AIP Journal of Applied Physics

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Citation: Journal of Applied Physics **97**, 10M503 (2005); doi: 10.1063/1.1847291
View online: http://dx.doi.org/10.1063/1.1847291
View Table of Contents: http://scitation.aip.org/content/aip/journal/jap/97/10?ver=pdfcov
Published by the AIP Publishing

Magnetic properties of $YGdFe_{17-x}(Ga,Al)_x$ (x=0–8)

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(Presented on 11 November 2004; published online 16 May 2005)

The effect of Ga/Al substitution on the structural and magnetic properties of $YGdFe_{17}$ has been investigated. A structural transformation from hexagonal to rhombohedral has been observed. The saturation magnetization increases up to x=1 (Ga)/2 (Al) and then decreases with further increase of x. Curie temperature increases from 476 K for $YGdFe_{17}$ to 595 K for $YGdFe_{14}Ga_3$ and 495 K for $YGdFe_{14}Al_3$ and decreases with further substitution of Ga/Al. The easy magnetization direction is planar up to x=6 for Ga- and 7 for Al-substituted compounds and shifts to along c axis for x=8. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1847291]

INTRODUCTION

Rare-earth-iron intermetallic compounds of the type R_2Fe_{17} (R=rare earth) have attracted significant attention as possible candidates for high-performance permanent magnet materials.[1,2] These compounds have been reported to crystallize in the rhombohedral Th_2Zn_{17}-type structure for rare earths lighter than Gd and in the hexagonal Th_2Ni_{17}-type structure for rare earths heavier than Tb with low Curie temperatures.[3] By the partial substitution of nonmagnetic elements, such as Al, Ga, and Si for iron, and by the interstitial doping with N and C, it has been reported that there is an enhancement in large extent in the T_C and magnetocrystalline anisotropy of these compounds.[4,5] Suresh and Rama Rao[6] have reported that substitution of Al for Fe in $ErPrFe_{17}$ has increased T_C from 285 to 435 K for Al=3 and with further increase of Al, T_C has decreased. Venkatesan *et al.*[7] have reported an increase in T_C in $HoErFe_{17-x}Ga_x$ with increasing concentration of Ga up to x=4. Huang and Ching[8,9] explained the enhancement of T_C for Al-, Ga-, and Si-substituted Nd_2Fe_{17} compounds on the basis of change in electronic structure of the parent compound upon substitution. Sabirianov and Jaswal[10] showed that there is a good agreement of the experimental and the theoretical results for T_C by considering the Mohn and Wohlfarth model.[11] Some of these investigations have been reviewed recently by Rama Rao *et al.*[12] Recently, substitution of Ga and Si for Fe in $ErPrFe_{17}$ has been reported to increase the T_C by about 250 K.[13] The variation of planar anisotropy of iron due to the substitution elements, in the absence of rare-earth anisotropy, can be investigated if the anisotropy at the rare-earth site is zero. In this paper the effects of substitution of Al and Ga on the structure, magnetization, magnetic anisotropy, and Curie temperature of $YGdFe_{17}$ compounds are presented.

EXPERIMENTAL DETAILS

Compounds with nominal compositions of $YGdFe_{17-x}(Al/Ga)_x$ (x=0–8) were prepared using an arc furnace and in argon atmosphere, starting from Y and Gd of 99.9% purity, Fe of 99.95% purity, and Al and Ga of 99.99% purity. The constituents were melted several times to ensure homogeneity. The ingots were homogenized in a vacuum (10^{-6} torr < pressure < 10^{-5} torr) at 950 °C for 7 days and furnace cooled. Structural characterization was carried out by taking x-ray diffraction patterns of sample powders employing Fe $K\alpha$ radiation. Magnetization and Curie temperature were determined using a vibrating-sample magnetometer (Model No. PAR 155) up to an applied field of 12 kOe. The powders were aligned in a magnetic field of 2.5 T to investigate the anisotropy and easy magnetization direction (EMD). Powders aligned perpendicular to the substrate were examined by x-ray diffraction in order to determine the EMD and those that are aligned parallel to the substrate were used to determine the anisotropy fields from magnetization measurements.

