Neutron powder diffraction of Tb1-xGdxB2C2(x=0.15,0.2)

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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<0.075) 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. The neutron diffraction experiments of Tb0.94Gd0.06B2C2 have revealed that the magnetic structure of AFM1 phase is a long periodic one whose wave vector is [1+delta delta 0] with delta~0.114 [3]. The magnetic structure below TO (phase IV) is described by the main wave vector of [1 0 1/2] in addition to the long-periodic component [3]. The results of neutron diffraction support the assumption proposed in ref. [2] that the antiferro-octupolar (AFO) order occurring at TO forces to align the magnetic moments with their wave vector of [1 0 1/2]. This assumption explains satisfactorily the anomalous properties of TbB2C2 and the Gd-substitution effects [2].

TO decreases very rapidly and disappears at x = 0.075, while TN increases with x. For compounds with x > 0.075, a new transition temperature T1 appears below TN. Although the magnetic phase for T1<T<TN is considered to be the same to AFM1 phase described above, that for T<T1 is not phase IV. The magnetic phase below T1 is called as AFM2 [2]. In this study, neutron powder diffraction experiments of Tb0.85Gd0.15B2C2 (x = 0.15) have been performed using HERMES installed at the JRR-3M reactor in JAEA to determine the magnetic structures for T1<T<TN and T<T1. Neutrons with a wavelength of 1.8204(5) 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 Tb0.85Gd0.15B2C2 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 (101) and (211) are observed at 17 K (T1<T<TN) as shown in Fig. 1(b). The positions of these satellite peaks can be explained by considering a long periodic one whose wave vector is [1+delta delta 0] with delta~0.11, implying that the magnetic structure at T1<T<TN is almost identical to AFM1 for Tb0.94Gd0.06B2C2. These satellite peaks disappears at 3.8 K and the other magnetic Bragg peaks appears as shown in Fig. 1(c). The magnetic Bragg peaks at 3.8 K (T<T1) can be explained by considering the wave vector of (100). Therefore, the magnetic structure of AFM2 is identical to that of GdB2C2.

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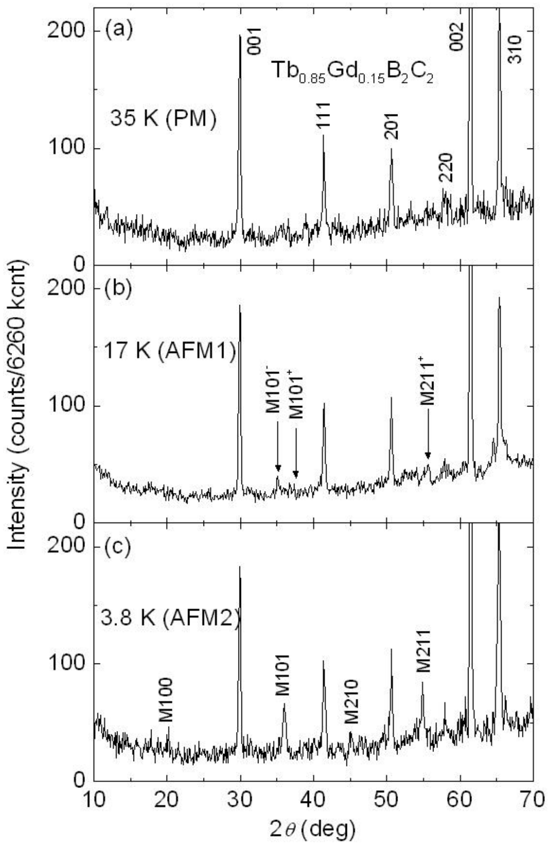

Fig. 1. Neutron powder diffraction patterns of Tb0.85Gd0.15B2C2 measured at several temperatures.