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Crystal and Magnetic Structure of $ErRh_3B_2$ Studied by Neutron Diffraction

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Single crystals of $ErRh_3{}^{11}B_2$ were investigated by neutron scattering. The compound crystallizes in space group $C2/m$ with cell dimensions $a = 5.358(5)$ Å, $b = 9.25(1)$ Å, $c = 6.194(5)$ Å and $\beta = 90.35°$. Because of twinning the structure could not be properly refined. Magnetic neutron scattering shows ferromagnetic ordering and a second order phase transition at $T_c = 26.411(7)$ K. There are indications of a small antiferromagnetic moment in the basal plane.

KEYWORDS: $ErRh_3{}^{11}B_2$, Ferromagnet, superstructure, neutron scattering

1 Introduction

Since the discovery of reentrant superconductivity in $ErRh_4B_4$[1,2], the ternary system RE-Rh-B (RE = Rare earth elements) have attracted much interest. The $RERh_3B_2$ systems[3,4] display unusual magnetic properties.

$ErRh_3B_2$ is known to be ferromagnetic and to crystallize in a base-centered monoclinic structure (space group $C2/m$), which is slightly distorted from hexagonal symmetry[5]. Recent X-ray and magnetic susceptibility studies show that the system is more complex[6,7]. Magnetization measurements show considerable anisotropy, with a large magnetic moment along the crystallographic c-axis and a very small moment in the basal plane. X-ray oscillation film technique observations on a single crystal of $ErRh_3B_2$ show a superstructure with a six doubling of the c-axis.

Based on these X-ray and magnetization measurements we have performed a single crystal neutron diffraction study of the $ErRh_3{}^{11}B_2$ compound.

2 Nuclear Scattering

2.1 *Unit Cell*

X-ray powder experiments[5] determined $ErRh_3B_2$ to crystallize in $C2/m$ and with unit cell: $a = 5.362$Å, $b = 9.288$Å, $c = 3.099$Å and $\beta = 90.9°$.

Single crystal X-ray oscillation film[6] of $ErRh_3B_2$ showed weak reflections positioned at $c^*/6$, indicating a six doubling of the c-axis. Because the crystals showed twinning in the a-b-plane, it was not possible to determine the crystal structure in the supercell, but the average positions were determined from powder measurements to be: Er$(0,0,0)$; Rh$_1(0,\frac{1}{2},\frac{1}{2})$; Rh$_2(\frac{1}{4},\frac{1}{4},\frac{1}{2})$; B$(0,0.336(7),0)$.

We performed a four circle neutron diffraction experiment on $ErRh_3{}^{11}B_2$ and found, surprisingly, weak reflections along $c^*/2$, that means only a doubling of the c-axis. The space group seems to be unchanged, $C2/m$, and the unit cell is $a = 5.358(5)$Å, $b = 9.25(1)$Å, $c = 6.194(5)$Å and $\beta = 90.35(7)°$.

We collected a data set and have tried to refine it. It turned out to be extremely difficult, though, due to the twinning, and gave unrealistic thermal parameters. It is therefore very difficult to conclude anything from the analysis, but our present result indicates that the supercell is due only to the Rh- and the B-sites.

2.2 *Structure*

The neutron scattering experiment on $ErRh_3^{11}B_2$ shows a doubling of the c-axis, while the previous X-ray diffraction experiment on $ErRh_3B_2$ shows a six doubling of the c-axis. There can be two possible explanations for that:

1. The difference is due to the two different techniques. The X-rays only probe the surface of the sample

while the neutrons probe the bulk. This explanation indicates that the surface structure is slightly different from the bulk structure.

2. The difference is due to different samples. The sample prepared with enriched ^{11}B is more pure than the sample prepared with natural occuring B, and the structure is not necessarily the same. The different modulations could, for example, be due to different vacancies of the B-sites.

Which one of the explanations that is correct can only be determined unambiguously by doing an X-ray study of $ErRh_3{}^{11}B_2$ or a neutron study of $ErRh_3B_2$.

3 Magnetic Scattering

If the magnetic structure were a simple ferromagnet with the moments located at the Er-atoms directed along the crystallographic c-axis there would be magnetic scattering at $hkl, l = 2n$ and $h + k = 2n$. Because the susceptibility measurements show a small magnetic moment in the basal plane, we were looking for magnetic scattering at unexpected positions.

3.1 *Reflections*

A triple axis neutron scattering experiment ($\lambda = 2$Å) performed on a single crystal mounted with the **b-c** plane horizontal showed magnetic scattering on all the $(0k0)$ reflections. These reflections might be $\lambda/2$ contamination from $(0, 2k, 0)$ reflections that are very strong; we will check this by measurements at the 4-circle diffractometer ($\lambda = 1$ Å) as well.

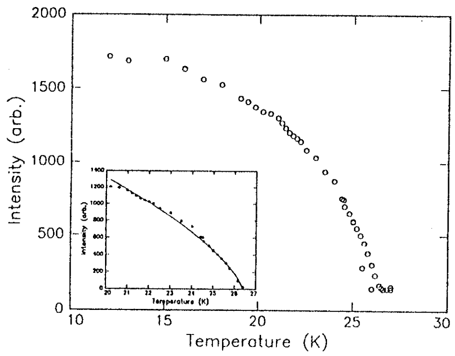

Fig. 1. The intensity (nuclear and magnetic) of the (020) reflections versus temperature. In the inset the best fit to $|(T - T_c)/T_c|^{2\beta}$ in the region close to T_c is shown.

In Fig. 1 the intensity of the (020) reflection is given versus temperature. The region for the (020) reflection close to T_c is shown in the inset, with the solid line being the best fit proportional to $|(T - T_c)/T_c|^{2\beta}$, where we found: $T_c = 26.411(7)$ K and $2\beta = 0.70(2)$. The size of the magnetic moment is difficult to determine precisely, because the precise structure is unknown; hence, the factor converting magnetic intensity to magnetic moment is undetermined.

As expected for a ferromagnet with moments directed along the c-axis, we did not observe magnetic scattering in the $(00l)$ reflections. However, magnetic scattering was observed at $hkl, l = 2n + 1$ positions on top of the nuclear scattering.

3.2 *Magnetic Structure*

It is reasonable to assume that the two Er-atoms in the unit cell have magnetic moments of equal magnitude. A model where $ErRh_3B_2$ is a simple ferromagnet with all the magnetic moments localized on Er-atoms and directed along the c-axis can therefore not give rise to scattering on the $(hkl), l = 2n + 1$ reflections.

If we combine this information with the susceptibility data that shows a small magnetic moment in the basal plane (the a-b-plane), it leads us to suggest that the magnetic struture is a ferromagnet with a weak antiferromagnetic moment in the basal plane. The magnetic moment at the Er-atoms at the (000) and $(\frac{1}{2}\frac{1}{2}0)$ reflections could be (μ_a, μ_b, μ_c) and consequently the moment at the Er-atoms at the $(00\frac{1}{2})$ and $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ would be $(-\mu_a, -\mu_b, \mu_c)$.

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