



# Magnetic anisotropy of $\text{YFe}_{11}\text{Ti}$ single crystal and its hydride

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## Abstract

The magnetocrystalline anisotropies of  $\text{YFe}_{11}\text{Ti}$  and its hydride are studied by torque and pendulum magnetometer in the temperature range 4.2–700 K in magnetic fields up to 13 kOe both on single crystals and magnetically aligned powder samples. The temperature dependence of the anisotropy constants  $K_1(T)$  and  $K_2(T)$  is determined. The Curie temperature, saturation magnetization and easy *c*-axis anisotropy are increased by hydrogenation. © 1999 International Association for Hydrogen Energy. Published by Elsevier Science Ltd. All rights reserved.

## 1. Introduction

Rare-earth intermetallic compounds  $\text{RFe}_{11}\text{Ti}$  have been attracting interest as candidates for permanent magnets because of fairly high values of Curie temperature, saturation magnetization and magnetocrystalline anisotropy [1, 2]. Recently, interstitial atoms such as H, N and C have been introduced into the crystal to modify the magnetic properties [3, 4]. To understand this effect, it is important to examine the properties of the Fe sublattice magnetism. The purpose of the present paper is a detailed study of magnetocrystalline anisotropy of  $\text{YFe}_{11}\text{Ti}$  single crystal and its hydride.

## 2. Experimental

The  $\text{YFe}_{11}\text{Ti}$  alloy was prepared by induction melting under argon atmosphere of constituent elements of purity at least 99.95 wt%. The ingot was remelted for homogenization. X-ray diffraction was used to control the single phase in samples. The ingots were preheated and cooled slowly in order to increase the grain size. The single crystals were extracted from the solidified ingots and were oriented by the conventional back Laue reflection method. For investigation of the  $\text{YFe}_{11}\text{Ti}$  interaction with hydrogen, a procedure was employed as described

in Ref [5]. Magnetic measurements were made on single crystal and the magnetically aligned powder samples using a torque and pendulum magnetometer in the temperature range 78–700 K in magnetic fields up to 13 kOe. The magnetization curves of  $\text{YFe}_{11}\text{Ti}$  single crystal were also measured in impulse fields up to 100 kOe using the induction method in the temperature range 4.2–300 K.

## 3. Result and discussion

Figure 1 shows the temperature dependence of saturation magnetization  $\sigma_s$  for the  $\text{YFe}_{11}\text{Ti}$  single crystal specimens and its hydride. It is noted that for  $\sigma_s$  for  $\text{YFe}_{11}\text{Ti}$  is much smaller than  $\text{YFe}_{11}\text{Ti H}$  (see Table 1). Table 1 also lists the lattice parameters (*a* and *c*) and unit-cell volume *V* at *T* = 300 K for  $\text{YFe}_{11}\text{Ti}$  and its hydride. The unit-cell volume expansion is 0.9% upon hydrogenation. The increase of the saturation magnetization of the hydride results from the volume expansion. Thermomagnetic analysis was used to measure the Curie temperature *T<sub>c</sub>*. The *T<sub>c</sub>* = 538 K for  $\text{YFe}_{11}\text{Ti}$  and *T<sub>c</sub>* = 600 K for  $\text{YFe}_{11}\text{Ti H}$  (Fig. 1, inset). The  $\text{Y}^{3+}$  is non-magnetic and the Curie temperature of this compound is determined by the Fe–Fe exchange interactions. It can be seen from the experimental results, that the Fe–Fe exchange interactions increase upon hydrogenation. The exchange coupling constants were obtained earlier in Ref [4].

Figure 2 shows the experimental torque curve  $L(\varphi)$ , where  $\varphi$  is the angle between *H* and the *c*-axes, for aligned

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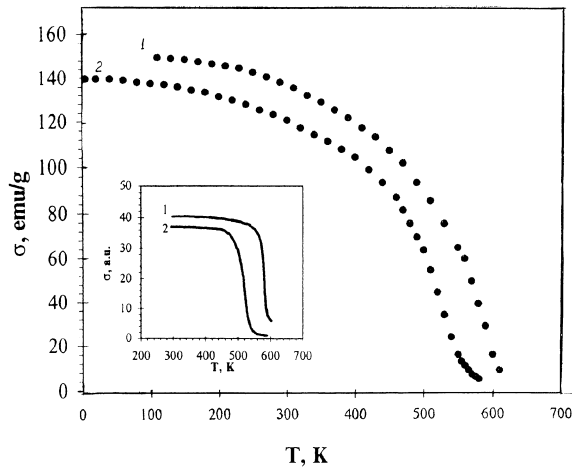


