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Study of the magnetocrystalline anisotropy of $\text{YFe}_{12-x}\text{Mo}_x$ and $\text{YFe}_{12-x}\text{Mo}_x\text{N}_y$ ($x = 1-3$, $y \simeq 1$)

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Abstract. The magnetocrystalline anisotropy of $\text{YFe}_{12-x}\text{Mo}_x$ and $\text{YFe}_{12-x}\text{Mo}_x\text{N}_y$ ($x = 1-3$, $y \simeq 1$) have been investigated by x-ray diffraction and the singular point detection technique. The uniaxial anisotropy of the $\text{YFe}_{12-x}\text{Mo}_x$ series decreases with increasing Mo concentration with a clear turning point at about $x = 1.6$. The anisotropy characteristic of the nitride $\text{YFe}_{12-x}\text{Mo}_x\text{N}_y$ changes into a canted-type anisotropy for $x < 1.5$ and a planar anisotropy for $x \geq 1.5$. The anisotropy reduction for $\text{YFe}_{12-x}\text{Mo}_x$ is mainly due to the substitution of Mo atoms on the 8i sites, while the further change in anisotropy for $\text{YFe}_{12-x}\text{Mo}_x\text{N}_y$ may be due to a change in the 3d orbital moment or to a change in crystal-field interaction by the interstitial N atoms.

1. Introduction

In recent years the rare-earth iron-rich nitrides $\text{RFe}_{12-x}\text{T}_x\text{N}_y$ ($\text{R} \equiv$ rare earth; $\text{T} \equiv \text{Ti}, \text{V}, \text{Cr}, \text{Mo}$ or W) with tetragonal ThMn_{12} -type structure have been studied extensively [1-6]. Of these compounds, $\text{RFe}_{12-x}\text{Mo}_x$ can be readily stabilized and the nitride $\text{RFe}_{12-x}\text{Mo}_x\text{N}_y$ ($\text{R} \equiv \text{Nd}$ or Pr) seems to be more suitable for permanent magnet fabrication [7, 8]. From studies of intrinsic magnetic properties on the $\text{RFe}_{10}\text{Mo}_2$ series, it has been observed that there is variety of magnetic phase transitions (MPTs) at low temperatures [9]. In order to obtain information on the influence of the element Mo on the intrinsic magnetic properties of the Fe sublattice, a detailed study of the $\text{YFe}_{12-x}\text{Mo}_x$ and its nitride is required. Recently, some intrinsic magnetic properties of $\text{YFe}_{12-x}\text{Mo}_x$ and its nitride were reported [10, 11]. In this work, we investigated the magnetocrystalline anisotropy of $\text{YFe}_{12-x}\text{Mo}_x$ and $\text{YFe}_{12-x}\text{Mo}_x\text{N}_y$ ($1 < x < 3$, $y \simeq 1$) in detail.

2. Experimental details

Ingots of $\text{YFe}_{12-x}\text{Mo}_x$ with $x = 1.0, 1.25, 1.5, 1.75, 2.0, 2.5$ and 3.0 were prepared by arc melting from 99.9% starting materials and then vacuum annealed at 1100°C for 24 h. By x-ray diffraction and thermomagnetic analysis, all alloys were found to be single phase with a ThMn_{12} -type structure. The nitrides were formed by heating the fine powders of parent alloys at 580°C for about 4 h in nitrogen. The nitrogen content was estimated by the weight difference before and after nitrogenation and the value y is about 1 in

$\text{YFe}_{12-x}\text{Mo}_x\text{N}_y$. The Curie temperature T_C was derived from the thermomagnetic curves in an applied field of 0.07 T. The saturation magnetization M_S was obtained using an extracting-sample magnetometer in the temperature range from 1.5 to 300 K in an applied field up to 7 T. The anisotropy characteristics was checked using aligned-powder x-ray diffraction. The anisotropy field B_a was determined by the singular point detection (SPD) technique [12] on the aligned samples magnetizing along the perpendicular direction, which was performed in a pulsed-field magnetometer with an available field of 10 T. The signal from the sample can be treated by the electronic system and then the magnetization curve $M(B_0)$ or derivatives $d^2(B_0)/dt^2$ can be plotted.

3. Results and discussion

Studies of x-ray diffraction patterns show that all annealed parent alloys are single ThMn_{12} -structure phase and their nitrides retained the structural symmetry of parent alloys, but with cell volume expansions and a small amount of α -Fe. The Curie temperature T_C varies with Mo concentration for both the parent alloys $\text{YFe}_{12-x}\text{Mo}_x$ and their nitrides $\text{YFe}_{12-x}\text{Mo}_x\text{N}_y$ and this is plotted in figure 1. These values are in agreement with those reported in literature [1, 10]. The values of T_C and other intrinsic magnetic properties are summarized in table 1.

