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HEiDi: Single crystal diffractometer at hot source

Heinz Maier-Leibnitz Zentrum
RWTH Aachen University, Institute of Crystallography
Forschungszentrum Jülich, Jülich Centre for Neutron Science

Instrument Scientists:
- Martin Meven, Institut für Kristallographie, RWTH Aachen and Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany, phone: +49(0) 89 289 14727, email: martin.meven@frm2.tum.de
- Andrew Sazonov, Institut für Kristallographie, RWTH Aachen and Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany, phone: +49(0) 89 289 11764, email: andrew.sazonov@frm2.tum.de

Abstract: The single crystal diffractometer HEiDi, which is operated by the Institute of Crystallography, RWTH Aachen University and JCNS, Forschungszentrum Jülich, is designed for detailed studies on structural and magnetic properties of single crystals using unpolarised neutrons and Bragg's Law: $2d_{\mathrm{hkl}} \sin\Theta = \lambda$ (typically 0.55 Å $< \lambda <$ 1.2 Å).

1 Introduction

Because of the large variety of short wavelengths and resolutions, HEiDi is suitable for studies on a lot of crystalline compounds – many of them of potential interest for energy or data storage technologies – like:

- HT superconductors (e.g. cuprates, FeAs-pnictides)
- Multiferroics (e.g. manganates) and other complex ferro- and antiferromagnetic compounds (e.g. olivines)
- Ionic conductors (e.g. nickelates)
- Ferroelectrics (e.g. KDP family)
- Mixed crystals (e.g. AsSe compounds)
- Highly absorbing compounds (e.g. with Gd, Sm, Eu, Dy)
- Frustrated magnetic materials (e.g. pyrochlores)

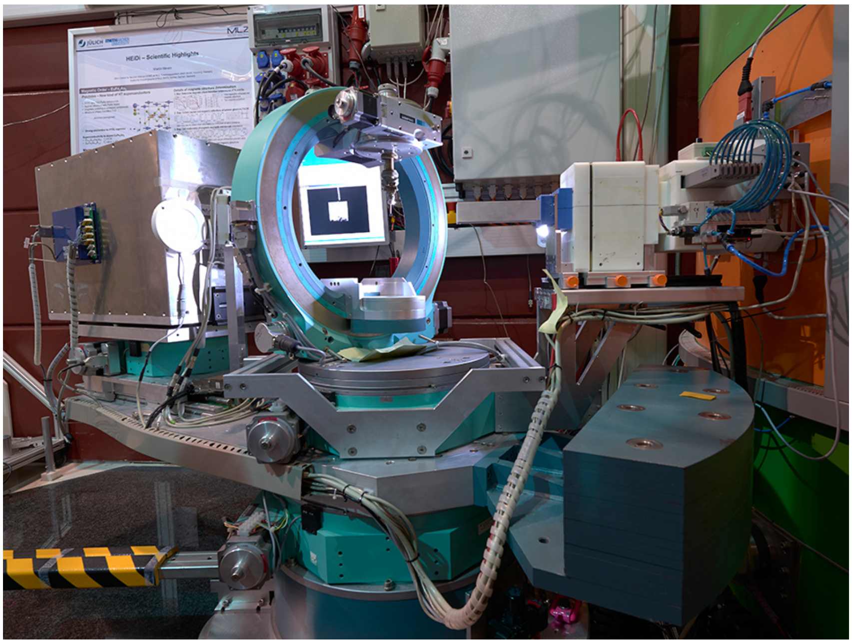

Figure 1: Instrument HEiDi (Copyright by W. Schürmann, TUM).

