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Redetermination of the incommensurately modulated magnetic structure of CrAs

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Chromium arsenide (CrAs) is considered a model system in which superconductivity and helimagnetism co-exist. The superconductivity is induced by pressure and forms a dome-like phase region with a maximum TC of 2.2 K at about 1 GPa. The superconductivity occurs in the vicinity of an antiferromagnetical phase of CrAs which is incommensurate and described as a double helix in the literature. This model was first proposed on the basis of neutron powder diffraction data and assuming an analogous magnetic structure as the one observed for MnP [1]. Since the model was in reasonable agreement with the powder diffraction data, it was henceforth considered to be correct for CrAs.

We have investigated the magnetic structure of CrAs for the first time by means of neutron high-pressure single-crystal diffraction in clamp cells. The results clearly show that the established model of the magnetic structure of CrAs is not in accordance with the measured intensities and can be discarded. While our data do not allow an unambiguous identification of one singular model, we identify four candidate models based on a stringent use of group theoretical considerations and the subsequent refinement using magnetic superspace groups with the program Jana2006 [2]. Details of these models will be presented.

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[1] H. Watanabe et.al., J. Appl. Phys. 40,1128-1129 (1969).

[2] V. Petricek et. al., Z. Kristallogr. 229, 345-352 (2014).

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