Study of H-T Phase Diagram of $ErNi_2B_2C$

H. Takeshita [a], M. Ochiai [b], E. Habuta [a], T. Nagata [b], H. Kawano-Furukawa [b,c], H. Yoshizawa [d], N. Furukawa [e], H. Takeya [f], K. Kadowaki [g]

[a] *G.S.H.S., Ochanomizu Univ., Bunkyo-ku, Tokyo 112-8610, Japan*
[b] *Department of Physics, Ochanomizu University, Bunkyo-ku, Tokyo 112-8610, Japan*
[c] *PRESTO, Japan Science and Technology Corporation, Kawaguchi, Saitama 332-0012, Japan*
[d] *Neutron Scattering Lab., I. S. S. P., Univ. of Tokyo, Tokai, Ibaraki 319-1106, Japan*
[e] *Department of Physics, Aoyama Gakuin University, Setagaya-ku, Tokyo 157-8572, Japan*
[f] *National Institute for Materials Science, Tsukuba, Ibaraki 305-0047, Japan*
[g] *Institute of Materials Science, University of Tsukuba, Tsukuba, Ibaraki 305-8573, Japan*

Abstract

A field dependence of magnetization of $ErNi_2{}^{11}B_2C$ at 1.8 K with a field parallel to the b axis indicates that three phase transitions occur at 0.6, 1.1 and 1.9 T. In the present study, we performed a neutron diffraction measurement and determined a detailed magnetic structure in a phase at 1.9 K and 0.85 T. Accompanied by odd number higher order peaks there appear strong SDW magnetic peaks with $q_1 = \frac{4}{7}a^*$, indicating that the size of the magnetic unit cell is $7a \times b \times c$.

Key words: weak ferromagnetism; superconductivity

Superconductivity and ferromagnetism are conventionally considered as antagonistic states, because superconductivity collapses when an external magnetic field is applied. However, it is theoretically predicted that superconductivity can coexist with ferromagnetism as far as an internal magnetic filed ($H_{\rm int}$) mediated by the ferromagnetism is lower than the critical magnetic field[1]. In particular, for type II superconductors, the theory predicts that a spontaneous vortex phase may exist if $H_{\rm int}$ further satisfies a following inequality, $H_{c1} < H_{\rm int} < H_{c2}$, where H_{c1} and H_{c2} are lower and upper critical magnetic field, respectively[2–4].

$ErNi_2B_2C$ is the first material in which coexistence of weak ferromagnetism and superconductivity was microscopically confirmed by neutron scattering techniques [5–7]. Previously we determined a weak ferromagnetic structure at 1.4 K in zero-field, which has a unit cell with $20a \times b \times c$[8]. To study details of the H-T phase diagram of this material, we further performed magnetization and neutron diffraction measurements with a field applied parallel to the b axis. In this paper, we shall report the magnetic structure in a phase at 1.9 K and 0.85 T.

Single crystals of $ErNi_2{}^{11}B_2C$ were grown by the floating zone method. To reduce neutron absorptions by ^{10}B, the ^{11}B isotope was used. A superconducting transition temperature (T_c), a Néel (SDW) temperature (T_N) and a weak ferromagnetic transition temperature ($T_{\rm WFM}$) of our pre-annealed sample are 8.6 , 6.0 and 2.75 K, respectively. Magnetization measurements were performed with a Quantum Design MPMS SQUID magnetometer. Neutron diffraction measurements were done with a triple axis spectrometer GP-TAS (4G) installed in the JRR-3M at JAERI, Tokai. Neutrons with $k_i = 2.57 Å^{-1}$ were used. In the present study, an external magnetic field was applied along the b axis.

In Fig. 1(a) is depicted a magnetization curve ($M(H)$ curve) observed at 1.8 K. Three jumps at 0.6, 1.1 and 1.9 T indicate three phase transitions take place at respective fields. From this curve, a saturation moment