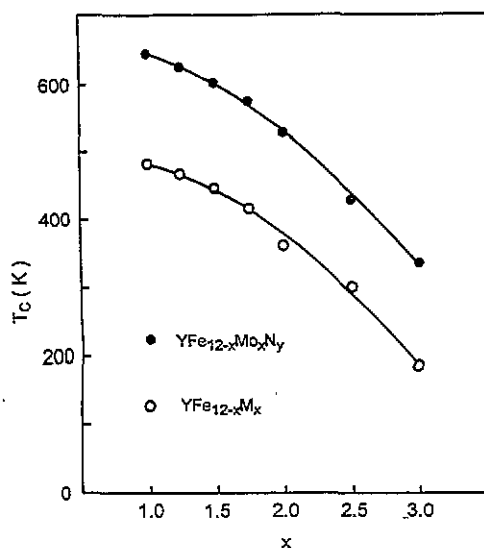


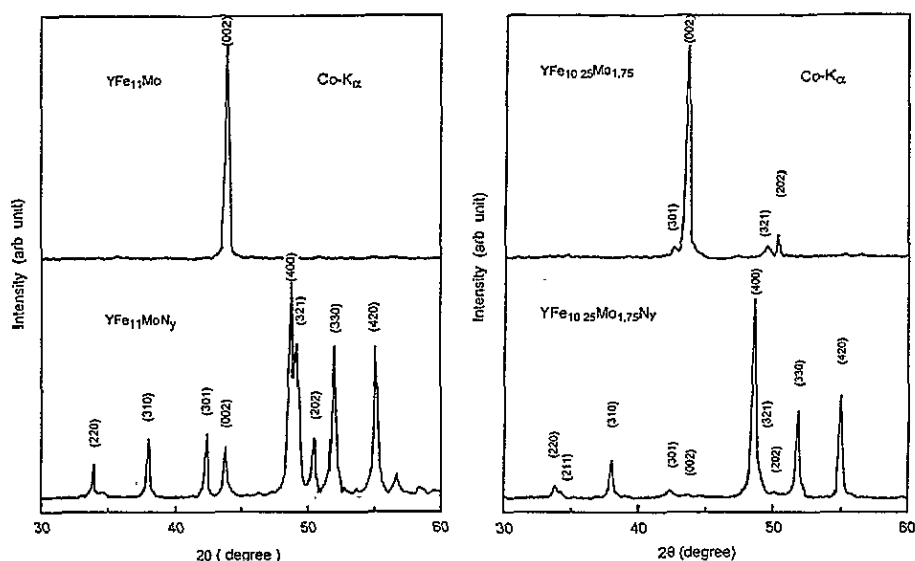
Figure 1. Mo concentration dependence of the Curie temperatures for $\text{YFe}_{12-x}\text{Mo}_x$ and $\text{YFe}_{12-x}\text{Mo}_x\text{N}_y$.

The x-ray diffraction patterns of the aligned samples indicate that all the parent alloys possess uniaxial magnetocrystalline anisotropy, while $\text{YFe}_{12-x}\text{Mo}_x\text{N}_y$ does not. Typical aligned-powder x-ray diffraction patterns at room temperature for $\text{YFe}_{12-x}\text{Mo}_x$ and $\text{YFe}_{12-x}\text{Mo}_x\text{N}_y$ with $x = 1.0$ and 1.75 are shown in figure 2.

The values of the anisotropy field B_a for parent alloys were derived using the SPD technique on aligned samples at a temperature of 293 K and a reduced temperature $T_r = T/T_C = 0.314$ (see table 1). In order to exclude the effect of the Curie temperature difference on the anisotropy field, we chose a series of measurements at a reduced temperature which was limited by the liquid-nitrogen condition of the SPD system. Figure 3 gives typical SPD measurement curves for YFe_{11}Mo at 151 K. The position of the cusp on

Table 1. The intrinsic magnetic properties of $YFe_{12-x}Mo_x$ and $YFe_{12-x}Mo_xN_y$. Some data are taken from [10] as indicated.

x	$YFe_{12-x}Mo_x$				$YFe_{12-x}Mo_xN_y$		
	T_C (K)	M_s (4.2 K) (A m ² kg ⁻¹)	B_a (T)		T_C (K)	M_s (4.2 K) (A m ² kg ⁻¹)	EMD 293 K
			0.314 T_C	293 K			
1.0	481	165.6 [10]	2.50	1.34	642	170.3 [10]	Canted
1.25	464		1.90	0.94	623		Canted
1.5	440	117.3	1.33	0.51	600	147.5	Planar
1.75	413		1.05	0.35	573		Planar
2.0	360	93.8 [10]	0.96	> 0	527	116.5 [10]	Planar
2.5	300	52.0	0.61	> 0	425	99.1	Planar
3	185		—	—	337	80.0	Planar

