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Magnetic structure and magneto-volume anomalies in $\text{Er}_2\text{Fe}_{17}$ compound

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Abstract. Neutron powder diffraction shows that the intermetallic $\text{Er}_2\text{Fe}_{17}$ compound with hexagonal crystal structure has a ferrimagnetic ground state ($T_C = 303$ K). At $T = 5$ K the magnetic moments of Fe sublattice ($\mu \sim 2 \mu_B$) are therefore antiparallel to those of the Er one ($\mu \sim 9 \mu_B$), all of them lying on the basal plane. This compound exhibits strong magneto-volume effects up to temperatures in the vicinity of T_C . Neutron thermo-diffraction experiments also show an anomalous temperature dependence of the cell volume, including a negative thermal expansion coefficient below 300 K. In addition, a positive spontaneous volume magnetostriction is observed up to $T \sim 400$ K, with a maximum ($\omega_s \sim 0.02$) located at $T = 5$ K.

1. Introduction

$\text{Er}_2\text{Fe}_{17}$ orders magnetically with Curie temperature, T_C , close to room temperature [1,2]. It crystallizes into the hexagonal $\text{Th}_2\text{Ni}_{17}$ -type crystal structure with iron atoms occupying four different crystallographic sites, 4f, 6g, 12j and 12k, and two non-equivalent positions for erbium, 2b and 2d (in Wyckoff notation) [3]. The magnetic behaviour of the R_2Fe_{17} compounds depends strongly on the local environment of the Fe atoms. This Fe-rich R-Fe family of intermetallic compounds displays a combination of relatively high values for the Fe magnetic moments (exceeding $2 \mu_B$), with rather low magnetic ordering temperatures (between 200 and 500 K) [3], and the existence of a moderate magneto-caloric effect [4,5]. In the case of hexagonal crystal structure, the Fe atoms located at the 4f positions possess the largest coordination number, which is likely related to their higher values for the magnetic moment compared with those of the rest of the Fe atoms occupying the other three non-equivalent positions [6]. For interatomic distances larger (or lower) than a critical distance of 2.45 Å positive (or negative) Fe-Fe magnetic exchange interactions are involved [7,8]. The strong link between the magnetic behaviour and the Fe-Fe interatomic distances gives rise to magneto-volume anomalies from low temperature to the vicinity of T_C , similar to those found in Fe-3d invar alloys, such as FeNi or FeCu [9-11].

In this work we show a preliminary study of the crystal and magnetic structures, together with the anomalous temperature dependence of the cell volume in $\text{Er}_2\text{Fe}_{17}$.

2. Experimental

As-cast $\text{Er}_2\text{Fe}_{17}$ ingots have been prepared from commercial (Goodfellow) 99.9% pure elements, mixed in the nominal molar ratio 2:17, by arc melting under Ar atmosphere, being remelted at least three times to ensure their homogeneity. An excess of 5% Er has been added to compensate the evaporation losses. Each specimen has been annealed during one week at 1373 K and water quenched directly from the furnace. Crystallographic information has been obtained by means of both x-ray (XRD) and neutron powder diffraction (ND). A room temperature XRD pattern was collected in a high-resolution powder diffractometer (Seifert XRD 3000 T/T), with scans performed from 5 to 25° in $\Delta 2\theta = 0.01^\circ$ steps using 40 s as counting time per step and Mo K_α radiation ($\lambda = 0.7107 \text{ \AA}$). The temperature dependence of the cell parameters has been determined from a neutron powder thermo-diffraction experiment [12] performed on the high-flux D1B two-axis powder diffractometer ($\lambda = 2.52 \text{ \AA}$). More than 100 patterns (10 minutes long) collected in temperature steps of 5 K in the temperature range 5 - 820 K were collected using a conventional orange cryostat and a vanadium furnace. Several 2-hour patterns have been collected at selected temperatures between 5 K and 325 K in order to show the evolution of the magnetic structure with temperature. In addition, a high resolution ND pattern above the ordering temperature have been collected on the two-axis D1A diffractometer ($\lambda = 1.91 \text{ \AA}$) at $T = 350 \text{ K}$. All neutron experiments have been performed at the ILL (Grenoble, France). Rietveld analysis of the diffraction patterns has been carried out by means of the Fullprof suite package [13]. Effects on the peak broadening due to small crystals and/or microstrain effects [14] were not observed.

3. Results and Discussion

3.1. Crystal and magnetic structure

The diffraction peaks can be indexed as the Bragg reflections associated with the hexagonal $\text{Th}_2\text{Ni}_{17}$ -type crystal structure, in agreement with those observed on the XRD pattern (not shown). As the Curie temperature of the compound is $T_C \sim 303 \text{ K}$, firstly we have refined the high resolution neutron diffraction pattern collected in the paramagnetic region (at $T = 350 \text{ K}$, see figure 1), in order to reduce the number of free parameters when refining the magnetic structure in the diffraction pattern collected at $T = 5 \text{ K}$ in the high-flux D1B diffractometer.

