. Thus an angular range of 0° - 2° is accessible.

The detector is an array of ^3He gas detectors with an efficiency higher than 90% for a neutron wavelength of 0.4 nm, moving in a vertical plane. Optionally, a two-dimensional position sensitive detector (PSD) can be used.

The sample-detector distance is variable between 1 m and 3 m. The instrument is capable to measure magnetic samples with



exit beam spin analyzing, thus all four spin-dependent reflectivities (spin flip and non-spin flip) can be studied. All instrument components and the sample environments are computer controlled.

Applications

- multilayers (anorganic or organic materials)
- liquid and solid surfaces
- magnetic penetration depth in superconductors
- magnetic properties of thin layers or multilayers
- properties of in-plane structured layers
- domain walls in spring magnet systems

Selected Examples

- Temperature dependent reflectivity of a Au (111) / 1.6 nm Co/W (Fig. 1)
- Reflectivity of a free floating polymer monolayer on a water surface (Fig. 2)

Instrument Data – V6 Reflectometer

Neutron guide	NL 4
Monochromator crystal	Pyrolythic graphite (002) mosaicity: $\Delta\lambda/\lambda = 2\%$
Wavelength	0.466 nm
Scattering plane	vertical
Polarization of neutron beam	98.5%
Guide field	permanent, horizontal
Detectors	48 ^3He -detector tubes, optionally multiwire position sensitive detector (180 x 180 mm, resolution 1.5 mm)
Detector angular range	10°
Angular range for liquids	0° - 2°
Vertical collimation	0.01° - 0.05°
Angular precision	0.001°
Typical flux at sample	$3 \cdot 10^4$ n/cm 2 s $1.5 \cdot 10^4$ n/cm 2 s (polarized 98.5%)
Typical accessible reflectivities	$2 \cdot 10^{-5}$ (with sample size 10 x 40 mm)
Typical q resolution	$2 \cdot 10^{-2}$ nm $^{-1}$ (depending on collimation)
Sample environment	horizontal magnetic field < 1 T sample rotation table (360°) closed cycle cryostat (10 K - 300 K) heatable cells for liquids Langmuir Blodgett trough
Instrument responsible	H. Fritzsche, fritzsche@hmi.de, direct dialing -3141 R. Steitz, steitz@hmi.de, direct dialing -2149

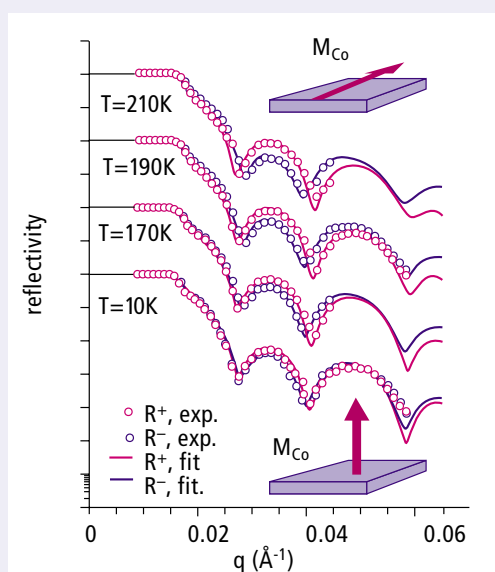


Fig. 1: Temperature dependent reflectivity of a Au (111) / 1.6 nm Co/W sample showing the spin reorientation from in-plane magnetization at 210 K to out-of-plane magnetization at 10 K.

