

DIFFRACTOMETERS FOR SINGLE CRYSTALS

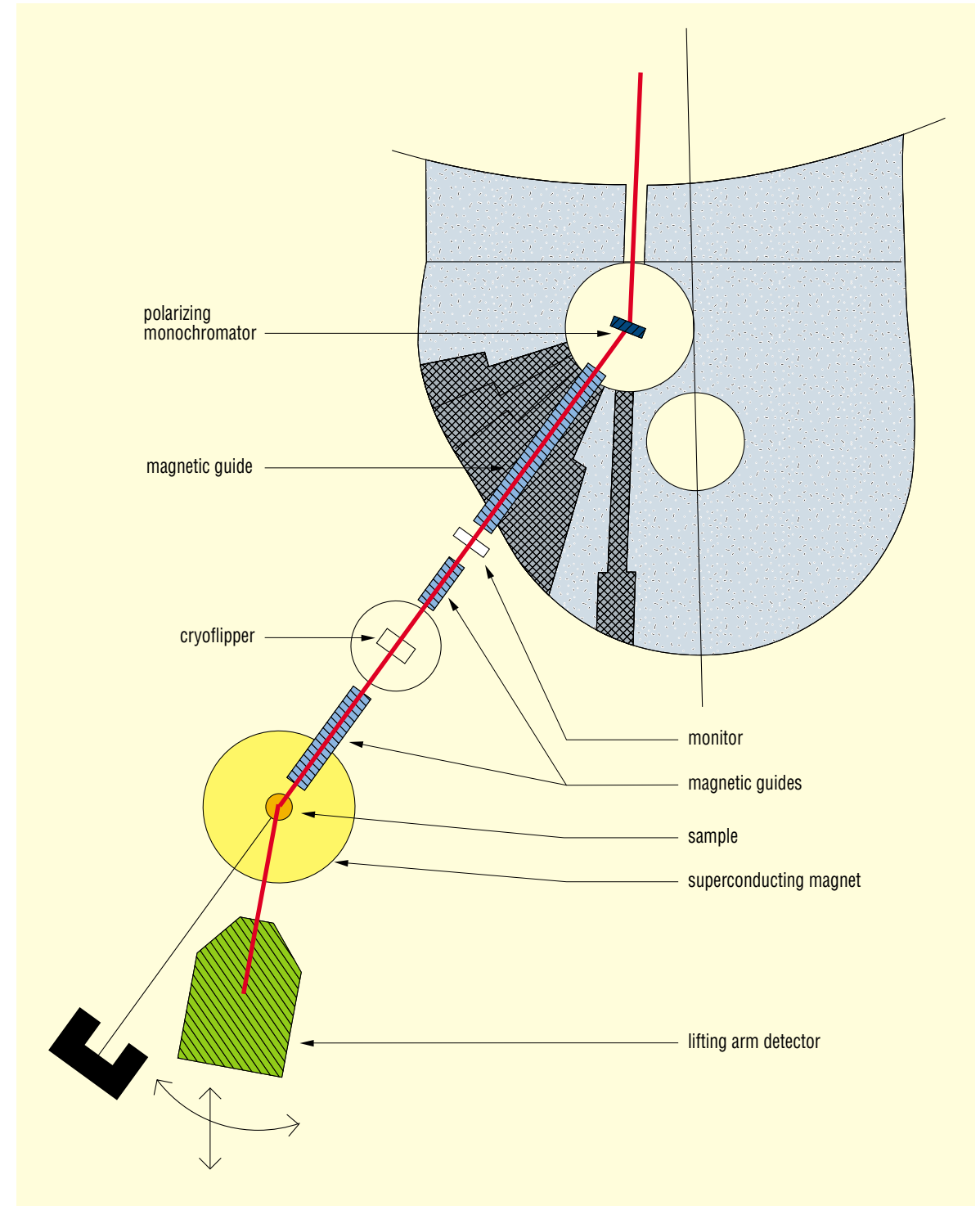
Beam tube	5 C1 Hot source
Monochromator	Heusler Cu ₂ MnAl (111)
Collimation	Horizontal divergence before the monochromator 58', 28' or 14'
Type of instrument	two-axis ; lifting arm detector polarized neutrons
Max. beam size at specimen	20 x 20 mm
Incident wavelength	$\lambda = 0.84 \text{ \AA}$
Angular ranges	Detector : 0, 120° in the horizontal plane -5, + 18° in the vertical plane
Minimum step size scan	0.01°
Detector	³ He counter
Data collection and Instrument control system	PC Data are transferred to a SUN computer for further treatment.
<u>Ancillary equipment</u>	★ Cryostat from 1.5 K → 300 K. ★ Cryomagnet H < 7.8 Tesla