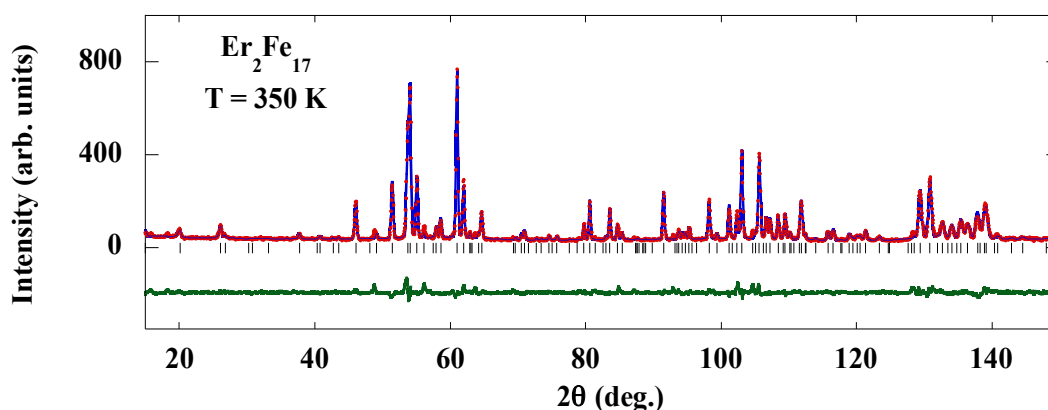


Figure 1. Observed (dots) and calculated (solid line) NPD pattern at $T = 350 \text{ K}$. Positions of the Bragg reflections are represented by vertical bars. The observed–calculated difference is depicted at the bottom of each figure.

The modus operandi was as follow: the cell parameters and the atomic coordinates have been refined, and then the atomic coordinates as well as the isotropic temperature factor, B, for each atom of Er [2b (0 0 1/4), 2d (1/3 2/3 3/4)] and Fe [4f (1/3 2/3 z); 6g (1/2 0 0); 12j (x y 1/4); 12k (x 2x z)]; labels for the Er and Fe atomic sites are those used in the International Tables for Crystallography for the space group $P6_3/mmc$ (#194) [15]. Attempts using a disordered hexagonal structure [16,17] have been carried out, leading to worse results.

The values for the magnetic moment at each crystallographic site have been obtained by refining the pattern collected at $T = 5$ K (D1B), and using as starting information those values for the Fe magnetic moment in the isostructural Y_2Fe_{17} compound [18], while the magnetic moments of Er remain as free parameters during the fitting procedure (see Table I). When the pattern corresponding to $T = 5$ K is properly fitted, the magnetic moments for the 6 non-equivalent sites (4 Fe and 2 Er) are left as free parameters for the rest of the patterns. The fit shows that Er_2Fe_{17} is a collinear ferrimagnetic with Er and Fe magnetic moments antiparallel to each other and all of them lying in the basal-plane. A further study of the magnetic structure will be published elsewhere.

TABLE I. Crystallographic data ($T = 350$ K) and magnetic moments ($T = 5$ K) of Er_2Fe_{17} obtained from neutron diffraction patterns collected on D1A and D1B, respectively.

a (Å)		8.4415 (1)
c (Å)		8.2480 (1)
V (Å ³)		509.00 (1)
Er (2b)	μ (μ_B)	9.03 (8)
Er (2d)	μ (μ_B)	9.03 (8)
Fe (4f)	μ (μ_B)	2.23 (8)
	z	0.1051 (4)
Fe (6g)	μ (μ_B)	2.04 (8)
Fe (12j)	μ (μ_B)	1.98 (9)
	x	0.3290 (4)
	y	0.9580 (3)
Fe (12k)	μ (μ_B)	1.73 (9)
	x	0.1660 (4)
	z	0.9822 (2)

3.2. Magneto-volume anomalies

In the three-dimensional plot of figure 2 we show the temperature evolution of the neutron powder diffraction patterns of the Er_2Fe_{17} compound between 5 K and T_C . The decrease of the magnetic intensity can be clearly observed in the three intense Bragg reflections found below 55° in 2θ as the temperature is raised. Moreover, Er_2Fe_{17} exhibits a cell contraction along the c-axis when heating from 5 K to around 325 K, whereas the cell dimensions on the basal plane remain almost unchanged in that temperature range, similar to that found in other R_2Fe_{17} compounds [7,8]. Consequently, the cell volume shows a decrease that reaches around 0.4 % between 5 and 325 K, giving rise to an anomalous and negative thermal expansion coefficient with minimum values in the vicinity of T_C . For temperatures above 400 K, the cell parameters a and $c(T)$ (not shown) increase linearly with temperature as it is expected for a conventional metal.

Figure 3 shows the cell volume vs. temperature curve. As the temperature goes up from 5 K up to the magnetic ordering temperature, the Fe magnetic moments decrease and the magneto-volume coupling loses strength progressively, giving rise to the above mentioned lattice contraction. The volume decreases down to the corresponding equilibrium value in the absence of magnetic order, which is reached above T_C .

