The new Single Crystal Diffractometer HEiDi at the FRM-II and its Applications

Martin Meven[a], Vladimir Hutanu[a,b], Gernot Heger[b], [a]*ZWE FRM-II, TU München, Germany.* [b]*Institut für Kristallographie, RWTH Aachen, Germany.* E-mail: martin.meven@frm2.tum.de

HEiDi, one of the new single crystal diffractometers of the research neutron source FRM-II, was designed to cover a wide area of scientific applications in crystal structure analysis. It uses the high flux of fast neutrons with short wavelengths from the hot source of the FRM-II. The enlargement of the visible reciprocal space (=Q-space) allows very accurate determinations of nuclear positions in single crystals as well as more detailed quantitative informations about mean square displacements and vacancies which is of interest in reference to static or dynamic disorder effects and phase transitions. The Q-dependences of the magnetic and the nuclear cross sections of neutrons are quite different. This can be used to determine the magnetic and the nuclear order in a crystal separately. Other advantages of shorter neutron wavelengths (1.4 Å down to 0.3 Å) are the significant reduction of absorption effects in compounds with highly absorbing elements (e.g. Sm, Gd) and the reduction of extinction effects.

During the nuclear commissioning of the FRM-II in 2004 started the adjustment and characterization of HEiDi with neutron radiation. First experimental results are quite promising, e.g. an excellent resolution function (<0.1° at min.) or a perfect alignment between the calculated and the measured gain factor of 2.5 of the monochromator focussing unit. Further experimental results from the instrument and typical applications like structural phase transitions, local disorder (H bonds in RDP) or magnetism will be presented on the conference.

Keywords: neutron and x-ray diffractometry, single crystal structure analysis, neutron instrumentation