

Structural and macroscopic investigation of CrAs at low temperatures and high pressures

A. Eich¹, A. Grzechnik², T. Müller³, C. Paulmann⁴, K. Frieze²

¹ Jülich Centre for Neutron Science–2/Peter Grünberg Institute–4 (JCNS-2/PGI-4), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

² Institute of Crystallography, RWTH Aachen University, 52056 Aachen, Germany

³ Jülich Centre for Neutron Science (JCNS), Forschungszentrum Jülich GmbH at Heinz Maier-Leibnitz Zentrum (MLZ), 85748 Garching, Germany

⁴ Mineralogisch-Petrographisches Institut, Universität Hamburg, 20146 Hamburg, Germany

Chromium Arsenide (CrAs) is the first Cr-based superconductor, exhibiting pressure-induced superconductivity with a maximum $T_c = 2.2$ K at around 1 GPa [1,2] and the dome-like shaped superconducting phase region existing in the vicinity of a magnetically ordered state. The magnetic structure is described as double helices propagating along the c^* direction with the spins in the (a,b) plane. The first-order phase transition from the helimagnetically ordered antiferromagnetic state to a paramagnetic state is clearly and consistently observed in our macroscopic measurements of magnetization, resistivity and heat capacity at $T_N \approx 267$ K. The transition is furthermore connected to an abrupt increase in unit cell volume of about 2.4%, though the symmetry of the crystal structure ($Pnma$, $Z = 4$) does presumably not change [3].

As the understanding of the behaviour of the crystal structure of CrAs so far is based primarily on powder data, the objective of our work is to precisely determine the crystal structure by single crystal diffraction at low temperatures as well as at high pressures. This knowledge will serve as base for further studies of the crystal and magnetic structures of CrAs at simultaneously low temperatures and high pressures, in particular within or in the vicinity of the superconducting phase.

For this, synchrotron x-ray diffraction experiments were performed on single crystals between 300 K and 20 K at ambient pressure, and between 0.92 GPa and 9.45 GPa at room temperature.

The preliminary refinements show a good agreement with the literature data for the room temperature phase. Below the transition temperature the symmetry $Pnma$ is preserved and the reflections can still be indexed with the orthorhombic cell, although a deterioration of the crystal quality is observed.

[1] R.Y. Chen, N.L. Wang, *Rep. Prog. Phys.* **82**, 012503 (2019)

[2] W. Wu, *et al.*, *Nat. Commun.* **5**, 5508 (2014)

[3] T. Suzuki, H. Ido, *J. Appl. Phys.* **69**, 4624 (1991)