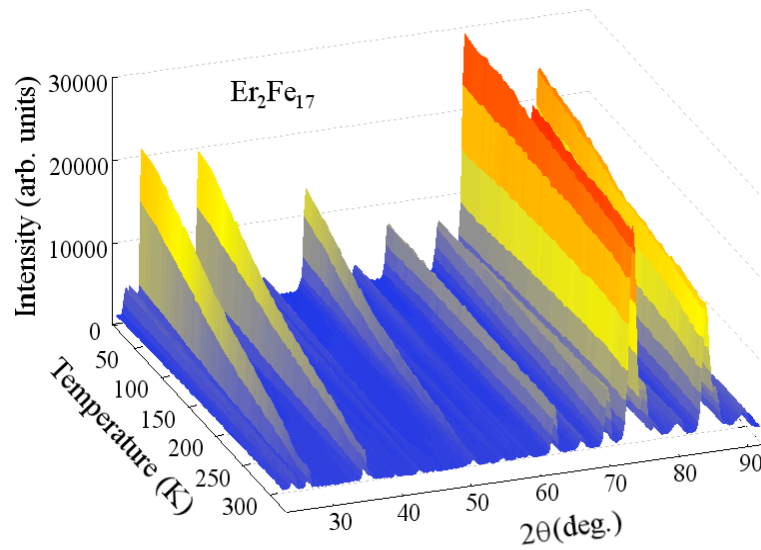


Figure 2. 3-D plot of neutron thermo-diffraction patterns.

This is a consequence of the strong dependence between the magnetic interactions and the Fe-Fe interatomic distances, and suggests the existence of short-range magnetic interactions in the paramagnetic state up to $T > 1.2 T_C$ [6,7,9,19].

The temperature dependence of the magnetostriction normalized to the value at $T = 5$ K [$\omega_s(5K) = 0.018$] is also shown in Figure 3. The value of $\omega_s/\omega_s(5K)$ increases progressively as the temperature decreases down to $T = 5$ K. It is worth noting that ω_s exhibits non-zero values even for temperatures $T > T_C$, therefore, the existence of magnetic short-range ordering in the paramagnetic region can be invoked [20-23].

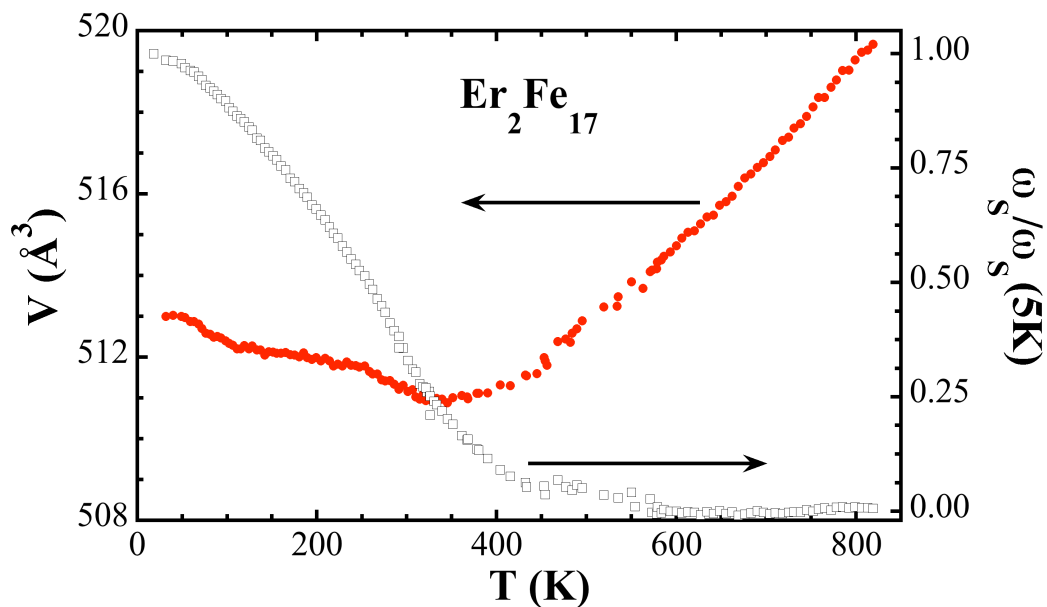


Figure 3. Temperature dependence of the cell volume and the normalized magnetostriction (for details about calculation, see text).

Summary and conclusions

The values for the magnetic moment of the different crystallographic sites in $\text{Er}_2\text{Fe}_{17}$ have been obtained at $T = 5$ K, showing that this compound is ferrimagnetic with the rare-earth moments ($\mu(\text{Er}) \sim 9 \mu_B$) antiparallel to those of the Fe-sublattice ($\mu(\text{Fe}) \sim 2 \mu_B$). Strong magneto-volume anomalies are present in $\text{Er}_2\text{Fe}_{17}$, evidenced throughout a lattice contraction on heating from 5 K up to around 325 K. The spontaneous magnetostriction increases upon cooling reaching a value of $\omega_s = 0.018$ at $T = 5$ K. A more exhaustive work on the variation of magnetic moments with temperature will be done in a further study.

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