

Instrument Development on HEiDi for Hot Topics and Extreme Conditions

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Single crystal diffraction is one of the most versatile tools for detailed structure analysis. 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 single crystal diffractometer HEiDi uses the hot source of FRM II to offer high flux, high resolution and large Q range, low absorption and high sensitivity for light elements.

In order to adapt this instrument to the most recent scientific topics its hardware, sample environment and data collection software are continuously extended and improved. For instance, temperature dependent multidimensional Q mapping at low temperatures down to 2.5 K in the multiferroic DyMnO₃ reveals accurately the evolution and interplay between the incommensurate magnetic sublattice of Mn and the commensurate magnetic sublattice of Dy.

At very high temperatures studies on Nd₂NiO_{4+δ} and Pr₂NiO_{4+δ} brownmillerites concerning their oxygen diffusion pathways reveal anharmonic displacements of the apical oxygens pointing towards the interstitial vacancy sites which create a quasicontinuous shallow energy diffusion pathway between apical and interstitial oxygen sites [1]. Recent studies use a special mirror furnace developed at MLZ which allows not only temperatures > 1300 K but also atmospheres with various oxygen content and pressure around the sample to study their influence to the evolution of the occupation of the interstitial sites.

Last but not least recently a BMBF funded project was launched in 2016 in order 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. on MgFe₄Si₃ compounds and their magnetic features [2]. For this reason new high pressure cells have been developed and different components of the neutron optics of HEiDi have been optimized.

[1] M. Ceretti et al.; Low temperature oxygen diffusion mechanisms in Nd₂NiO_{4+δ} and Pr₂NiO_{4+δ} via large anharmonic displacements, explored by single crystal neutron diffraction; J. Mater. Chem. A 3, 21140-21148 (2015).

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

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