[MS35-04] Nuclear and Magnetic Structure of HoNi2B2C at Room Temperature and 2.2 K

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Quarternary intermetallics of general composition $LnNi_2B_2C$ (Ln = La – Lu) have arisen much interest due to their superconducting and magnetic properties. Their structures are described in the literature in the tetragonal space group I4/mmm with the approximate lattice parameters $a_{tet} = b_{tet} \approx 3.5$ Å and $c_{tet} \approx 10.5$ Å [1]. They consist of two types of layers: The inverse PbO-type Ni_2B_2 layer, in which the Ni is tetrahedrally coordinated by four boron atoms and the NaCl-type LnC layer, where each lanthanide is in square planar coordination by carbon and vice versa. Much attention has been focused on $HoNi_2B_2C$ due to its complex behaviour at low temperatures. The compound becomes superconducting at ~ 8 K, then reenters the normal state at ~ 5 K and becomes superconducting again at lower temperatures [2-4]. Also at approximately 8 K two types of magnetic peaks initially develop indicating the co-existence of a commensurate antiferromagnetic structure and an incommensurate spiral state. Additional magnetic peaks corresponding to a modulation wave vector of δ = (0.55,0,0) begin to develop at 6.25 K. Below ~5 K the incommensurate magnetic phases are suppressed and only the commensurate antiferromagnetic phase is observed.

We investigated the nuclear and commensurate magnetic structure of HoNi2B2C at room temperature and 2.2 K, respectively, with x-ray and neutron diffraction, as well as spherical neutron polarimetry. The neutron measurements were performed on the 4-circle single crystal diffractometer HEiDi [5] and the polarized neutron single crystal diffractometer POLI [6] at the hot source of the neutron research centre FRM II in Garching. Single crystal x-ray diffraction data were measured in-house using a STOE IPDS II diffractometer. Observed extinction rules for the room temperature data are in accordance with a tetragonal I-centered lattice. Refinements performed with the program Jana2006 [7], in which the room temperature x-ray and neutron single crystal data were taken into account simultaneously, were carried out for all possible tetragonal space groups in accordance with the observed reflections conditions (*hkl: h + k + l = 2n*). A detailed comparison of the results showed the polar space group I4mm to be the best choice. Compared to the published structural data the main difference in our model is the significant displacement of the Ni and C atom from the mirror plane perpendicular to the c axis.

In the neutron data of the magnetically ordered phase at 2.2 K reflections h + k + l = 2n + 1 are clearly visible.

Several trial refinements using different magnetic space groups were carried out and showed the magnetic space group Cmm′2′ ($a_{ortho} \approx b_{ortho} \approx \sqrt{2}\, a_{tet} \approx 4.97$ Å, $c_{ortho} \approx c_{tet} \approx 10.52$ Å) to be the best choice. A 4-fold rotation had to be taken into account in the refinement as additional twin operation. The magnetic moment of Ho was refined to 7.98(10) μB.

The magnetic moments are coupled ferromagnetically in the *a,b* plane forming ferromagnetic sheets which are then stacked antiferromagnetically along the c axis. The spherical neutron polarimetry measurements show that the spins of Ho are aligned in the [110] direction. Trial refinements of the magnetic moment of Ni did not lead to any values significantly different from zero.

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