Journal of Alloys and Compounds 487 (2009) 116–120

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: www.elsevier.com/locate/jallcom

The isothermal section of the Nd–Fe–Ga ternary system at 773 K

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ARTICLE INFO

Article history:
Received 9 June 2009
Received in revised form 19 July 2009
Accepted 24 July 2009
Available online 3 August 2009

Keywords:
Rare earth alloys and compounds
Phase diagram
X-ray diffraction

ABSTRACT

The isothermal section of the Nd–Fe–Ga ternary system at 773 K was constructed using X-ray diffraction analysis. Ten binary compounds, Nd_2Fe_{17}, Nd_5Fe_{17}, Nd_9Ga_4, Nd_5Ga_3, NdGa, $NdGa_2$, $FeGa_3$, Fe_3Ga_4, α-Fe_6Ga_5 and α-Fe_3Ga, and three ternary compounds, $NdFe_2Ga_8$, $NdFe_5Ga_7$ and $Nd_6Fe_{13}Ga$ were existed in this isothermal section. The solid solutions $Nd_2Fe_{17.00-15.57}Ga_{0-1.43}$ (Th_2Zn_{17}-type structure, space group $R\bar{3}m$), $NdFe_{5.46-4.65}Ga_{6.54-7.35}$ ($ThMn_{12}$-type structure, space group $I4/mmm$) and $Nd_6Fe_{13.0-12.0}Ga_{1.0-2.0}$ ($La_6Co_{11}Ga_3$-type structure, space group $I4/mcm$) were formed by substitution of Ga for Fe in the compounds Nd_2Fe_{17}, $NdFe_5Ga_7$ and $Nd_6Fe_{13}Ga$ at 773 K, respectively. The ternary compound $NdFe_2Ga_8$ is $CaCo_2Al_8$-type (space group *Pbam*) with $a = 1.43742$ (4), $b = 1.24601$ (4), $c = 0.40479$ (1)). The homogeneity range of $NdGa_2$ is from 66.7 to 74.7 at.% Ga in Nd–Ga side but the solid solubility of Fe in this compound is very small. The homogeneity ranges of $Nd_6Fe_{13}Ga$ and $NdFe_5Ga_7$ are from 5.0 to 10.0 and from 50.3 to 56.5 at.% Ga, respectively. The maximum solid solubilities of Ga in Nd_2Fe_{17} is 7.5. The homogeneity ranges for the other compounds are small.

1. Introduction

Gallium has unique interactions with rare earth (R)–transition metal (T) alloys. The studies of the phase diagrams of the Ho–Co–Ga, Sm–Co–Ga, Er–Fe–Ga and Sc–Fe–Ga ternary systems show rich ternary compounds or substitution derivatives in R–T–Ga systems [1]. An investigation of the Nd–Fe–Ga is a part of a systematical study of the interaction of rare earth metals with gallium and iron. Recently, we reported the isothermal sections of the ternary systems Tb–Fe–Ga [2] and Gd–Fe–Ga [3] at 773 K. The room temperature saturation magnetization for $Nd_2Fe_{17-x}Ga_x$ increases with increasing Ga concentration, reaching maximum at $x = 1.0$, and then decreases [4]. Magnetic ordering of the $Nd_6Fe_{13-x}Ga_{1+x}$ ($x = 0$, 1) compounds studied by neutron diffraction has been reported [5]. The investigation of the Nd–Fe–Ga has not been reported so far. In this work, we investigated the isothermal section of this ternary system at 773 K.

Two intermetallic compounds, Nd_2Fe_{17} and Nd_5Fe_{17} formed peritectically at 1481 and 1025 K, respectively, were reported in the most recent assessed phase diagram of Nd–Fe binary system [6]. Five binary compounds, Nd_3Ga, Nd_5Ga_3, NdGa, $NdGa_2$, and $NdGa_6$ are given in the Nd–Ga phase diagram. The compound $NdGa_2$ melts congruently at 1761 K, while the compounds Nd_3Ga, Nd_5Ga_3, NdGa and $NdGa_6$ form peritectically at 1059, 1157, 1178 and 895 K, respectively [7]. $NdGa_6$ has a polymorphic transition from its high temperature structure to its lower temperature phase α-$NdGa_6$ with Ga_6Cu-type structure at 729 K during cooling. Yatsenko [8,9] pointed out the existence of the binary compounds Nd_3Ga_2 and Nd_9Ga_4 in this system. Gur and Kimmel [10] investigated the pairwise substitution of Nd atoms by gallium in the $Nd_{1-x}Ga_{2+2x}$ solid solution. They established the positional ordering of Ga_2 pairs located in the basal planes of this AlB_2 derivative type compound at the composition $Nd_{1-x}Ga_{2+2x}$ ($x = 0.18$). Four intermediate phases exist in the Fe–Ga system: $FeGa_3$, Fe_3Ga_4, Fe_6Ga_5 and Fe_3Ga, with polymorphic modifications for the last two: α-Fe_3Ga (cubic, $Pm3m$) for $T < 892$ K and β-Fe_3Ga (hexagonal, $P6_3/mmc$) for $T > 892$ K and α-Fe_6Ga_5 (monoclinic, $C2/m$) for $T > 1051$ K and β-Fe_6Ga_5 (rhombohedral, $R\bar{3}m$) for $T < 1051$ K [7]. The existences of ternary compounds $NdFe_2Ga_8$, $NdFe_5Ga_7$ and $Nd_6Fe_{11}Ga_3$ in the Nd–Fe–Ga ternary system and their structures have been reported [11].