R. Sellmann, H. Fritzsche (2000)

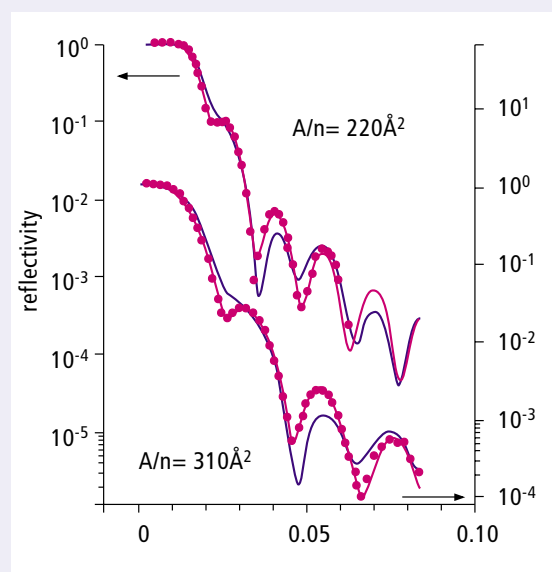


Fig. 2: Neutron reflectivity of a free floating polymer monolayer on a water surface before and after lateral compression (left). The solid lines show the theoretical expectation (blue) of the scattering length density profile (right) of the mixed layer of a long chain deuterated and a short chain protonated polymer and the best fit to the data (red).

W.A. Goedel, R. Steitz et al.,
Macromolecules 32 (1999) 7599.

V 10

Two-Axis Diffractometer for Low Temperature Studies

The two-axis diffractometer V10 is installed at the neutron guide NL 2 of which it uses the lower part.

Instrument description