The diffractometer is devoted to the determination of the magnetic structure factors, using an incident polarized neutron beam ; it is utilized for magnetic form factor and magnetization density studies on single crystals.

The polarization direction of the incident neutrons is defined by a magnetic guide field and can be inverted with the help of a cryogenic flipping device. A strong magnetic field is applied to the sample.

The intensities I₊ and I₋, diffracted by the sample, are measured when the incident neutrons are respectively polarized parallel (+) or antiparallel (-) to the applied magnetic field. The flipping ratio R = I₊/I₋, is thus measured for each Bragg reflection, and gives access to the magnetic structure factor, knowing previously the nuclear structure factor.

The wavelength is 0.84 Å (maximum of the flux of the hot source). This short wavelength allows the investigation of a large domain of reciprocal space.



General layout of the spectrometer 5 C1.

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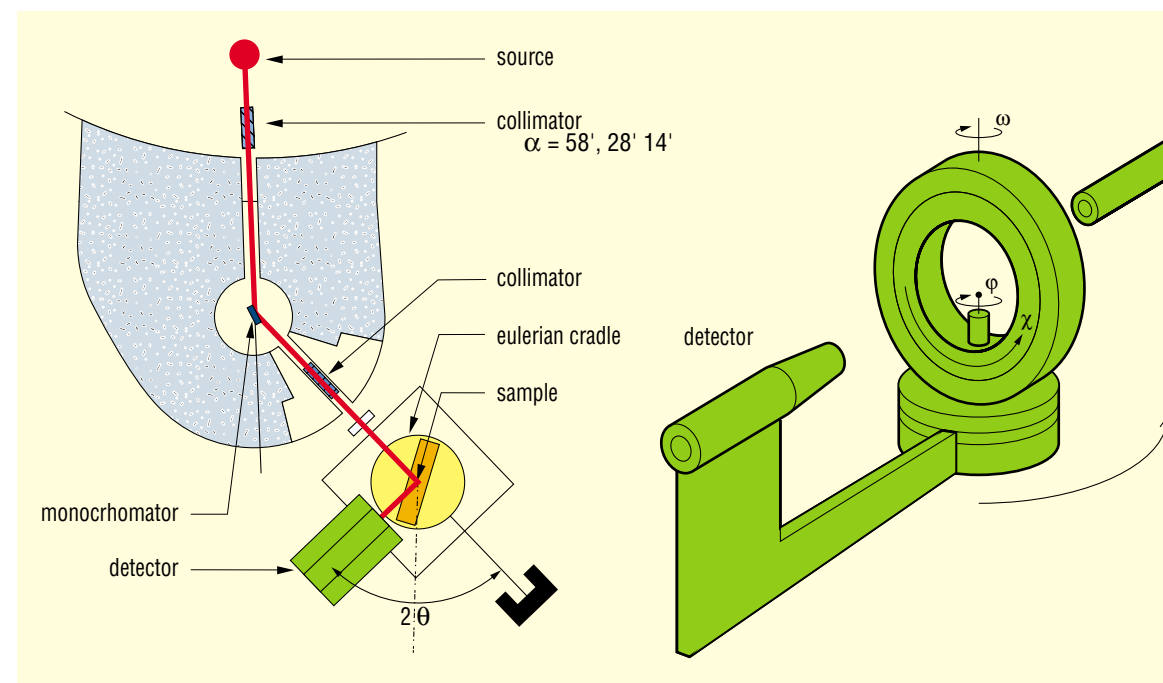
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Beam tube	5 C2 (hot source)
Monochromators	Cu (220) and GeSi (311), adjustable vertical focusing
Type of instrument	centric Eulerian cradle (Stoe)
Max. flux at specimen (n/cm ² s)	5.7 x 10 ⁶ (λ = 0.835 Å, α ₁ = 58')
	5.0 x 10 ⁶ (λ = 1.112 Å, α ₁ = 58')
Max. beamsize at specimen	∅ = 15 mm
Incident wavelength	0.835 Å (Cu 220), Erbium filter
	1.112 Å, GeSi (311)
λ/2 contamination	< 0.1% for λ = 0.835 Å
	0 for λ = 1.112 Å
Angular range	-100° ≤ 2θ ≤ 130°
	-60° ≤ ω ≤ 65°
	-180° ≤ χ ≤ 180°
	-180° ≤ φ ≤ 180°
Collimation α ₁	58', 28' or 14'
Resolution	Δω = 0.12°(FWHM) at 2θ = 40° for λ = 0.835 Å
	Δω = 0.20°(FWHM) at 2θ = 40° for λ = 1.112 Å
Detectors	³ He detector, position sensitive detector under construction
Data collection and instrument control system	PC (LINUX), modified and extended DIF4N software
Ancillary equipment	★ cryostat and furnace (5 K < T < 1400 K)