Fig. 1. Temperature dependence of saturation magnetization  $\sigma$  for 1—YFe<sub>11</sub>TiH; 2—YFe<sub>11</sub>Ti single crystal. Inset: thermomagnetic curves of YFe<sub>11</sub>Ti and its hydride.

powder samples YFe<sub>11</sub>Ti and YFe<sub>11</sub>TiH at  $T = 300$  K. The shape of the torque curve is a typical uniaxial type. The easy axis is  $c$  axis. We have also obtained the torque curves for the (110) disk of YFe<sub>11</sub>Ti single crystal at different temperatures. Anisotropy constants  $K_1$  and  $K_2$  were determined by using a procedure as described in Ref. [6]. The magnetization curves of the aligned samples were measured in magnetic fields applied parallel and perpendicular to the alignment direction for YFe<sub>11</sub>Ti and YFe<sub>11</sub>TiH at  $T = 300$  K (Fig. 2, inset). Anisotropy constants  $K_1$  and  $K_2$  were determined by using Sucksmith's method [7].

The temperature dependence of anisotropy constants  $K_1$  and  $K_2$  for the YFe<sub>11</sub>Ti single crystal is presented in Fig. 3 (open circles: Sucksmith–Thompson method, closed circles: method of analysis of the corrected torque curves). The magnetic anisotropy constant  $K_2$  ( $K_2 = 0.096 \times 10^7$  erg cm<sup>-3</sup> at  $T = 4.2$  K) is negligible

Table 1

Lattice parameters  $a$  and  $c$ , unit-cell volume  $V$ , second-order anisotropy constant  $K_1$  and saturation magnetization  $\sigma_s$  at  $T = 300$  K for YFe<sub>11</sub>Ti and its hydride

	$a$ [Å]	$c$ [Å]	$V$ [Å <sup>3</sup> ]	$c/a$	$K_1 \times 10^7$ [erg cm <sup>-3</sup> ]	$\sigma_s$ [emu/g]
YFe <sub>11</sub> Ti	8.509	4.783	346.6	0.56211	0.85	120
YFe <sub>11</sub> TiH	8.547	4.786	349.6	0.55996	1.25	138

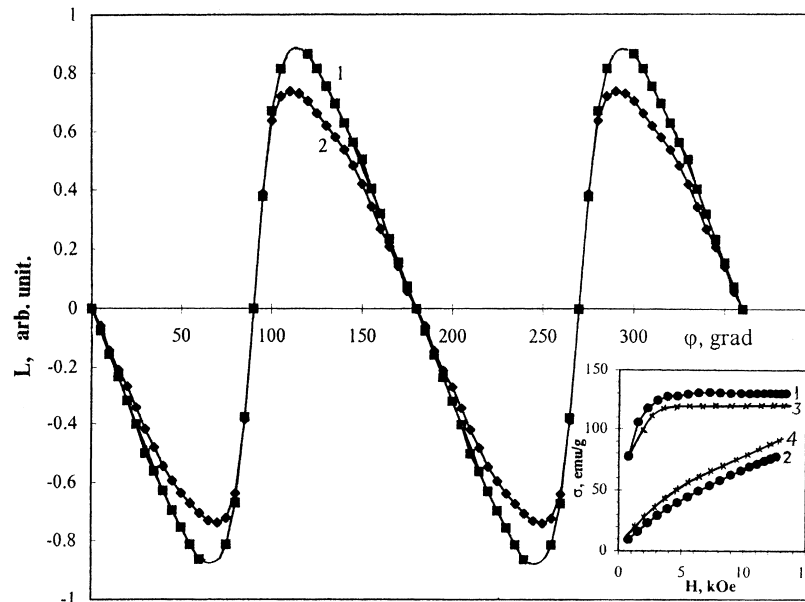


Fig. 2. Observed torque curves  $L$  obtained in an applied field of 13 kOe for 1—YFe<sub>11</sub>TiH; 2—YFe<sub>11</sub>Ti aligned powder samples at  $T = 300$  K. Inset: magnetization curves of YFe<sub>11</sub>Ti [3, 4] and its hydride [1, 2] along and perpendicular to the alignment direction at  $T = 300$  K.