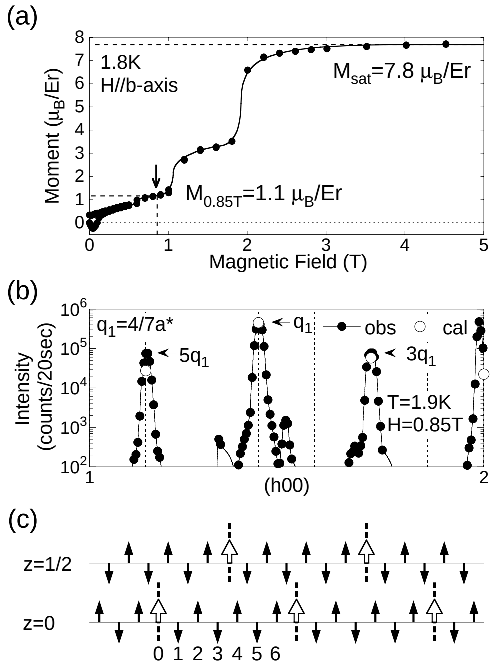

Fig. 1. (a) A field dependence of magnetization at 1.8 K and with an applied field parallel to the *b* axis. (b) Neutron diffraction profile along the (h00) direction at 1.9 K and 0.85 T. Data at 0 T and 10 K were subtracted as a background. Open circle symbols are calculated intensities with a model shown in (c). A large discrepancy between observed and calculated intensities at (200) was attributed to a change of the nuclear intensity due to the crystallographic phase transition at 6 K. (c) The model of the magnetic structure at 1.9 K and 0.85 T. The number of 0, 1, 2, $\cdots$ stands for x positions of Er the atoms.

($M_{\rm sat}$) and a magnetization value at 0.85T ($M_{0.85{\rm T}}$) are evaluated to be 7.8 and 1.1 $\mu_{\rm B}$/Er, respectively. These values are consistent with those reported by Canfield *et al.*[9] and indicate that one from seven Er moments contributes the weak ferromagnetism at 0.85 T.

A neutron diffraction profile observed along the (h00) at 1.9 K and 0.85 T is shown in Fig.1 (b). The magnetic peaks with $q_1 = \frac{4}{7}a^*$ are observed with odd number higher order peaks. The result indicates that the size of the magnetic unit cell in this phase is $7a \times b \times c$. In $ErNi_2B_2C$, Er ions form a body centered lattice, and the magnetic unit cell contains 14 Er ions. By combining the magnetization results, one can expect that the magnetic unit cell contains two excess up spins than down spins, namely 8 up and 6 down spins. With these facts in mind, we tried to determine a precise magnetic structure with two different approaches described below.

First, we focused on the fact that the strong magnetic peaks appear at positions with $q_1 = \frac{4}{7}a^*$, which indicates that the Er spins at the position x feel an effective field $h(x) = h_0\sin(2\pi\frac{4}{7}x)$ and that spins are aligned along this field direction. The existence of odd number higher harmonics further indicates the spins form a squared up structure. With this q_1, the $h(x) = 0$ sites appear at every 7 Er sites as indicated by black dashed lines in the Fig. 1(c). We considered that Er spins at these node sites comply with an external magnetic field to gain the Zeeman energy. An obtained model for the magnetic structure is illustrated in Fig. 1(c). The calculated intensities (open circles) with this model are in good agreement with the observed ones (filled circles) as shown in the Fig. 1(b). Note that this model gives an average net moment of 1.1 $\mu_{\rm B}$/Er.

As a second approach, a computational analysis was performed. In addition to the conditions mentioned above, we assumed that the numbers of up and down spins on the $z = 0$ layer are the same with those on the $z = \frac{1}{2}$ layer because of a disappearance of the (100) reflection, cf. an extinction rule. Namely, four up spins and three down spins were assumed for both $z = 0$ and $\frac{1}{2}$ layers. We calculated all possible spin configurations and found that the best-fit model is the same with the one obtained by the first approach.

From these analyses, we conclude that the phase at 1.9 K and 0.85 T has the magnetic structure depicted in Fig. 1(c). The spin alignment on the $z = 0$ layer is identical with that on the $z = \frac{1}{2}$ layer with a shift of three and a half atoms. Such a spin structure gives a total net moment of $\frac{1}{7}M_{sat} \sim 1.1\mu_{\rm B}$/Er.

In summary, by using neutron scattering technique, we determined the magnetic structure of $ErNi_2B_2C$ at 1.9 K and 0.85 T as the one depicted in Fig. 1(c). The size of the magnetic unit cell in this phase is seven times larger than the crystal unit cell along the a axis and that one from seven Er spins contributes weak ferromagnetism. The structure gives a net moment of 1.1 $\mu_{\rm B}$/Er which is consistent with the magnetization data.

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