The ω -module of the diffractometer carries a low temperature cryostat which is equipped with a powerful dilution refrigerator (model 600 Oxford Instruments) and a copper demagnetization stage with a 9 T magnet. The dilution refrigerator pre-cools

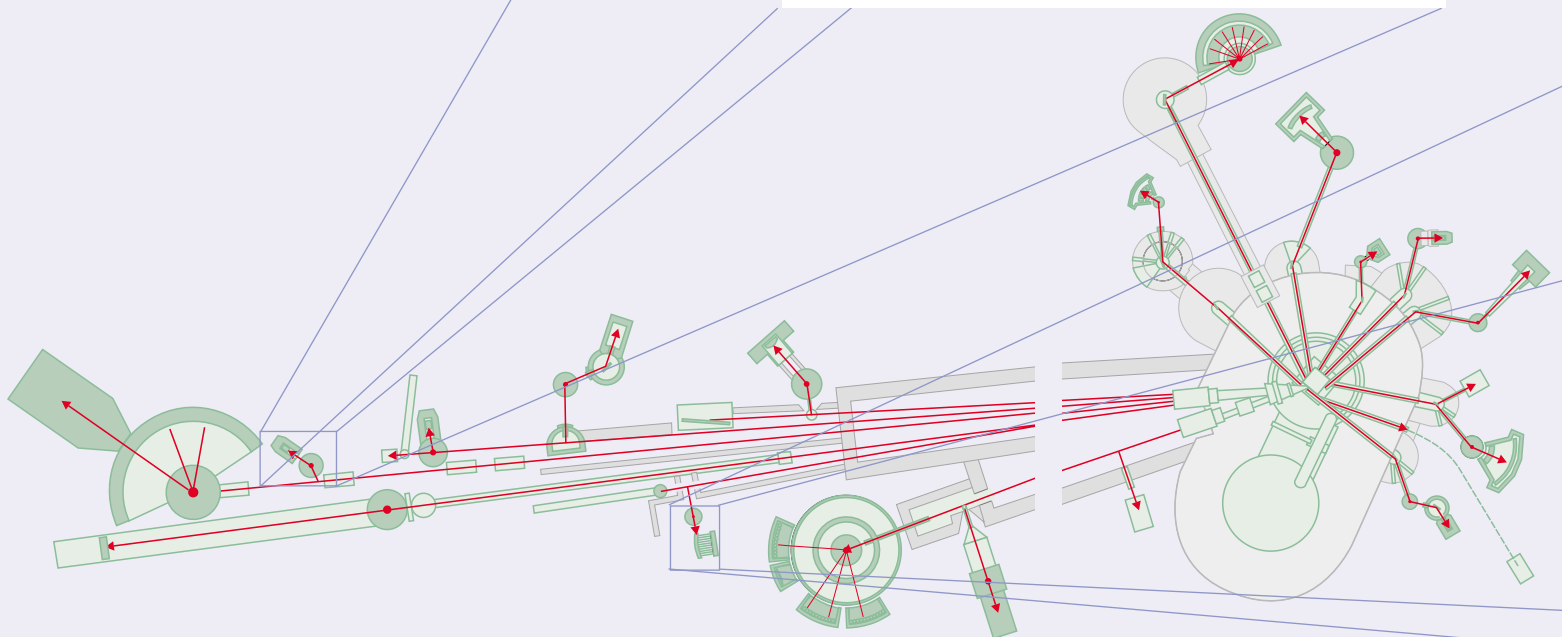
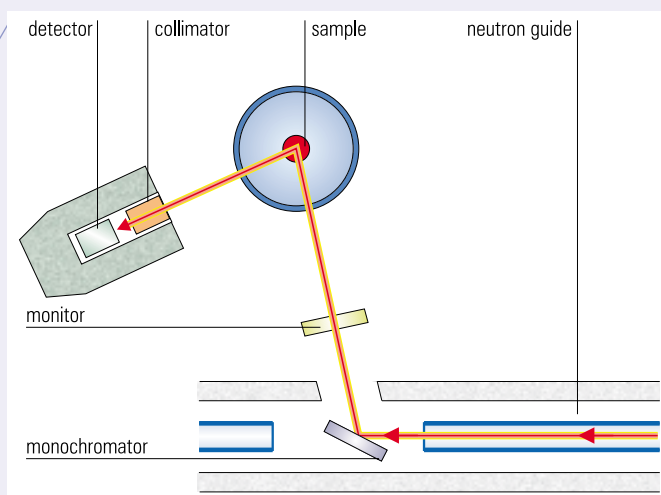
the copper nuclear stage to a temperature of about 10 mK. The extremely low sample temperature can be reached by demagnetization of the first nuclear stage (copper) to at least 200 μ K and in a second demagnetization cycle using a 7 T split pair magnet which has a 360° neutron beam access. The diffractometer is mounted on top of a vibration isolated platform, in order to minimize mechanical disturbances of the cryostat and the sample. In principle, metallic samples can be pre-cooled below 200 μ K and then further cooled by nuclear demagnetization to still lower temperatures.

