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Magnetic structure and dipolar interaction in antiferromagnetic superconductor BCT-$ErRh_4B_4$

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Abstract

Metamagnetic transitions in the antiferromagnetic superconductor BCT-$ErRh_4B_4$ have been analyzed on the basis of the magnetic dipolar interaction by applying the group theoretical method of Luttinger and Tisza. The analyses allowed us to uniquely determine the magnetic structures of the ground state and the intermediate states.

Keywords: Dipolar interactions; Metamagnetism; Magnetic structure; Superconductivity – magnetic

It is well-known that the primitive tetragonal (PT) phase of $ErRh_4B_4$ is a typical ferromagnetic superconductor with $T_S = 8.7$ K, which shows re-entrant behavior at $T_C = 0.95$ K [1]. Making a marked contrast, the body-centered tetragonal (BCT) phase of $ErRh_4B_4$ is an antiferromagnetic superconductor with $T_S = 7.8$ K and $T_N = 0.65$ K, and superconductivity and antiferromagnetism coexist below T_N [2, 3]. We previously reported peculiar metamagnetic transitions in the BCT-$ErRh_4B_4$ single crystal under four-fold anisotropy in the c-plane, which is reproduced in Fig. 1. As can be seen in the figure, the magnetization jumps on two steps with applied field in the [1 0 0] (and [0 1 0]) direction, while it takes a one-step jump in the [1 1 0] direction. The magnetization of the intermediate state is one half of the saturation moment M_0 in the [1 0 0] direction and that in the [1 1 0] direction is $M_0/\sqrt{2}$. The easy magnetization axes are the [1 0 0] and [0 1 0] axes and the [0 0 1] axis is the very strong hard magnetization axis. Since T_N of BCT-$ErRh_4B_4$ is as low as 0.65 K and the magnetic moment μ of Er^{3+} ion is pretty large ($\mu = 9.6\ \mu_B$ in free-ion state), the magnetic dipolar interaction should play a role of fundamental importance to determine the magnetic structure in this compound [4, 5]. We analyze the metamagnetic transitions in BCT-$ErRh_4B_4$ by

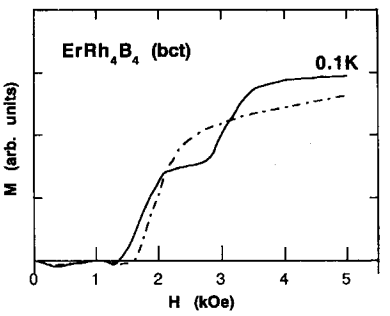

Fig. 1. Solid line represents magnetization with $H \| [1\ 0\ 0]$ and dashed line with $H \| [1\ 1\ 0]$ [2].

applying the method and results of Luttinger and Tisza (LT) [6] for the dipolar energy of the cubic lattice.

If we direct our attention only to Er atoms in BCT-$ErRh_4B_4$, they are located almost on face-centered cubic (FCC) lattice points. Let Γ be the group of cubic translations, $\Gamma = l_1 i + l_2 j + l_3 k$. Here l_1, l_2, l_3 are integers and i, j, k are cubic lattice vectors in the x, y, z directions. We consider the general ordered arrays which are invariant under translations of the form, $\Gamma^2 = l_1(2i) + l_2(2j) + l_3(2k)$. Γ^2 is the subgroup of Γ. For simple cubic (SC) lattice, any ordered array of the class Γ^2 can be represented as a linear combination of the 24 basic arrays, X_i, Y_i, Z_i, $i = 1, 2, \ldots, 8$ (see Fig. 2). The

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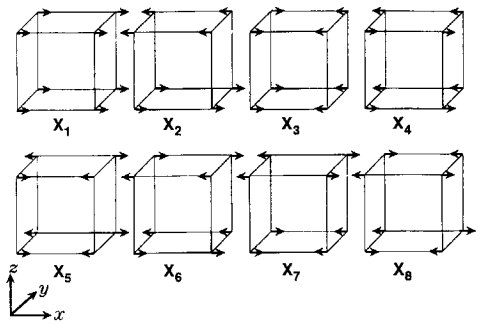

Fig. 2. The eight basic arrays for the x component of the magnetic moment. X_i and the similar basic arrays Y_i and Z_i span the class I^{12} magnetic structures [6].