**Figure 2.** Typical x-ray diffraction patterns (Co $K\alpha$) for magnetically aligned samples of $YFe_{12-x}Mo_x$ and $YFe_{12-x}Mo_xN_y$ for $x = 1.0$ and 1.75 , respectively.

the curve of the second-order time derivative $d^2M(B_0)/dt^2$ of the magnetization indicates the anisotropy field B_a of the sample. At 293 K, $B_a = 1.34$ T for $YFe_{11}Mo$, which is lower than $B_a = 2.1$ T for $YFe_{11}Ti$ [13, 14]. This difference may be attributed to the Curie temperature difference (481 K for the former and 524 K for the latter), since these two compounds have similar unit-cell volumes (0.3469 nm⁻³ for the former and 0.3456 nm⁻³ for the latter).

In figure 4 is plotted the Mo concentration dependence of B_a for $YFe_{12-x}Mo_x$ at 293 K and reduced temperature T_r . It can be seen that, at both temperatures, the variation in magnetocrystalline anisotropy field B_a with Mo concentration x has a clear turning point at $x \simeq 1.6$, before which B_a decreases rapidly and after which B_a decreases slowly. According to a neutron diffraction experiment [15], the Mo occupation is 0.8 on 8i sites and 0.2 on 8f sites for $YFe_{11}Mo$ and is 2.6 on 8i sites and 0.4 on 8f sites for YFe_9Mo_3 . Since the uniaxial anisotropy of the Fe sublattice in $ThMn_{12}$ -structure compounds is dominantly contributed by

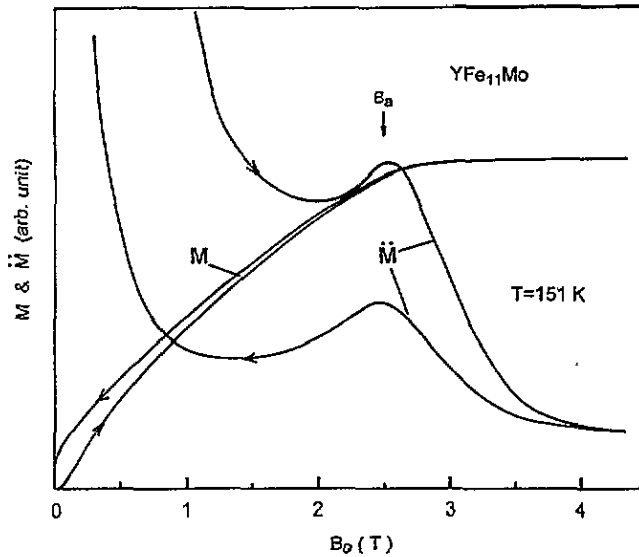


Figure 3. Magnetization $M(B_0)$ and derivative $\dot{M}(B_0) = d^2M(B_0)/dt^2$ curves for $YFe_{11}Mo$ at a temperature of 151 K by the SPD technique. The arrow indicates the position of the anisotropy field.

the Fe atoms at 8i sites [16], the anisotropy of $YFe_{12-x}Mo_x$ must decrease with increase in Mo substitution. However, the turning point at $x \approx 1.6$ cannot be explained by the simple dilution effect of Mo atoms. A possible reason could be that the effect on the Fe-sublattice anisotropy of Mo substitution is stronger when $x < 1.6$ than when $x > 1.6$.

From figure 2 we can also see that the $(hk0)$ reflections dominate and the (400) line becomes the strongest on the nitrides. When $x < 1.5$, the intensities of the (001) inflections of aligned samples are almost the same as the corresponding inflections of isotropic samples. When $x \geq 1.5$, the (001) inflections of the aligned samples almost disappear. These characteristics of x-ray diffraction patterns indicate that the nitrides may have canted anisotropy when $x < 1.5$ and planar anisotropy when $x \geq 1.5$. The easy magnetization direction (EMD) is indicated by the ratio of I_{002}/I_{400} , where I_{002} and I_{400} are the intensities of (002) and (400) reflections respectively. Figure 5 gives the Mo concentration dependence of the ratio I_{002}/I_{400} , which was derived from the x-ray diffraction patterns of aligned nitride samples at room temperature. With increase in the Mo concentration, the ratio I_{002}/I_{400} has a high value up to $x \approx 1.5$ and then drops to almost zero. The nitrogenation effects on the magnetocrystalline anisotropy for $YFe_{12-x}Mo_x$ compounds have also been observed in [11], but it was found that $YFe_{12-x}Mo_xN_y$ with $x = 1.0$ has the same uniaxial anisotropy as its parent compound, which is different from our result.