2. Experimental details

The alloy samples for this study each with a total weight of about 2 g, were prepared from Nd (99.9 wt.%), Fe (99.99 wt.%), and Ga (99.99 wt.%) and melted them in an electric-arc furnace using a nonconsumable tungsten electrode and a water-cooled copper tray in an atmosphere of pure argon. To ensure homogeneity, the alloy buttons were remelted at least three times. No composition analysis was carried out since the weight lost of the sample was less than 1% during the preparation. The homogenization was performed at 800 °C for 20 days for the alloys near Fe corner with Nd less than 10.5 at.% and Ga less than 40 at.%, and at 600 °C for 25 days

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doi:10.1016/j.jallcom.2009.07.154

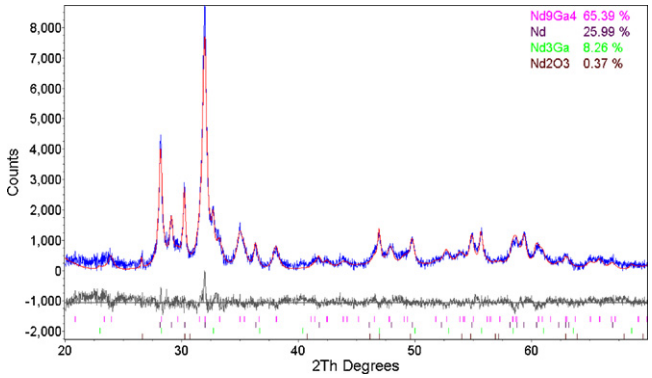

Fig. 1. Rietveld refinement for the XRD pattern of the alloy with composition of Nd_3Ga.

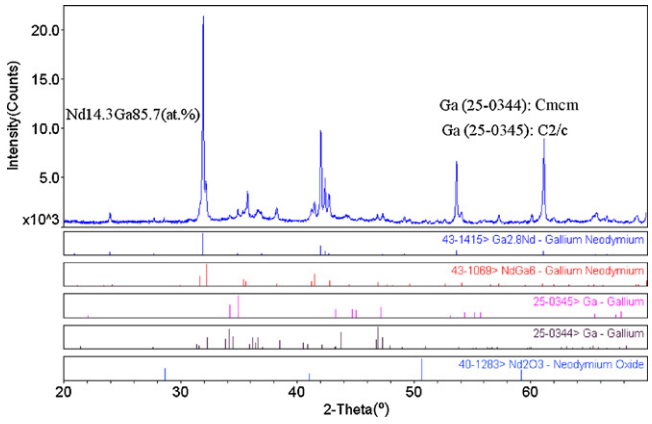

Fig. 2. XRD pattern for the alloy with composition of $NdGa_6$.

for the other alloys. They were cooled from their homogenization temperatures to 500 °C, kept at 500 °C for 3 days and then quenched in liquid nitrogen. About 168 samples in total were prepared for this investigation. X-ray powder diffraction (XRD) data were collected by a Bruker D8 Advance SS/18 kW diffractometer with CuKα radiation. JADE 5.0 and Topas 3.0 software were used for phase analysis and structure determination.

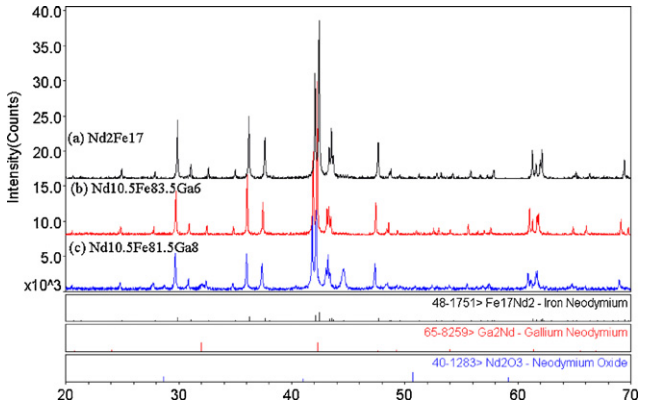

Fig. 3. XRD patterns of compound $Nd_2Fe_{17-x}Ga_x$ with various Ga, showing this compound keeps its Th_2Zn_{17}-type structure, but increases its lattice parameters with increase of Ga content.

