Experimental report

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Proposal: 5-41-977 **Council:** 4/2018

Title: Crystallographic and magnetic structure of UNi4B

Research area: Physics

This proposal is a continuation of 5-41-903

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Samples: UNi_4B

Instrument	Requested days	Allocated days	From	To
D10	8	6	14/09/2018	20/09/2018

Abstract:

The uranium intermetallic UNi_4B, originally reported to crystallize in a hexagonal lattice, was proposed to represent a prime example of a magnetically frustrated metallic f-electron compound. Yet, recently, from a reinvestigation of the crystal structure it was concluded that the crystal structure is orthorhombic, which possibly would be inconsistent with the concept of UNi_4B being a geometrically frustrated system. As well, it raises questions about the proposed magnetic structure of a partially ordered (2 out of 3 uranium moments) system below T_N = 20K. The unresolved issue of the crystallographic and magnetic structure is of relevance in the context of the observation of a magnetoelectric effect for UNi_4B, i.e., the detection of a current induced magnetization. Therefore, to understand the appearance of magnetoelectricity in UNi_4B, it requires a determination of the crystallographic and magnetic symmetries of this compound.

Experimental report: Crystallographic and magnetic structure of UNi_4B

Summary

The frustrated intermetallic magnet UNi_4B has been reported to crystallize in a hexagonal crystallographic structure with a magnetic transition at $T_N = 20\,\mathrm{K}$ [1]. Recently, synchrotron x-ray diffraction data have indicated that the structure is orthorhombic and not hexagonal [2]. The best description of the crystal structure at 300 K was obtained with the space group 63 (*Cmcm*) [2].

Experimental procedure and results

A single-crystal with a mass of 0.8592 g has been used for the experiment, which had already been investigated in the previous neutron diffraction experiment at the D10 diffractometer. The 4-circle cryostat was installed in order to reach the required measurement temperature of 1.8 K.

We refined the measurement data with the space group 63 using the software FullProf (see Fig. 1). The agreement of the refinement with the observed scattering intensities is already good, but shows a mismatch in some details. Furthermore, we detected various structural Bragg peaks forbidden for the Cmcm symmetry. So we assume that the actual space group has to be a subgroup of 63 with a lower symmetry and we limited the number of possible space groups to the following four: 17, 25, 26 and 57.

Further, we have found a lot of magnetic Bragg peaks below T_N and characterized the propagation vector of magnetic structure, which is $q = (0\ \frac{1}{3}\ 0)$. The temperature dependence of the $(0\ 2.67\ 0)$ peak is shown in Fig. 2 and confirms the transition temperature of $T_N = 20\,\mathrm{K}$. Further investigations are required to determine the crystallographic and magnetic structure of UNi_4B.

References

[1] S. Mentink et al., *Phys. Rev. Lett.* **73**, 1031 (1994)

[2] Y. Haga et al., *Physica B* **403**, 900 (2008).

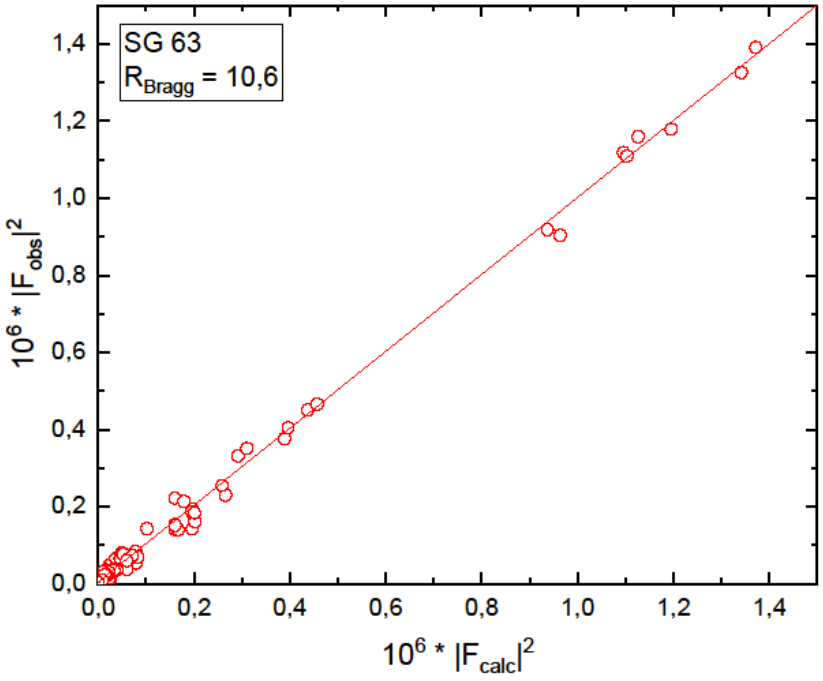
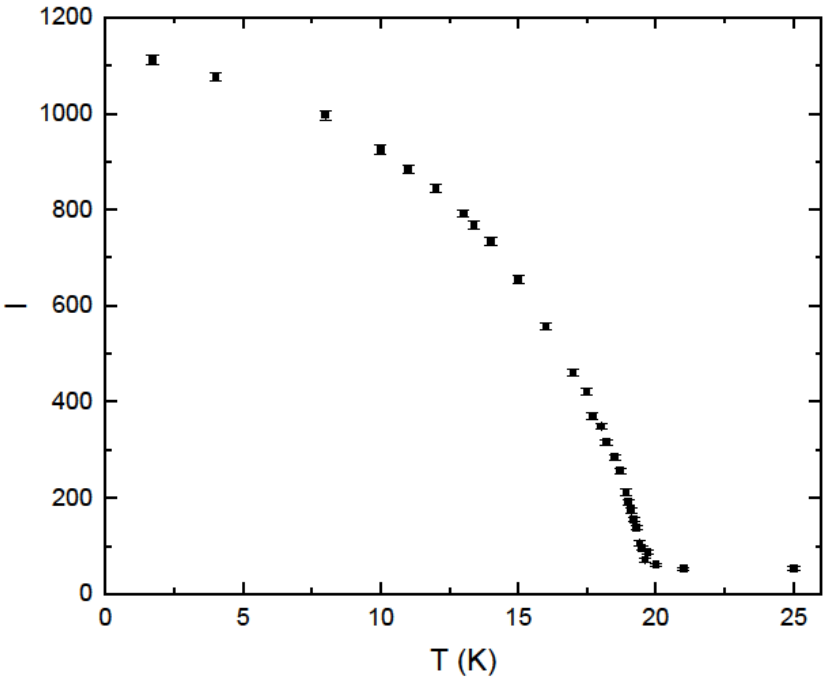


Fig. 1: The result for the refinement for the Cmcm symmetry (space group 63) at 1.8 K.



. Fig. 2: Temperature dependence of the magnetic $(0\ 2.67\ 0)$ peak.