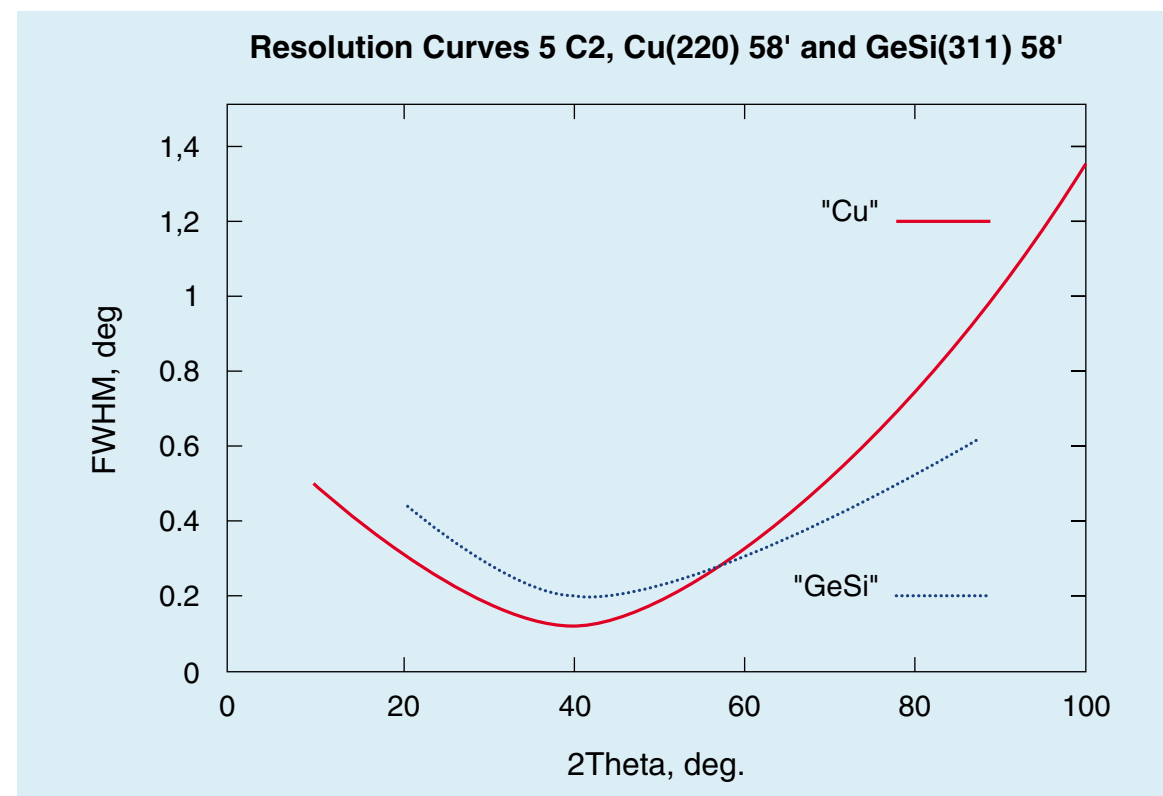
The purpose of this four-circle diffractometer is the measurement of Bragg-reflections for the evaluation of structure factors. It allows to determine crystal structures and magnetic structures of twinned or untwinned single crystals. Typical applications are the localisation of hydrogen in inorganic and organic compounds, the analysis of disordered crystal structures and anharmonic displacement parameters, structural phase transitions, magnetic structures, high-Tc superconductors or related materials, and quasicrystals. The shorter wavelength is used to study small unit cells (V < 2000 Å³) up to high (sin θ/λ) values, which allows to obtain very precise information on thermal displacement parameters. The longer wavelength is used to collect data of even larger unit cells (V < 8000 Å³) with a high resolution.

