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Single Crystal Diffraction Experiments under High Pressure with Hot Neutrons at MLZ

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Due to their specific peculiarities neutrons are a very useful probe for structural studies on various hot topics related to physics, chemistry and mineralogy. The neutron single crystal diffractometer HEiDi at the Heinz Maier-Leibnitz Zentrum (MLZ) offers high flux, high resolution and large q range, low absorption and high sensitivity for light elements. These properties apply in a similar way to its polarized sister diffractometer POLI, which is optimized for magnetic structure determinations.

In 2016 a project was launched in order to allow studies on tiny samples $< 1 \text{ mm}^3$ and to develop new pressure cells for HEiDi which can be combined with its existing low temperature equipment in order to study structural properties down to temperatures below 10 K, e.g. MnFe_4Si_3 compounds and their magnetic features [1]. As part of this project (funded by the BMBF, No. 05K16PA3), various neutron-optical components (Cu220-monochromator, solid state collimators, neutron guides) were developed and optimized in order to generate a sufficiently high flux density at the sample location at the wavelength $= 0.87 \text{ \AA}$. Very tiny single crystal samples ($< 0.1 \text{ mm}^3$) were successfully studied using various newly developed diamond anvil cells up to several GPa, either with a panoramic pressure cell in combination with low temperatures [2] or in a transmission pressure cell, which allows simultaneous studies of the same sample using neutron, synchrotron as well as laboratory x-ray sources [3].

This project is now followed up by a second one (BMBF No. 05K19PA2) focusing on further improving the high pressure capabilities on HEiDi and POLI (including the installation of a 2-dimensional detector) and the development of optimized pressure cells for further instruments at the MLZ, namely POLI, DNS and MIRA (see contribution by A. Eich).

[1] A. Grzechnik et al.; Single-Crystal Neutron Diffraction in Diamond Anvil Cells with Hot Neutrons; J. Appl. Cryst. 51, 351-356 (2018).

[2] A. Eich et al.; Magnetocaloric Mn_5Si_3 and MnFe_4Si_3 at variable pressure and temperature; Mater. Res. Express 6, 096118 (2019).

[3] A. Grzechnik et al.; Combined X-ray and neutron single-crystal diffraction in diamond anvil cells; J. Appl. Cryst. 53(1), 1 - 6 (2020).

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