Instrument Data – V 10

Neutron guide	NL 2 (lower part) beam cross section: 55 mm (height) x 30 mm (width)
Monochromator	PG 002
Wavelength	0.44 nm
Range of scattering angle at sample table	$-45^\circ < 2\theta < 160^\circ$
Detector	^3He single detector or 2D position-sensitive detector
Flux at sample position	$5 \cdot 10^5$ n/cm ² s (PG 002, flat, open collimation)
Software	PC LAB
Instrument responsible	K.Siemensmeyer, siemensmeyer@hmi.de direct dialing -2757

Applications

The instrument is dedicated to the study of nuclear magnetic order at extremely low temperatures. Present applications include the study of nuclear magnetism in Ag, where ^{109}Ag nuclei are being cooled to a temperature as low as 600 pK.



Double-Crystal Diffractometer

The double-crystal diffractometer V12a is installed at the curved neutron guide NL 3B. It allows the measurement of the scattered neutron intensity with a very high angular resolution (in an angle range from seconds of arc up to 34 minutes of arc) and provides possibilities for the study of large scale structures from 30 nm to 30 μm in solid state physics, chemistry and biology.

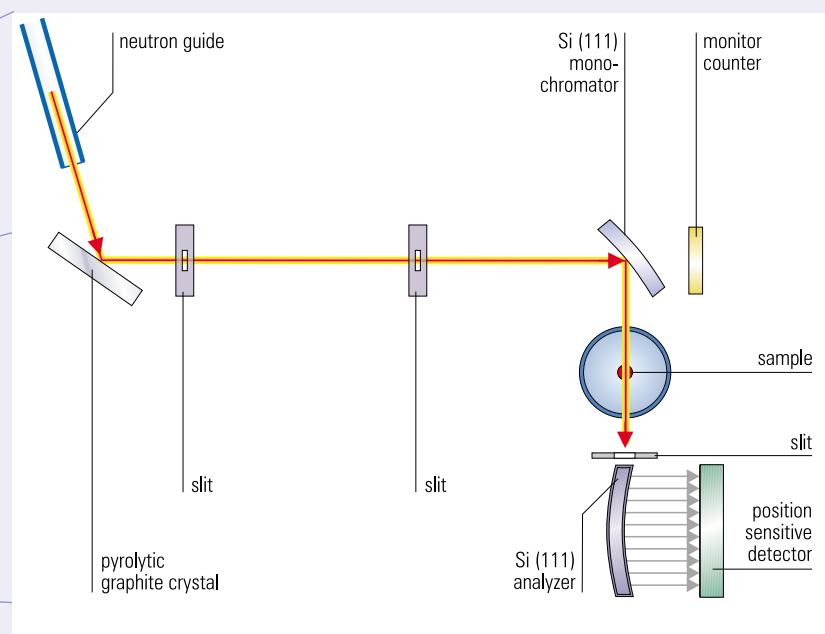
Instrument description

The incident neutron beam is deflected to the diffractometer by a pyrolytic graphite premonochromator. Main components of the instrument are two elastically bent crystals in the (111) Bragg reflection and a one-dimensional position sensitive detector. The neutron beam, monochromatized by the Bragg diffraction at monochromator, enters the end face of an asymmetrically cut analyzer crystal and propagates along its longest edge.

The analyzer crystal reflects the neutron beam only in the case the scattered beam fulfils the Bragg-condition. For the neutrons which are scattered by a sample this takes place at different parts of the bent analyzer crystal, so that the scattering diagram can be recorded as a whole by the position-sensitive detector. This fact is important for investigations of time-depending processes.

It is possible to change curvatures of the monochromator and the analyzer within a rather wide range (see table). By this way one can modify both the resolution (monochromator) and the Q-range available (analyzer). It allows the optimization of the instrumental resolution as well as the luminosity according to experimentalist's requirements.

A sample unit allows a fine adjustment of the sample (transverse translation, rotation and tilt). The sample position and data acquisition are controlled by the PC based control system, which operates in automatic mode.



Instrument Data – V12a

Neutron guide	NL 3B, curved R = 500 m
Premonochromator crystal	PG (002)
Wavelength	0.478 nm
Diffractometer crystals	monochromator Si (111) - symmetric Bragg case analyzer Si (111) - completely asymmetric case
Neutron flux	5000 n/cm ² s (R _M = 13 m) 540 n/cm ² s (R _M = 360 m)
Resolution in Q-space	4.5 · 10 ⁻³ nm ⁻¹ (R _M = 13 m) 1.5 · 10 ⁻⁴ nm ⁻¹ (R _M = 360 m)
Q-range	3.6 · 10 ⁻³ nm ⁻¹ - 2.6 · 10 ⁻¹ nm ⁻¹ for RA = 11.4 m 7.6 · 10 ⁻⁵ nm ⁻¹ - 5.3 · 10 ⁻³ nm ⁻¹ for RA = 547.7 m
Detector	one-dimensional position sensitive detector ORDELA 1250N, ³ He filled, length 250 mm (resolution < 1mm)
Instrument responsible	W. Treimer (TFH Berlin), treimer@hmi.de direct dialing -2221

Applications

- small-angle scattering study of:
 - porous materials (hydrating cement paste, rocks, coal)
 - inhomogenous metallic alloys
 - particles (polymers, ceramics)
 - material inhomogeneities from 30 nm to 30 μm
- investigations of neutron optical components
- investigations of reflection from surfaces
- the study of diffraction and refraction at magnetic domains, etc.