RESULTS AND DISCUSSION

The compounds have formed in hexagonal Th_2Ni_{17} structure for Ga (Al) concentration up to 2 and in rhombohedral Th_2Zn_{17} structure for higher concentrations, evidenced by the changes in the values of a and c in both the cases, as seen in Fig. 1.

The saturation magnetization (M_S) values were found from Honda plots. The value of M_S increases from 83 emu/g for x=0 to 103 emu/g for x=1 and then decreases to 40

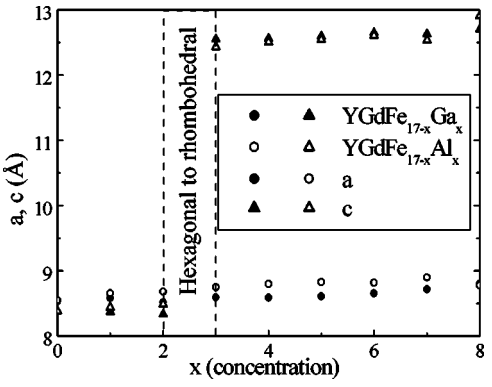

FIG. 1. Lattice parameters of $YGdFe_{17-x}(Ga/Al)_x$, showing the transition from hexagonal to rhombohedral structure.

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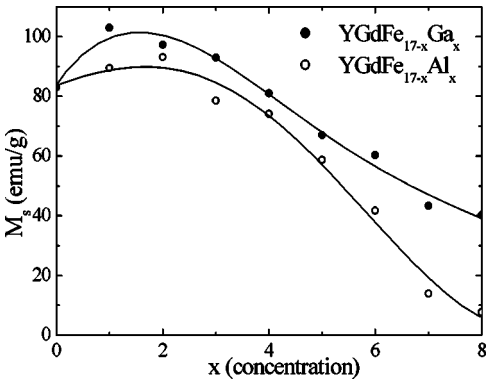

FIG. 2. Saturation magnetization of $YGdFe_{17-x}(Ga/Al)_x$. The lines are only guides to the eye.

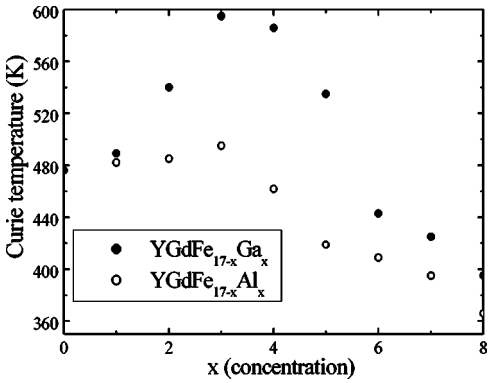

FIG. 3. Curie temperatures of $YGdFe_{17-x}(Ga/Al)_x$.

emu/g for $x=8$ in the case of Ga series whereas in the case of Al-substituted compounds M_S increases with increase of x from 83 emu/g for $x=0$ to 93 emu/g for $x=2$ and then decreases to 8 emu/g for $x=8$, as shown in Fig. 2.

The substitution of metal or metalloid, such as Ga and Al, changes the density of states (DOS) of the $3d$ band differently through the $3d-(4p,4s)$ hybridization and $3d-(3p,4s)$ hybridization, respectively. Huang and Ching[8,9] have carried out band-structure calculations in Nd_2Fe_{17} by substituting Fe with Ga, Si, and Al and obtained partial density of states (PDOS) of Ga, Si, and Al. They have reported that the $4p$ band of Ga is more delocalized and extends up to E_F whereas, in the case of Al and Si, the $3p$ band is very narrow and lies almost near the bottom of the $3d$ band. Thus, the modification of the $3d$ band by Ga is more than by Al, reflecting a larger increase of magnetization of Fe sublattice in Ga-substituted compound than in the Al-substituted compound. At higher concentrations the magnetization decreases faster in Al-substituted compounds than in the Ga-substituted compounds probably due to a faster reduction in the integrated DOS (area covered by the DOS) in the former compared to the latter. It is also seen that the relative variations in the magnetization with substitution of Ga/Al are independent of whether there is crystallographic transition (as in the present case) or not.[6,14]