strength and the symmetry of the fields at the lattice points and face-centers of a cube ($\boldsymbol{f}_1 - \boldsymbol{f}_8$, $\boldsymbol{h}_1 - \boldsymbol{h}_4$) are tabulated in Tables I and II of Ref. [6]. One FCC lattice can be decomposed into four SC lattices and the dipolar energy of various magnetic structures can readily be calculated because we know the fields of the lattice points and face-centers. We now introduce the notation $[P, Q, R, S]$ to denote the FCC magnetic structure with P a basic array at lattice points, Q at XY face-centers, R at YZ face-centers and S at ZX face-centers. As LT pointed out, the ground-state spin configuration (g-state) is $[X_8, Y_8, -X_8, Y_8]$, energy U_g per spin being given by

$$U_g = -\boldsymbol{h}_4\mu^2/2\boldsymbol{a}^3 = -7.232\mu^2/\boldsymbol{a}^3 = -0.48\ \mathrm{K}, \quad (1)$$

where we used the measured value $\mu = 5.3\ \mu_B$ for the saturation moment [2], and $\boldsymbol{a} = 7.4$ Å for the FCC lattice constant. The U_g value seems to be consistent with $T_N = 0.65$ K of this compound.

The lowest dipolar energy state with moment $M_0/2$ in the [1 0 0] direction (I_1-state) is $[X_8, Y_8, X_1, X_1]$ with the dipolar energy

$$U_{I1} = -(\boldsymbol{h}_1 + \boldsymbol{h}_4)\mu^2/4\boldsymbol{a}^3 = -4.699\mu^2/\boldsymbol{a}^3 = -0.31\ \mathrm{K}. \quad (2)$$

This I_1-state is realized from g-state by changing the array at YZ and ZX face-centers to ferromagnetic basic array X_1.

The state with moment $M_0/\sqrt{2}$ in the [1 1 0] direction (I_2-state) is $[X_1, X_1, Y_1, Y_1]$ and the dipolar energy is given by

$$U_{I2} = -\boldsymbol{h}_1\mu^2/2\boldsymbol{a}^3 = -2.167\mu^2/\boldsymbol{a}^3 = -0.15\ \mathrm{K}. \quad (3)$$

If we assume a spherical sample, the metamagnetic transition between g-state and I_1-state should take place at $H_{1d} = 1000$ Oe, between g-state and I_2-state at $H_{2d} = 1300$ Oe and between I_1-state and the final ferromagnetic state ($U_F = 0$) at $H_{3d} = 1700$ Oe, respectively. These values are favorably compared with the experimental values, $H_1 = 1120$ Oe, $H_2 = 1250$ Oe and $H_3 = 2770$ Oe. The minor discrepancy can be remedied by introducing very weak exchange interaction between Er moments. The proposed magnetic structures are schematically presented in Fig. 3. Low-temperature neutron diffraction studies to confirm these structures are highly desirable.

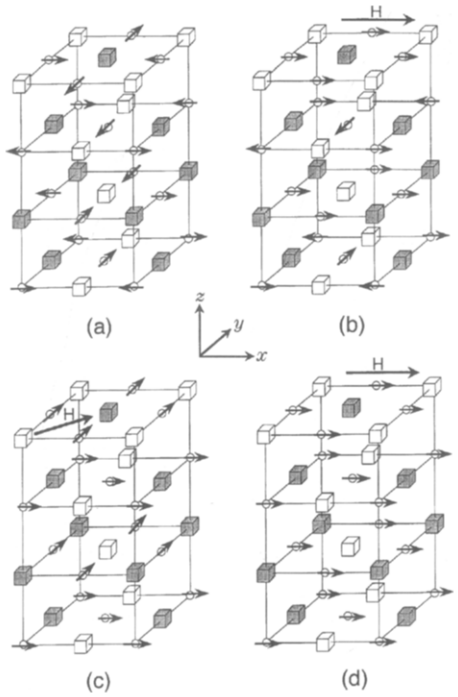

Fig. 3. Proposed magnetic structures, (a) the ground state, (b) the intermediate ferromagnetic state with $M_0/2$ for $H\|[1\ 0\ 0]$; (c) the canted ferromagnetic structure with $M_0/\sqrt{2}$ for $H\|[1\ 1\ 0]$, (d) the final ferromagnetic state for $H\|[1\ 0\ 0]$. Cubes (shaded and not shaded) represent Rh_4B_4 units.

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