Sample Environment

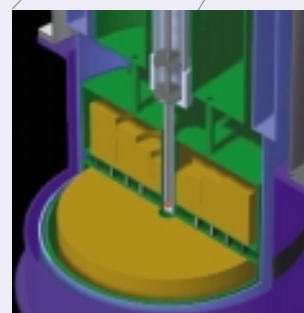
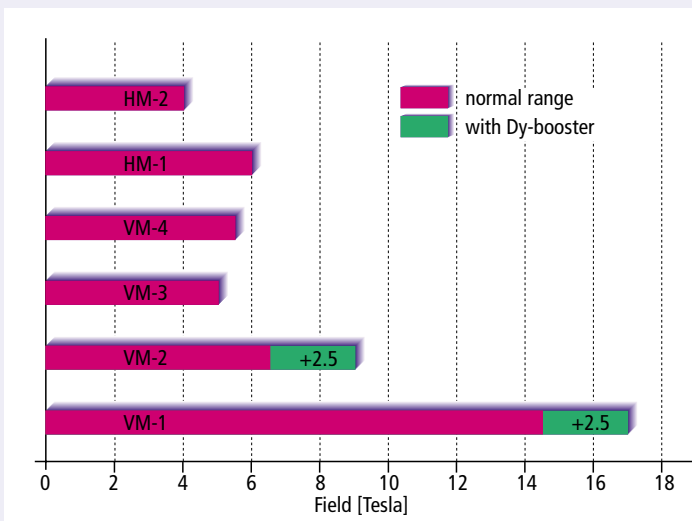
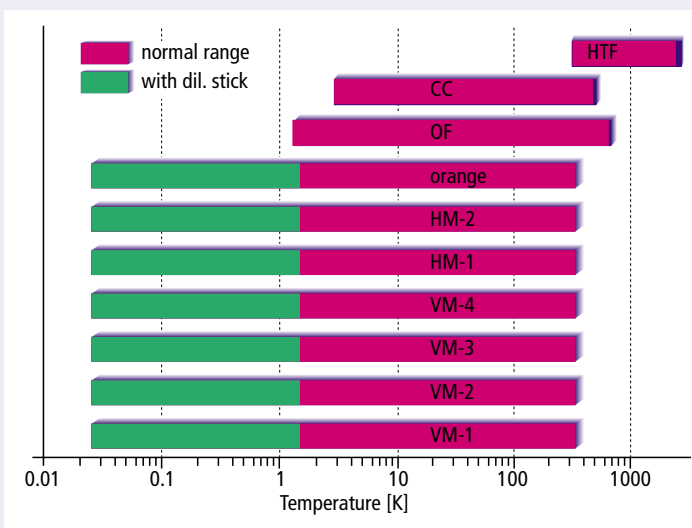
A broad range of equipment is available to provide different sample environments for neutron scattering experiments with a wide temperature range, $T = 25 \text{ mK} - 2000 \text{ K}$, and with variable magnetic fields up to $B = 17 \text{ Tesla}$ and with pressure up to $p = 40 \text{ kbar}$. The components are mutually compatible and can be used on most of the instruments both in the experimental and the neutron guide hall.

For experiments down to 25 mK two Dilution Refrigerator Sticks can be combined with a variety of Magnet Cryostats and Orange Cryostats. This technique provides a cryostat set-up for a temperature range, $T = 30 \text{ mK} - 300 \text{ K}$, combined with Vertical Magnetic Field up to 14.5 Tesla (17 T with Dy-pole tips and 14.5 T external field and $T = 1.5 \text{ K} - 80 \text{ K}$; 7 Tesla for studies with polarized neutrons) or Horizontal Magnetic Field up to 6 Tesla .

The standard low-temperature equipment consists of Orange Cryostats ($T = 1.5 \text{ K} - 300 \text{ K} / 600 \text{ K}$) or Closed Cycle Cryocoolers ($T = 3 \text{ K} - 420 \text{ K}$) permanently at the instrument or for schedule on most of the instruments. High Temperature Furnaces for temperatures as high as 1600°C are available as well.

