s1.m2.p4 **HEiDi, New Single Crystal Diffractometer at the Hot Source of FRM-II.** Martin Meven[a] and Gernot Heger[b], *[a]TU München, ZWE FRM-II, Lichtenbergstraße 1, 85747 Garching, Germany, and [b]RWTH Aachen, Institut für Kristallographie, Jägerstraße 17-19, 52056 Aachen, Germany. E-mail: martin.meven@frm2.tum.de*

Keywords: Neutron Diffraction; Single Crystals; Instrumentation

HEiDi, one of two new single crystal diffractometers at the research neutron source FRM-II, was developed in collaboration between the RWTH Aachen and the TU Munich. It was designed to cover a wide area of scientific applications using the specific advantages of the hot source of this facility. This year, after the launch of the FRM II, the instrument will start its work. Apart from the general advantage of a more accurate determination of atomic positions of light atoms like hydrogen (compared to X-ray diffraction) the large available Q space gives the opportunity to perform structural investigations which are not limited to the determination of atomic positions in single crystals only. For instance, temperature dependent determinations of anisotropic mean square displacements of a structure yield accurate statements about possible static and dynamic disorder effects and anharmonicities in the temperature areas of structural phase transitions. The reduction of absorption for shorter wavelengths allows investigations of compounds with highly absorbing isotopes like samarium or gadolinium. Furthermore, the different Q-dependence of the magnetic and the core interactions of the neutrons can be used to determine both the magnetic order and the order of the atomic cores in a crystal separately (derivation of magnetic data from Bragg data sets at low Q space and core data from Bragg data at high Q space) and therefore very accurately. Other possible investigations concern wavelength dependent extinction effects.

In order to fulfil the high expectations on the flexibility and the quality of the data measurements with this instrument, its components were selected with special care. Also new concepts were developed. Examples for this are very radiation-resistant collimators (developed at the HMI), a focusing monochromator unit with up to four different monochromator crystals to cover a broad range of wavelengths, an analyzer for purely elastic scattering, a multi-detector unit specially designed for fast neutrons to improve underground correction and a complex multi axes controller system for rapid data collection of Bragg reflections. Further details to these and other components of the instrument will be presented on the conference as well as our plans to extend its usability to further scientific applications in the future, e.g. investigations on magnetic structures using polarized neutrons.

s1.m2.p5 **Strategy of data collection based on statistic modelling.** Alexander Popov[a] and Gleb Bourenkov[b], *[a]EMBL Hamburg Outstation, c/o DESY, Notkestrasse 85, 22603 Hamburg, Germany, [b]Max-Plank-Arbeitsgruppen fur Strukturelle Molekular-biologie, Arbeitsgruppe Proteindynamik, Notkestrasse 85, 22603 Hamburg,. E-mail: sasha@embl-hamburg.de*

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We present new developments in method and program BEST for optimal and automatic planning of data collection. The method is based on modelling of the statistical results of data collection taking into account characteristics of a particular crystal, X-ray equipment and time available for measurement [1]. Statistical methods are further developed for optimisation of anomalous data collection. A few initial images taken with short exposure time are required to make predictions. The set of parameters, which provide minimal data collection time or radiation dose is selected. Anisotropy in the diffraction, geometrical restrictions (e.g. spot overlapping) and already collected data are taken into account. On the basis of the resolution and $\hat{I}/\sigma$ ratio requested by the user, the program proposes the plan of data collection. The plan defines the total rotation range, scan speed and rotation range per frame, detector distance and the detector mode. Contrary to traditional data collection strategy, the rotation range per frame and scan speed vary with the rotation angle in a way to make the distribution of statistics over reciprocal space as uniform as possible. The program estimates the data statistics (mean intensity, mean sigma, R-merge, as a function of resolution) for the data that will be collected according to the plan. The program can also predict data statistics for any set of data collection parameters defined by the user. The software proved to be extremely useful in using the available data collection time in the most efficient way. The methods are directly applicable for ranking the crystals. Applications for automatic selection of the best quality crystal will be discussed.

[1] Popov, A.N. & Bourenkov, G.P. (2003). *Acta Cryst.* D**59**, 1145-1153.