The Fe-Nd (Iron-Neodymium) System

W. Zhang, G. Liu, and K. Han
University of Science and Technology Beijing

Equilibrium Diagram

An Fe-Nd binary phase diagram was proposed initially by [65Ter]; several investigations on the structure and magnetism of some Fe-Nd alloys had been made previously [61Gsc, 64Ray]. [65Ter] investigated the Fe-Nd system by means of thermal and X-ray analyses, metallography, microhardness tests, and measurements of the electrical resistance. Fe of 99.9 wt.% and Nd of 99.0 wt.% purity were used as starting materials. [65Ter] concluded that this system comprises two peritectic reactions, and one eutectic reaction, and two intermetallic compounds—$Fe_{17}Nd_2$ and Fe_2Nd. [82Kub] reviewed this system and based her diagram mainly on the results of [65Ter].

The existence of Fe_2Nd has not been confirmed by later investigations. From systematic analyses with differential thermal analysis and X-ray diffraction, [87Sch] concluded that $Fe_{17}Nd_2$ is the only intermetallic compound in the system. Fe_2Nd was not found either in a diffusion couple held at 800 °C for reaction between Fe and Nd to form Fe_2Nd, or in specimens annealed for 300 h at 900 and 600 °C and quenched. The assessed Fe-Nd phase (Fig. 1) is based on the works of [65Ter], [87Sch], [85He], [87Wan], and

[65Ter] (1185 ± 10 °C). The "Fe_7Nd" compound obtained by [64Wei], [64Ray], and [65Ray] is now believed to be $Fe_{17}Nd_2$ [66Ray, 87Sch].

(Nd) Solid Solutions

The $\alpha \leftrightarrow \beta$ transformation temperature of Nd is 863 °C [86Gsc]. The maximum solid solubility of Fe in (αNd) was reported to be 4 wt.% [65Ter], which appears to be improbably high, compared with results from other Fe-RE systems.

Fe_2Nd

Both [61Gsc] and [65Ter] reported the existence of Fe_2Nd as a stable phase, but this was not confirmed by later investigations [87Sch].

Metastable Phases

$Fe_{5+x}Nd$ was obtained by splat cooling [86Sta] at rates estimated to be 10 °C/s. The samples were analyzed by X-ray. The exact composition is not yet known; it is represented as $Fe_{5+x}Nd$, where x is less than 3.5, but not near zero [86Sta]. The Fe-Nd compound

[85Bus]. [65Ter] further pointed out that the structure analysis of $Fe_{17}Nd_2$ was originally carried out by [63Kri] with $Fe_{17}Nd_2$ in the rhombohedral representation. Available evidence favors the view that $Fe_{17}Nd_2$ is monomorphic and not dimorphic, as are some other $Fe_{17}RE_2$ compounds.