A helium cryostat and a furnace allow temperature dependent structure investigations in the temperature range from 5 K to 300 K and from 300 K to 1400 K. Special sample environments (like uniaxial or hydrostatic pressure, electric or magnetic fields) can be adapted individually.

This diffractometer was built by german scientists in cooperation between the FZ Karlsruhe and the LLB. It is currently operated by the RWTH Aachen and the LLB under the "Verbundforschung" program of the Federal Ministry of Education and Research "BMBF".



General layout of the diffractometer 5 C2.



Resolution Curves 5 C2, Cu (220) 58' and GeSi (311) 58'.

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Beam tube	6T (thermal source)
Monochromators	Cu 220 P.G. 002
Incident wavelength	0.90 Å, 1.55 Å, 2.35 Å
Collimation	$\alpha_1 = 14', 28', 57'$ $\alpha_2, \alpha_3 = 10', 30'$
Range of monochromator angles	$2\theta = 27^\circ$ or 42°
Ranges of spectrometer angles	$-28^\circ < 2\theta < 140^\circ$ $-90^\circ < \omega < 90^\circ$ $-180^\circ < \chi < 180^\circ$ $-180^\circ < \varphi < 180^\circ$ $-5^\circ < \nu < 26^\circ$
Detector	^3He
Ancillary equipment	<ul style="list-style-type: none"> ★ Displex 5 K - 300 K ★ ^4He cryostat 1.5 K - 300 K ★ Cryomagnet 7.5 T, 12 T ★ Dilution cryostat 30m K ★ High pressure cell

The diffractometer is equipped with two vertically focusing monochromators :

