Magnetic structure of an antiferro-octupolar ordering compound Tb0.94Gd0.06B2C2

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The compound TbB2C2 shows an antiferromagnetic (AFM) ordering at TN = 21.7 K with a main [1 0 1/2] propagation vector and field-induced antiferroquadrupolar transitions [1]. The AFM phase in TbB2C2 that has been called phase IV shows some anomalous features in its magnetic behavior. The [1 0 1/2] wave vector in phase IV is peculiar to TbB2C2 since the other RB2C2 exhibit [1 0 0]-type AFM structure. Furthermore, the magnetic susceptibility anomalously increases below TN without any spontaneous magnetization. To obtain more precise information with respect to the anomalous magnetic behavior, effects of substitution of Tb3+ ions by Gd3+ have been examined and the T-x phase diagram of Tb1-xGdxB2C2 has been constructed [2]. The Gd substitution with a small content (x<0.07) induces drastic change of magnetic properties, namely, an intermediate magnetic phase named AFM1 appears at TO<T<TN. Here, TO is a transition temperature from AFM1 to phase IV. In ref. [2], the following assumption has been proposed: although the magnetic structure of AFM1 is a [1+delta delta 0]-type long periodic one, the antiferro-octupolar (AFO) ordering at TO forces to align the magnetic moments with their wave vector of [1 0 1/2]. The proposed assumption explains satisfactorily for the anomalous properties of TbB2C2 and the Gd-substitution effects [2].

To examine the assumption proposed in ref. [2], neutron powder diffraction experiments of Tb0.94Gd0.06B2C2 has been performed by using HERMES installed at the JRR-3M reactor in JAEA. Neutrons with a wavelength of 1.82646 A were obtained by the 331 reflection of the Ge monochromator. Since the natural boron is a strong neutron absorber, the 11B-enriched boron was used for the sample preparation.

Fig. 1 shows the neutron diffraction patterns of Tb0.94Gd0.06B2C2 measured at several temperatures. At paramagnetic region (T>TN), all of the Bragg peaks can be indexed as a LaB2C2-type tetragonal structure as shown in Fig. 1(a). On the other hand, weak satellite peaks around (100) and (101) are observed at 18 K (TO<T<TN) as shown in Fig. 1(b). The positions of these satellite peaks are almost identical to those observed in phase IV of TbB2C2 [1] as expected in ref. [2], implying that the magnetic structure of AFM1 is a long periodic one whose wave vector is [1+delta delta 0] with delta~0.11. It is noteworthy that similar long periodic structure is observed for the intermediate magnetic phase of ErB2C2 [3]. In addition to the satellite peaks, strong magnetic peaks indexed by the wave vector of [1 0 1/2] are observed at 2.5 K (T<TO) as shown in Fig. 1(c). The results of present neutron diffraction support the assumption proposed in ref. [2].

[1] K. Kaneko et al., J. Phys. Soc. Jpn. 70 (2001) 3112.
[2] E. Matsuoka et al., J. Phys. Soc. Jpn. 75 (2006) 123707.
[3] K. Ohoyama et al., J. Phys. Soc. Jpn. 71 (2002) 1746.

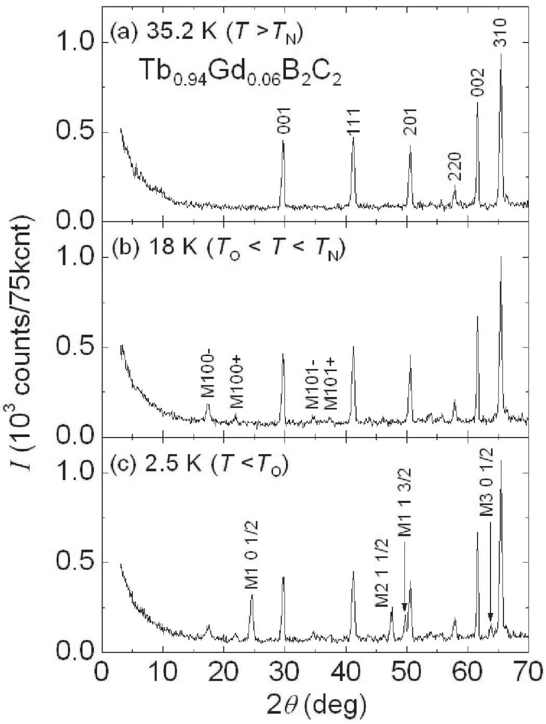

Fig. 1. Neutron powder diffraction patterns of Tb0.94Gd0.06B2C2 measured at several temperatures.