Experimental report

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Proposal: 5-11-433 **Council:** 10/2018

Title: Crystallographic structure of UNi_4B

Research area: Physics

This proposal is a new proposal

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Samples: UNi_4B

Instrument	Requested days	Allocated days	From	To
D10	6	6	03/07/2019	09/07/2019

Abstract:

The precise symmetry of the crystallographic structure of UNi_4B needs to be established in order to associate an unusual magnetoelectric effect observed in this material to the possible existence of a toroidal moment. From a very recent neutron scattering experiment on the crystallographic and magnetic low temperature symmetry of this material we found evidence of a lattice symmetry that is even lower than previously suggested. Therefore, in order to unambiguously and fully establish the crystallographic lattice we propose to carry out a neutron diffraction study on single crystalline UNi_4B (with 11B) with low wavelength neutrons.

Experimental report: Crystallographic structure of UNi_4B

Summary

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

Previously, we have studied the crystallographic symmetry of an ^{11}B enriched single crystalline sample UNi_4B using the diffractometers CYCLOPS and D10 with a neutron wavelength $\lambda = 2.36\,\text{Å}$ (proposal no. 5-41-977). Various structural Bragg peaks forbidden for the *Cmcm* symmetry have been detected during this experiment and indicate that the symmetry is even lower. Because of the good description of the synchrotron x-ray diffraction data with the *Cmcm* symmetry, we assume that the actual space group is a subgroup of the space group 63. With this assumption and the neutron data we have limited the number of possible space groups to the following four: 17, 25, 26 and 57. To fully characterize the material we have proposed another low-temperature Bragg peak mapping with a smaller neutron wavelength of $\lambda = 1.26\,\text{Å}$.

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 to reach the required measurement temperatures of 1.8 K and 30 K. We measured around 2700 reflections at both temperatures. The analysis of the data reveal many reflections forbidden in *Cmcm* (see an example in Fig. 1) and confirm the assumption from our previous neutron diffraction experiments. We measured further reflections to check the list of subgroups and only for space group 25 we found no forbidden reflections. So we conclude that the crystallographic symmetry of UNi_4B is most likely the orthorhombic *Pmm2* (space group 25).

To verify the symmetry we used the software FullProf to refine the structure with the space groups 25 and 63 and compare the results shown in Fig. 2. From our refinement, we find that the *Pmm2* symmetry ($R_{Bragg} = 12.2$) shows a much better agreement with the experimental data than the refinement with the *Cmcm* symmetry ($R_{Bragg} = 22.8$). Thus, according to our neutron diffraction experiment, we conclude that UNi_4B

crystallizes in an orthorhombic lattice with space group 25 ($a = 14.7908$ Å, $b = 6.9281$ Å and $c = 17.1077$ Å).

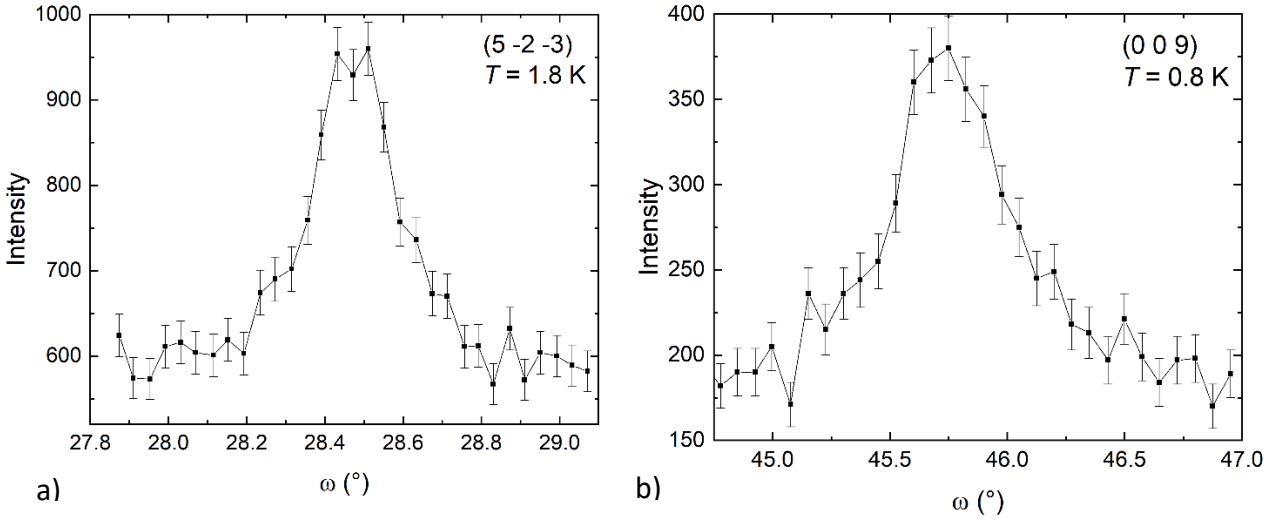

Fig. 1: Rocking curve of the a) (5 -2 -3) peak and b) (0 0 9) peak. The (5 -2 -3) peak violates the condition $h + k = 2n$ for the space group 63 and the (0 0 9) peak the condition $l = 2n$ for the space groups 17, 26, 57 and 63.

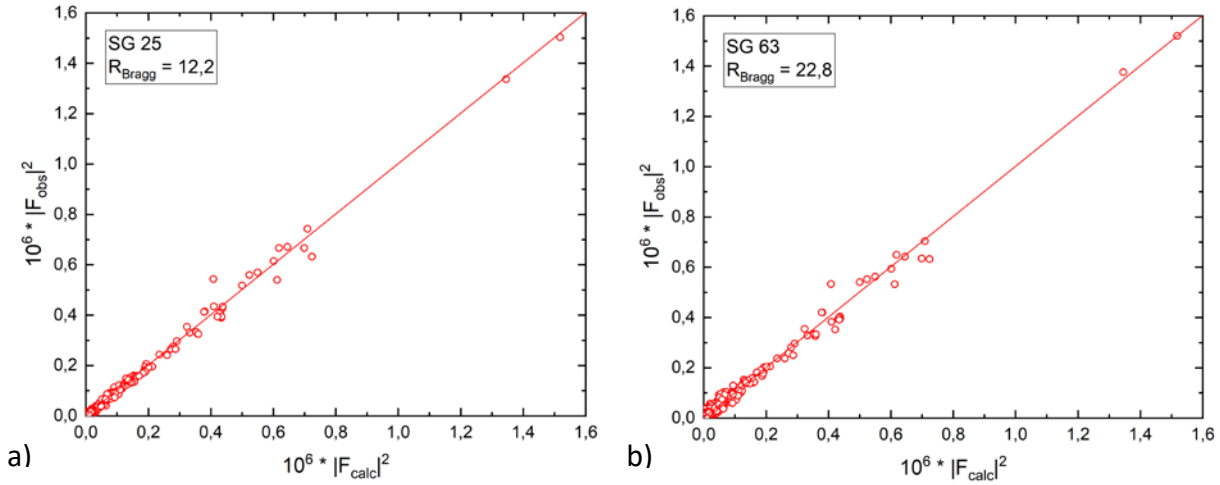

Fig. 2: The result for the refinement for the a) Pmm2 symmetry (space group 25) and b) Cmcm symmetry (space group 63) at 1.8 K.

References

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

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