2 Applications (in general)

- Structure analysis
- Hydrogen bonds
- Static and dynamic disorder
- Harmonic and anharmonic mean square displacements
- Twinning
- Magnetic structure and order
- Structural and magnetic phase transitions
- Incommensurate structures

3 Applications (in detail)

- Studies of atomic positions and bond distances in compounds with heavy and light elements or elements of similar electron shells
- Temperature dependent studies for determination of phase transitions
- Studies of order – disorder phase transitions, e.g. H bonds by determination of anisotropic mean square displacements using large Q range up to $\sin(\Theta)/\lambda > 1$
- Structure determination of compounds with highly absorbing elements (Gd, Sm, Cd, Dy) with short wavelengths
- Studies on magnetic phase transitions and T dependencies (ferri, ferro and antiferro magnets, multiferroics)
- Studies on HT superconductors (e.g. cuprates, FeAs pnictides)
- Sample characterisation by profile analysis
- Determination of sample orientation, e.g. for preparation of experiments on three axes instruments
- Presentation of fundamentals of crystallography and structure analysis for education

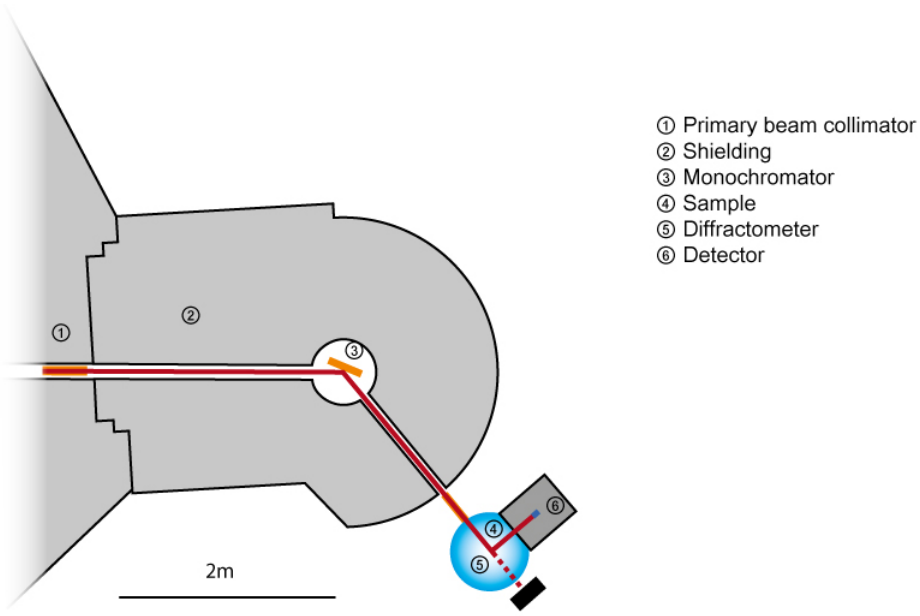

Figure 2: Schematic drawing of HEiDi.

4 Sample Environment

- Closed cycle cryostat (2 K – RT)
- Mirror furnace (RT – 1500 K)
- Micro furnace (RT – 500 K)
- Uniaxial pressure cell (from PUMA)

5 Technical Data

5.1 Beam-tube

- SR-9b (hot source)
- Flux at sample $1.4 \cdot 10^7$ n cm^{-2}s^{-1} ($\lambda \approx 1.17$ Å)
- Gain by hot source x 10 ($\lambda \approx 0.6$ Å)

5.2 Wavelength

$2\Theta_M$	Ge(311)	Cu(220)	Ge(422)	Cu(420)
20°	0.503	0.443	0.408	0.280
40°	1.168	0.870	0.793	0.552
50°	1.443	1.079	0.993	0.680

5.3 Q-range

$2\Theta_M$	Ge(311)	Cu(220)	Ge(422)	Cu(420)
20°	1.46	1.95	2.12	3.09
40°	0.74	0.99	1.09	1.57
50°	0.60	0.80	0.87	1.27

5.4 Optical components

- Single detector optimised for small wavelengths (sensitivity $>$ 90% at 0.3 Å)
- Analyzer PG(002); optional for studies of purely elastic scattering and background suppression
- Neutron filters for suppression of $\lambda/2$- or $\lambda/3$-contamination of the monochromatised beam