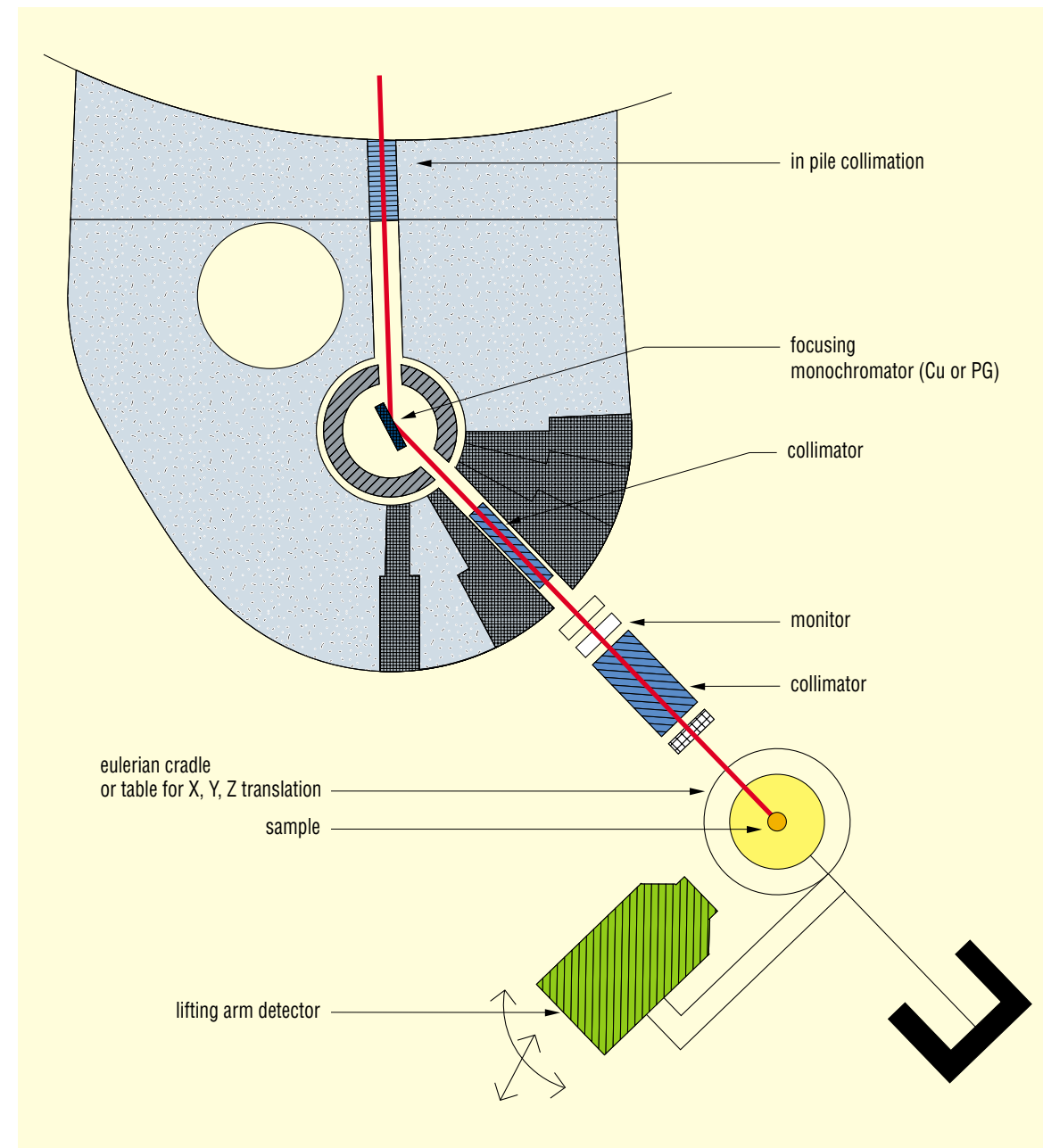
- 1) Copper (220) $\lambda = 0.90 \text{ \AA}$ (Er filter)
- 2) pyrolytique graphite (002) $\lambda = 1.55$ and 2.35 \AA (PG filter).

Depending on the aim of experiment a high flux configuration (bent monochromator, relaxed collimation) or high resolution configuration (planar monochromator, short wavelength, tight collimation) can be easily used.

Two types of diffractometer can be mounted :

- 1) 4-circles geometry : with an Eulerian (deported) cradle for structural studies of large unit cells (cell volumes of more than 1000 \AA^3) and high resolution studies (phase transitions, etc...).
- 2) Lifting counter geometry using cryomagnet, dilution cryostat and high pressure cell for magnetic studies.

The spectrometer is controlled by a Windows NT PC computer.



General layout of the diffractometer 6 T2.

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