For powder samples two High Pressure Cells have been developed in collaboration with the Institut für Mineralogie und Kristallographie of the Universität Kiel and are now available for experiments in a pressure range $p = 0 - 40 \text{ kbar}$ (for temperatures $T = 25^\circ\text{C} - 400^\circ\text{C}$). Two clamped pressure Cells for $p < 10 \text{ kbar}$ can be used in the Orange Cryostats providing a temperature range $T = 2 \text{ K} - 300 \text{ K} / 600 \text{ K}$.

More detailed information on the equipment specifications can be found on the BENSC webpages.



Sample

Fig. 1: Overview of the sample environment equipment available at BENSC

Fig. 2: Magnet-Cryostat VM-1

Specifications of Sample Environment: Standard Equipment

Orange Cryostats

System Code	Temperature Range	Sample Space Dia./Height	Thermometry Sensors	Permanent on Instrument X
OS-X	1.5 K – 300 K	<50 mm / <30 mm	RhFe, SiD	E1...E4, E6, E9, V1, V2, V4, V5
OM-1, OM-2	1.5 K – 300 K	<100 mm / <50 mm	RhFe, SiD	see below
OF-1, -2, -3	1.5 K – 600 K	<50 mm / <30 mm	RhFe	see below
OFM-V3	2 K – 600 K	<80 mm / <80 mm	RhFe	V3

OM-1, OM-2, OF-1, OF-2, OF-3 can be posted for E1, E2, E3, E4, E6, E9, V1, V2, V4, V5.

Closed Cycle Refrigerators

System Code	System Construct.	Temperature Range	Sample Space Dia./Height	Thermometry Sensor	Permanent on Instrument X
CC-E1	Leybold	10 K - 300 K	<50 mm / <30 mm	Si-Diode	E1
CC-E5	Air Products	10 K - 300 K	<50 mm / <30 mm	Si-Diode	E5
CC-V6	Air Products	10 K - 300 K	<50 mm / <30 mm	Si-Diode	V6
CC-A1	Air Products	5 K - 300 K	<50 mm / <30 mm	Si-Diode	see below
CC-A2	Air Products	5 K - 430 K	<50 mm / <30 mm	Si-Diode	see below
CC-S1	Sumitomo	3 K - 300 K	<50 mm / <30 mm	Si-Diode	see below

CC-A1, CC-A2, CC-S1 can be posted for E1, E2, E3, E4, E6, E9, V1, V2, V4, V5.

High Temperature Furnaces

System Code	System Construct.	Temperature Range	Sample Space Dia./Height	Thermometry Sensor
HTF-1, HTF-2	ILL/AS	400 K - 2000 K	<50 mm / <30 mm	Type C (WRe5 % / WRe26 %)
HTF-J1	IFF Jülich	300 K - 1500 K	<10 mm / <10 mm	Type K (Chromel/Alumel)

HTF-1, HTF-2 can be posted for E1, E2, E3, E4, E6, E9, V1, V2, V4, V5;

HTF-J1 can be posted for E5 and for the above instruments using the 4-circle-cradle.

High Pressure Cells

System Code	System Construct.	Temperature Range	Pressure Range	Sample Space Dia./Height	Thermometry Sensor
HPC-1	U. Kiel/HMI	25°C - 400°C	0 - 17 kbar	7 / 20 - 12 mm	K-type (NiCr-Ni)
HPC-2	U. Kiel/HMI	25°C - 400°C	0 - 17 kbar	7 / 20 - 12 mm	K-type (NiCr-Ni)
CPC-1	IP Prague	1.5K - 300 K (OS)	0 - 5 kbar	3.5 / 20 mm	RhFe / Pb-wire
CPC-2	ILL	1.5K - 600 K (OF)	0 - 10 kbar	6 / 10 mm	RhFe

HPC-1 can be posted for E1, E2, E3, E4, E6, E9, V1, V2, V4;

HPC-2 can be posted for E1, E2, E3, E4, E6, E9, V1, V2;

Clamped cells CPC-1, CPC-2 can be posted with any Orange Cryostat OS, OF, OM, OFM.