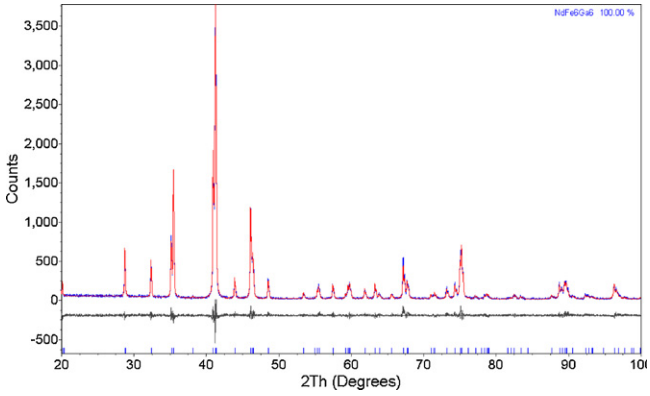

Fig. 4. Rietveld refinement for the XRD pattern of the compound $NdFe_{4.85}Ga_{7.15}$.

3. Results and discussion

3.1. Phase analysis

The boundary binary systems, Nd–Fe, Nd–Ga and Fe–Ga, studied in this work confirmed the existence of the binary compounds, Nd_2Fe_{17} (Th_2Zn_{17}-type) and Nd_5Fe_{17} (Nd_5Fe_{17}-type) in Nd–Fe system; Nd_9Ga_4 (Sm_9Ga_4-type), Nd_5Ga_3 (Cr_5B_3-type), NdGa (CrB-type) and $NdGa_2$ (NdB_2-type) in Nd–Ga system; and α-Fe_3Ga (Cu_3Au-type), α-Fe_6Ga_5 (Fe_6Ge_5-type), Fe_3Ga_4 (Fe_3Ga_4-type) and

Table 1
Structure, refined parameters for the ternary compounds $NdFe_{4.85}Ga_{7.15}$ and $Nd6Fe_{13}Ga$.

Sample	$NdFe_{4.85}Ga_{7.15}$			$Nd_6Fe_{13}Ga$			
Space group	*I4/mmm*			*I4/mcm*			
Structure type	$ThMn_{12}$			$La_6Co_{11}Ga_3$			
Cell parameters (nm)	$a = 0.87358\ (2)$, $c = 0.50998\ (1)$			$a = 0.80686\ (4)$, $c = 2.2937\ (1)$			
Volume of unit cell (nm^3)	$V = 0.3892\ (2)$			$V = 1.4933\ (2)$			
Calculated density (gcm^{-3})	7.84 (3)			7.3890 (8)			
Reliability factors	$R_p = 9.68$, $R_{wp} = 12.99$, $R_B = 4.804$			$R_p = 7.83$, $R_{wp} = 10.14$, $R_B = 4.415$			
	$R_{exp} = 11.39$, GOF = 1.19			$R_{exp} = 13.10$, GOF = 0.77			
Atomic parameters							
$NdFe_{4.85}Ga_{7.15}$ ($ThMn_{12}$-type, *I4/mmm*)				$Nd_6Fe_{13}Ga$ ($La_6Co_{11}Ga_3$-type, *I4/mcm*)			
Atom	Position	Occ.	B	Atom	Position	Occ.	B
Nd	2a (0, 0, 0)	1	0.10	Nd1	8f (0, 0, 0.10641)	1	0.2365
$Fe_{0.89}Ga_{0.11}$	8f (1/2, 1/2, 1/2)	1	0.10	Nd2	16l (0.16324, 0.66324, 0.18678)	1	1.229
Ga	8i (x, 0, 0), $x = 0.3398\ (3)$	1	0.10	Fe1	4d (0, 0.5, 0)	1	0.2181
				Fe2	16k (0.06621, 0.20851, 0)	1	0.6347
$Fe_{0.22}Ga_{0.78}$	8j (x, 1/2, 0), $x = 0.2773\ (3)$	1	0.10	Fe3	$16l_1$ (0.17871, 0.67871, 0.05925)	1	0.7184
				Fe4	$16l_2$ (0.61386, 0.11386, 0.09416)	1	1.36
				Ga	4a (0, 0, 0.25)	1	0.2181