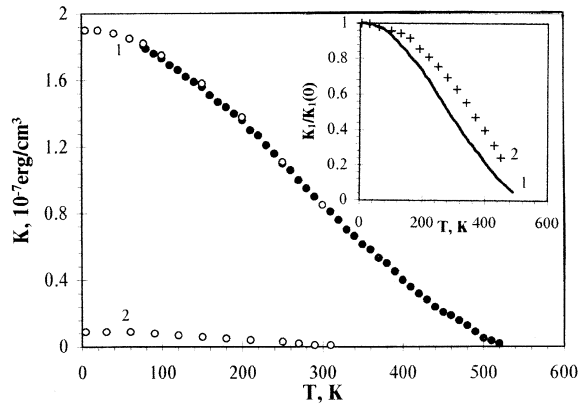


Fig. 3. Experimental temperature dependence of the magnetic anisotropy constants: 1,  $K_1$ ; 2,  $K_2$  for  $\text{YFe}_{11}\text{Ti}$  single crystal (open symbols—Sucksmith–Thompson method, and filled symbols—method of analysis of the corrected torque curves). Inset: 1— $K_1(T)/K_1(0)$  approximations by 2—calculated curve for a localized model [8].

compared to  $K_1$  ( $K_1 = 1.9 \pm 0.1 \times 10^7 \text{ erg cm}^{-3}$  at  $T = 4.2 \text{ K}$ ). The decrease of  $K_1$  with increasing temperature is faster than the predicted theory of localized magnetic moment system, namely  $K_1(T)/K_1(0) = [M_s(T)/M_s(0)]^3$  (Fig. 4 inset) [8].

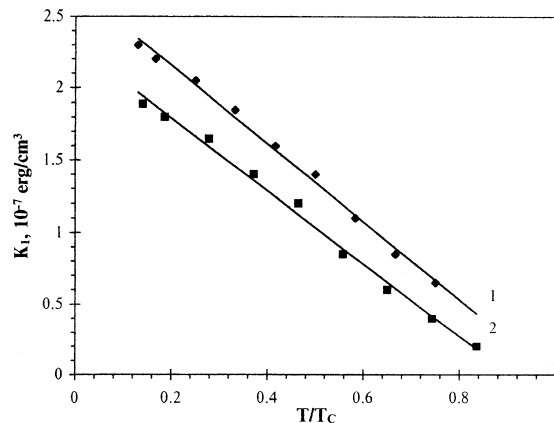


Fig. 4. Dependence of anisotropy constants  $K_1$  vs the  $T/T_c$  for: 1— $\text{YFe}_{11}\text{TiH}$ ; 2— $\text{YFe}_{11}\text{Ti}$ .

Figure 4 shows the dependence of anisotropy constants  $K_1$  vs the  $T/T_c$  for  $\text{YFe}_{11}\text{Ti}$  and its hydride. It is noted that hydrogenation enhances the easy  $c$ -axis anisotropy of the  $\text{YFe}_{11}\text{Ti}$  compound. From pure crystal-field consideration the second-order anisotropy constant  $K_1$  is expected to be proportional to  $(1 - \alpha(c/a)^2)$  [9]. Comparing the experimental data with calculated data shows that the change of  $c/a$  ratio and saturation magnetization by hydrogenation cannot adequately explain the change of value of second-order anisotropy constant  $K_1$ .

Interstitial hydrogen effect on the crystal field parameters is complex. Hydrogen atoms are located at the  $\text{YTi}_2\text{Fe}$  tetrahedral sites [4]. From experimental data (Table 1), it follows that introduction of H increases the lattice parameters and the unit-cell volume. This leads to the narrowing 3d band [4]. The change of local environment of Fe ions resulting from hydrogenation makes valency bonds between Fe ions weaker and rearranges electron density of valency electrons [10]. These effects are probably responsible for the significant increase of magnetic anisotropy in  $\text{YFe}_{11}\text{TiH}$  which is reported in this paper.

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