Explanation of terms and abbreviations used in the tables:

Acc.: Construction design which influences the 360°-access to the sample
 Ang.: Angle of vertical aperture above and below horizontal magnet split
 Asy.: Non-zero field profile in n-beam path (for polarized neutrons)
 Dia.: Diameter of sample given by sample tube diameter
 Height: Maximum sample height for n-beam

Max.: Maximum magnetic field strength
 Rings: Concentric aluminium rings in the split area which attenuate n-beam
 Split: Maximum height for n-beam through magnet split (= sample height)
 Wedges: provide dead angle of significant size which reduce the 360°-access to the sample; details are shown in the relevant section of the U.S.E. handbook

Specifications of Sample Environment: Special Equipment

Magnet Cryostats with Vertical Field

System Code	System Construct.	Temperature Range	Magnetic Field Max./Asy./Acc.	Sample Space Dia./Split/Angle	Thermometry Sensors
VM-1	OI	1.5 K - 300 K	14.5T (+2.5T) /no/rings	<20 mm/20 mm/2°	Cernox®
VM-2	OI	1.5 K - 300 K	7T /yes/rings	<50 mm/30 mm/5°	Cernox®
VM-3	AS / OI	1.5 K - 300 K	5T /no/3x5°wedges	<50 mm/30 mm/0°	Cernox®
VM-4	AS / Thor	1.5 K - 300 K	5.5T /yes/3x55°wedges	<50 mm/40 mm/+35°	Cernox®

VM-1 can be posted for E1, E4, E6, V2;

VM-2 can be posted for E1, E2, E4, E6, V1, V2;

VM-3, VM-4 can be posted for E1, E2, E4, E6, E9, V1, V2, V4.

Magnet Cryostats with Horizontal Field

System Code	System Construct.	Temperature Range	Magnetic Field Max./Asy./Acc.	Sample Space Dia./Split/Angle	Thermometry Sensors
HM-1	AS / RMC	1.5 K - 300 K	6T/2-coil/wedges	<50 mm/see U.S.E. book	Cernox®
HM-2	OI	1.5 K - 300 K	4T/4-coil/wedges	<40 mm/40mm/0°	Cernox®

HM-1 can be posted for E1, E4, E6, E9, V1, V2, V4;

HM-2 can be posted for E1, E4, E6, E9, V1, V2.

³He/⁴He Dilution Cryostat Inserts ("Dilution Stick")

System Code	Temperature Range	Sample Space* Dia./Height	Thermometry Sensors	Insert suitable to cryostat
DS-2	25 mK - 1.4 K	<35 mm / <30 mm	RuO ₂	AS-type: OS, VM-3, VM-4, HM-1 OI-type: VARIOX, VM-1, VM-2, HM-2
DS-3	25 mK - 1.4 K	<35 mm / <30 mm	RuO ₂	

DS-2, DS-3 can be posted in combination with the cryostats (and instruments) listed above

* For use with OS and VARIOX only; for use with magnets contact the sample environment staff.

Information on equipment supplied by users

Electrical interfaces:

220/380 V power supply (plugs, cables, etc.) must be to German VDE-Standard

Mechanical interfaces:

For details of the various instrument interfaces (device flanges, sample mounting, cooling water, gas supply) please contact the instrument responsible.

Safety aspects:

Containers and supply lines under vacuum or under pressure have to be approved by the Research Reactor BER-II safety engineer. For use of toxic, flammable and explosive gases a gas detector with actuator-logic and magnet valve operation has to be approved by the BER-II safety engineer. Please contact Mr. Köring, phone +49-30-8062-2690).

Berlin Neutron Scattering Center – BENSC, March 2001