The Curie temperatures of these compounds are found to increase initially until $x=3$–595 K and 495 K from 476 K for the parent compound, in the case of Ga- and Al-substituted compounds, respectively, and then found to decrease with the further increase of x (Fig. 3).

This behavior can be attributed to the decrease in the DOS at E_F (more for Ga-substituted system) in both the compounds as per the model of Mohn and Wohlfarth,[11] at least in the low-concentration (of Ga/Al) region. At higher concentrations of Ga/Al, the band narrowing as well as the magnetic dilution could decrease the T_C.

Al or Ga or Si, partially replacing Fe in Nd_2Fe_{17}, has been reported to preferentially occupy the $12j$ ($18h$) site.[8,9] Using this information, Sabirianov and Jaswal[10] have investigated the electronic structure and T_C of Sm_2Fe_{16}(Al/Ga/Si) by means of a self-consistent spin-polarized band-structure calculation on the basis of a model proposed by Mohn and Wholfarth[11] and have shown a behavior similar to the present results.

The x-ray diffraction patterns for the magnetically oriented samples are shown in Fig. 4. In $YGdFe_{17}$ only peaks corresponding to (300), (220) are seen, indicating the presence of planar anisotropy. The anisotropy is planar up to $x=6$ in $YGdFe_{17-x}Ga_x$. In $x=7$ compound, the anisotropy begins to become axial as seen by the development of (006) peak and is completely axial in the $x=8$ compound. In the $YGdFe_{17-x}Al_x$ compound, up to $x=7$, planar anisotropy is seen and in the $x=8$ compound, axial anisotropy is seen. Ga and Al are known to decrease the planar anisotropy of the Fe sublattice in Gd_2Fe_{17} (Ref. 15) and also in Y_2Fe_{17}.[16] Suresh and Rama Rao, on the other hand, observed an easy cone in $ErPr(Fe,Al)_{17}$.[6] The cone could be due to the anisotropy of the Er/Pr sublattice that is absent in the present system.

CONCLUSIONS

Structural transformation from hexagonal to rhombohedral when Ga or Al is substituted for Fe in $YGdFe_{17}$ is observed. The values of saturation magnetization for small Ga/Al substitutions increase and decrease for further increase of Ga/Al. Curie temperature increases from 476 K for $YGdFe_{17}$ to 595 K for $YGdFe_{14}Ga_3$ and to 495 K for $YGdFe_{14}Al_3$ and decreases with the further substitution of Ga/Al, which is discussed with respect to the PDOS of the substitutional elements. The easy magnetization direction is found to be in $a-b$ plane up to Ga/Al substitution of $x=6$ and 7, respectively, and completely axial for $x=8$.

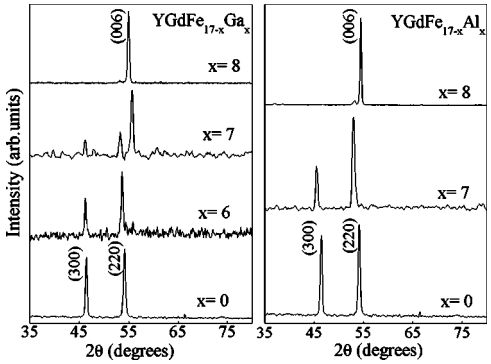

FIG. 4. X-ray diffraction (XRD) patterns of magnetically aligned particles of $YGdFe_{17-x}(Ga/Al)_x$.

ACKNOWLEDGMENT

One of the authors (R.S.) is thankful to Indian Institute of Technology Madras for the financial support.

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