

Investigation of the Crystal Structure of CrAs at Low Temperatures and High Pressures

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Chromium Arsenide (CrAs) is the first Cr-based superconductor, exhibiting pressure-induced superconductivity with a maximum $T_c = 2.2$ K at about 1 GPa [1,2]. The superconducting phase region with a dome-like shape lies in the vicinity of a helimagnetically ordered antiferromagnetic state, with a region of coexistence of magnetism and superconductivity below ~ 0.7 GPa [3]. Short-range magnetic fluctuations are assumed to play an essential role for the pairing mechanism of the superconductivity, and CrAs is considered to be a model system for the interplay of superconductivity and helimagnetism.

Up to now, most studies on CrAs in and near the superconducting phase region were focused on magnetic and resistive properties. The crystal structure of CrAs, however, has not been conclusively investigated yet, especially in dependence on the temperature, with only a few isolated data points existing for the full structure. The aim of our investigation is thus to give an overview of the complete structural behaviour of CrAs in dependence on temperature and on pressure to serve as reference for later studies in the two-parameter field.

For this, synchrotron and laboratory X-ray diffraction experiments were performed on single crystals between 400 K and 35 K at ambient pressure, and between 0.92 GPa and 9.45 GPa at room temperature. In accordance with the literature, the first-order phase transition from the paramagnetic to the antiferromagnetic state at $T_N \approx 267$ K is accompanied by an abrupt change in the lattice parameters without a change in the symmetry of the crystal structure (MnP-type $Pnma$, $Z = 4$), but moreover also in the atom coordinates. Our results show that in the paramagnetic phase, the crystal structure is changing around a nearly constant nearest-neighbor Cr–Cr distance which is hardly affected by neither temperature nor pressure (Fig. 1). Hence, this particular distance is assumed to play a key role in the properties of CrAs, which might eventually help in understanding the underlying mechanisms of the superconductivity.

In addition to the changes in the crystal structure, the experiments also show that the magnetostructural phase transition induces a change in the microstructure of CrAs, which has so far not been reported in the literature.

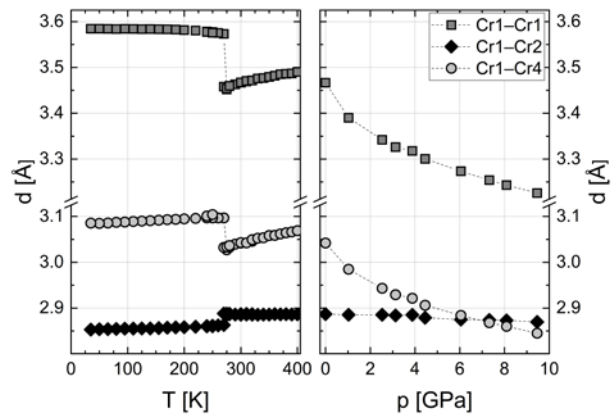


Figure 1: Interatomic Cr–Cr distances in CrAs as function of temperature (left) and pressure (right).

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References:

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