DIFFRACTOMETERS FOR SINGLE CRYSTALS
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.

The diffractometer is operated with two instruments:

- **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
- **Max. beam size at specimen:** 20 x 20 mm
- **Incident wavelength:** $\lambda = 0.84$ Å
- **Angular ranges:** Detector:
  - 0, 120° in the horizontal plane
  - $-6°, +18°$ in the vertical plane
- **Minimum step size scan:** 0.01°
- **Detector:** He counter
- **Data collection and Instrument control system:** PC
  - Data are transferred to a SUN computer for further treatment.
- **Ancillary equipment:**
  - Cryostat from 1.5 K → 300 K.
  - Cryomagnet $H < 7.8$ Tesla

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**General layout of the spectrometer 5 C1.**

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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 (N < 2000 Å) up to high (sin t/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 (N < 8000 Å) 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”.

The diagram shows the general layout of the diffractometer 5C2, including the beam tube, monochromators, detector, collimators, and Eulerian cradle. The diagram is labeled Hot Neutron Four-Circle Diffraotometer.

### Table: Instrument Specifications

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam tube</td>
<td>Cu (220) and GeSi (311), 5C2 (hot source)</td>
</tr>
<tr>
<td>Monochromators</td>
<td>Cu (220) and GeSi (311), adjustable vertical focusing</td>
</tr>
<tr>
<td>Type of instrument</td>
<td>Centric Eulerian cradle (Stoe)</td>
</tr>
<tr>
<td>Max. flux at specimen (n/cm² s)</td>
<td>5.7 x 10⁶ (λ = 0.835 Å, θ = 58°)</td>
</tr>
<tr>
<td>Max. beamsize at specimen</td>
<td>0.20° (FWHM) at 2θ = 0.835 Å</td>
</tr>
<tr>
<td>Incident wavelength</td>
<td>0.835 Å (Cu 220), Erbium filter</td>
</tr>
<tr>
<td>λ/2 contamination</td>
<td>1.112 Å, GeSi (311)</td>
</tr>
<tr>
<td>Angular range</td>
<td>0.1% for λ = 1.112 Å</td>
</tr>
<tr>
<td>-100° ≤ 2θ ≤ 130°</td>
<td></td>
</tr>
<tr>
<td>-60° ≤ ω ≤ 65°</td>
<td></td>
</tr>
<tr>
<td>-180° ≤ θ ≤ 180°</td>
<td></td>
</tr>
<tr>
<td>Collimation α</td>
<td>0° for λ = 1.112 Å</td>
</tr>
<tr>
<td>Resolution</td>
<td>58°, 28° or 14°</td>
</tr>
<tr>
<td>Δω = 0.12° (FWHM) at 2θ = 40° for λ = 0.835 Å</td>
<td></td>
</tr>
<tr>
<td>Δω = 0.2° (FWHM) at 2θ = 40° for λ = 1.112 Å</td>
<td></td>
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<tr>
<td>Detectors</td>
<td>He detector, position sensitive detector under construction</td>
</tr>
<tr>
<td>Data collection and instrument control system</td>
<td>PC (LINUX), modified and extended DIF4N software</td>
</tr>
<tr>
<td>Ancillary equipment</td>
<td>Cryostat and furnace (5 K &lt; T &lt; 1400 K)</td>
</tr>
</tbody>
</table>

### Resolution Curves

The resolution curves for Cu (220) and GeSi (311) are shown in the graph. The curves are labeled “Cu” and “GeSi”.

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Beam tube .................................................. 6 T (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 .................. \( 28 = 27° \) or \( 42° \)
Ranges of spectrometer angles .................... \( -28' < \chi < 140° \)
                                      \( -90° < \omega < 90° \)
                                      \( -180° < \chi < 180° \)
                                      \( -5° < \varphi < 26° \)
Detector .................................................. \(^3\)He
Ancillary equipment  

<table>
<thead>
<tr>
<th>Instrument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displex 5 K - 300 K</td>
<td></td>
</tr>
<tr>
<td>(^3)He cryostat 1.5 K - 300 K</td>
<td></td>
</tr>
<tr>
<td>Cryomagnet 7.5 T, 12 T</td>
<td></td>
</tr>
<tr>
<td>Dilution cryostat 30m K</td>
<td></td>
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<tr>
<td>High pressure cell</td>
<td></td>
</tr>
</tbody>
</table>

The diffractometer is equipped with two vertically focusing monochromators:

1) Copper (220) \( \lambda = 0.90 \) Å (Er filter)
2) Pyrolytique graphite (002) \( \lambda = 1.55 \) and 2.35 Å (P.G. 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 Å³ 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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