Obviously, the interstitial N atoms not only markedly modify the anisotropy of the rare-earth sublattice [1–6] but also have some influence on the anisotropy of the Fe sublattice as seen in $YFe_{10}V_2N_y$ [3] and $YFe_{11}TiN_{1-\delta}$ [17]. The uniaxial anisotropy of the Fe sublattice in these compounds with $ThMn_{12}$ -type structure was reduced by the introduction of interstitial N atoms as observed for $YFe_{12-x}Mo_xN_y$. However, $YFe_{12-x}Mo_xN_y$ has a smaller value than $YFe_{10}V_2N_y$ and $YFe_{11}TiN_{1-\delta}$ so that the effect of interstitial N atoms turns its uniaxial anisotropy into a canted-type or planar anisotropy. The interstitial N effect on the Fe sublattice in 2:17 compounds has also been investigated for $Y_2(Fe_{1-x}Co_x)_{17}N_{3-\delta}$ [18], where the planar anisotropy of the Fe sublattice was reduced. The opposite effects of

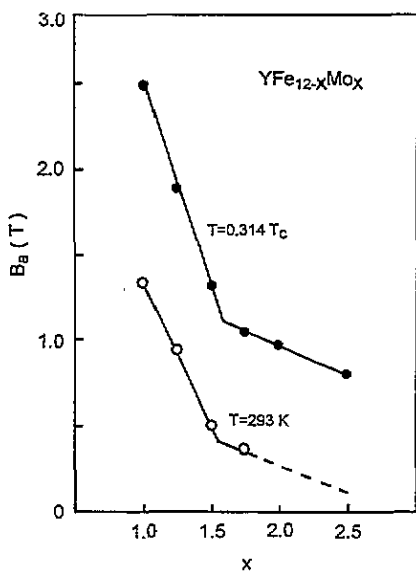


Figure 4. Mo concentration dependence of the anisotropy field B_a of $YFe_{12-x}Mo_x$ at 293 K and reduced temperature $T_r = T/T_c = 0.314$, respectively.

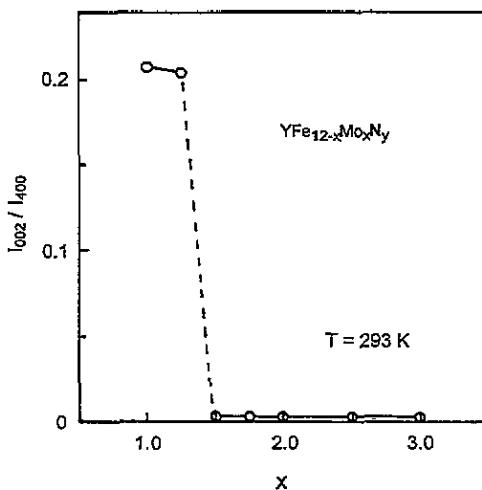


Figure 5. Mo concentration dependence of the intensity ratio I_{002}/I_{400} of x-ray diffraction patterns for magnetically aligned samples of $YFe_{12-x}Mo_xN_y$ at room temperature.

interstitial N on the 1:12 and 2:17 Fe sublattices can be understood because the c axes in these two compounds are orthogonal [16]. The anisotropy reduction for the nitrides may be due to a change in the 3d orbital moment or to a change in crystal-field interaction by the interstitial N atoms.

A distinct change in the magnetocrystalline anisotropy for both $YFe_{12-x}Mo_x$ and $YFe_{12-x}Mo_xN_y$ shows that $x = 1.6$ for the former and $x = 1.5$ for the latter are the critical Mo concentrations. The phenomenon observed for the $NdFe_{12-x}Mo_x$ series where there is uniaxial anisotropy when $x < 1.56$ and canted anisotropy when $x > 1.56$ at room temperature [19] may originate from the anisotropic anomalous variation in its Fe sublattice.

4. Conclusions

The magnetocrystalline anisotropy of $YFe_{12-x}Mo_x$ and $YFe_{12-x}Mo_xN_y$ ($x = 1-3$, $y \approx 1$) has been studied systematically. The uniaxial anisotropy of $YFe_{12-x}Mo_x$ decreases with increasing Mo concentration with two linear parts at a turning point of $x = 1.6$. After nitrogenation, the interstitial compound $YFe_{12-x}Mo_xN_y$ has canted-type anisotropy when $x < 1.5$ and planar anisotropy when $x \geq 1.5$. The anisotropy reduction for the parent alloy is mainly due to the substitution of Mo atoms for Fe on 8i sites, while the further anisotropy change for the nitride may be due to a change in the 3d orbital moment or to a change in crystal-field interaction by the interstitial N atoms.

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