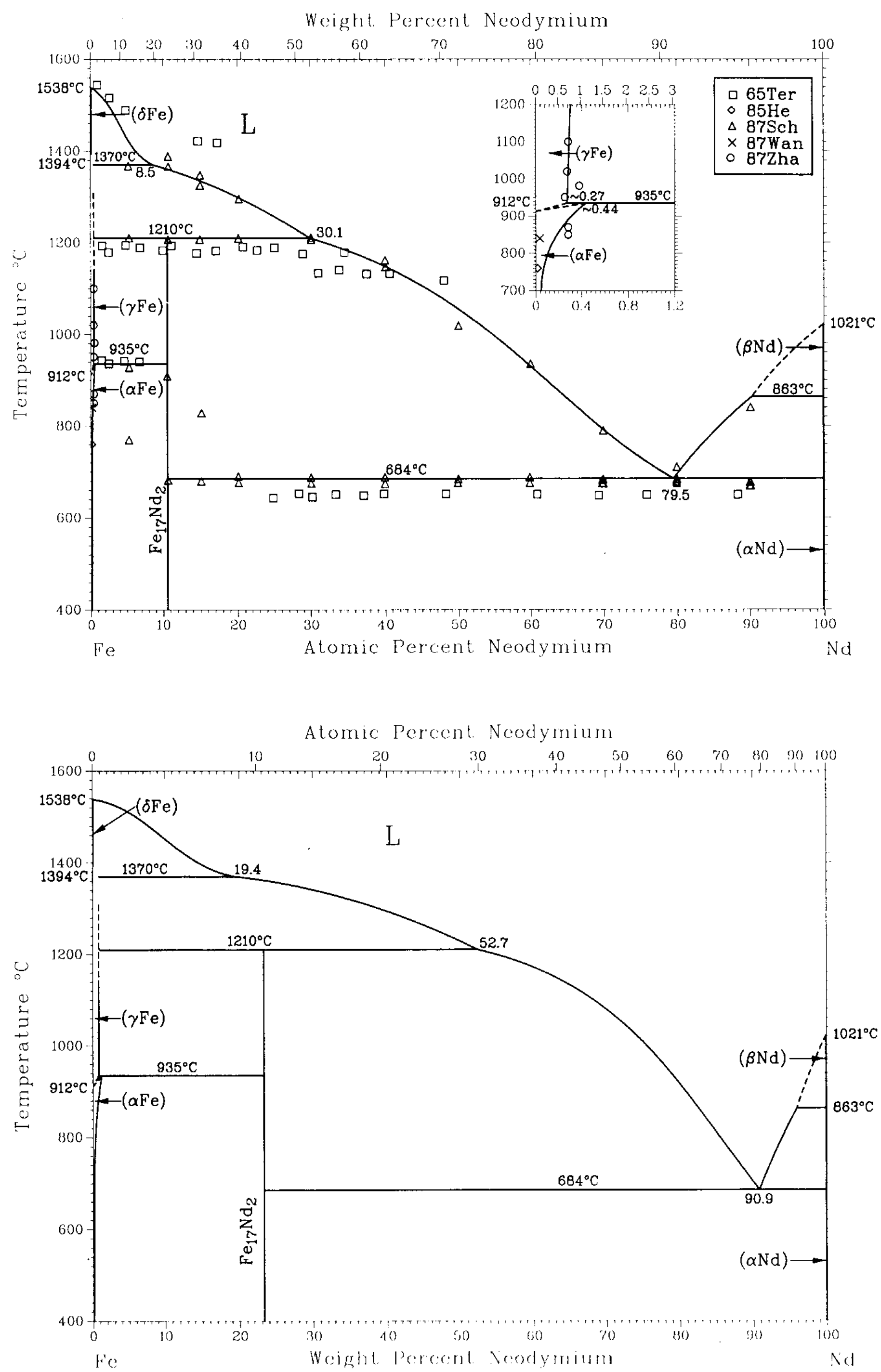

Fig. 1 Assessed Fe-Nd phase diagram.

Table 2 Fe-Nd Crystal Structure Data

Phase	Composition, at.% Nd	Pearson symbol	Space group	Strukturbericht designation	Prototype	Reference
δFe(a)	0	*cI2*	*Im$\bar{3}$m*	*A2*	W	[Massalski2]
γFe(b)	0	*cF4*	*Fm$\bar{3}$m*	*A1*	Cu	[Massalski2]
αFe(c)	0	*cI2*	*Im$\bar{3}$m*	*A2*	W	[Massalski2]
$Fe_{17}Nd_2$	10.5	(d)	*R$\bar{3}$m*	...	Th_2Zn_{17}	[86Sta,65Ter, 63Kri,66Ray]
βNd(e)	100	*cI2*	*Im$\bar{3}$m*	*A2*	W	[86Gsc]
αNd(f)	100	*hP4*	*P6₃/mmc*	*A3'*	αLa	[86Gsc]
Metastable phase						
$Fe_{5+x}Nd$	...	*hP6*	*P6/mmm*	*$D2_d$*	$CaCu_5$	[86Sta]

(a) From 1538 to 1394 °C. (b) From <1394 to 912 °C. (c) Below <912 °C. (d) Rhombohedral. (e) From 1021 to 863 °C. (f) Below <863 °C.

Table 3 Fe-Nd Lattice Parameter Data

Phase	Composition, at.% Nd	Lattice parameters, nm a	c	Comment	Reference
δFe	0	0.29315	...	At >1394 °C	[Massalski2]
γFe	0	0.36467	...	At >912 °C	[Massalski2]
αFe	0	0.28665	...	At 25 °C	[Massalski2]
$Fe_{17}Nd_2$	10.5	0.8567(5)	1.2443(5)	...	[82Her]
		0.859	1.247	...	[63Kri,65Ter]
		0.8578	1.2462	For "Fe_7Nd"	[64Ray,65Ray]
βNd	100	0.413	...	At >863 °C	[86Gsc]
αNd	100	0.36582	1.17966	At 25 °C	[86Gsc]
Metastable phase					
$Fe_{5+x}Nd$	...	...	...	...	[86Sta]

Thermodynamics

The thermodynamic optimization of the Fe-Nd phase diagram was carried out by [87Sch]. They summarized the phase stability parameters of Fe and Nd (as shown in Table 4), among which those of Fe are quoted from [85Gui] and those of Nd are their optimized results based on the information from [77Bar]. These data do not include ferromagnetic terms. The excess Gibbs energies (see Table 5) of the liquid also were extracted from their experimental work. The enthalpy of formation of $Fe_{17}Nd_2$ referring to Fe(bcc) and Nd(cph) was obtained as $G(T) = -97\,166 + 61.110\,T$ J/mol^{-1}.

Magnetism

$Fe_{17}Nd_2$

The Curie temperature, T_C, is 327 K [86Bus], which agrees well with the results obtained by [64Wei] and [64Ray] (326 K, originally reported as T_C of "Fe_7Nd") and [82Her] (330 K).

$Fe_{5+x}Nd$

$Fe_{5+x}Nd$ has a T_C of about 370 K. Its magnetic properties ($M_S \approx 0.80\,T$, $T_C \approx 370$ K) are not expected to make a useful contribution to permanent magnet behavior [86Sta].

Cited References

61Gsc: K.A. Gschneidner, Jr., *Rare Earth Alloys,* D. Van Nostrand Co., New York (1961). (Equi Diagram; Review)

63Kri: P.I. Kripyakevich, V.F. Terekhova, O.S. Zarechnyuk, and I.V. Burov, "Crystal Structures of Several Intermetallic Compounds of Gd and Nd," *Kristallografiya,* 7(2), 268 (1983) in Russian. (Crys Structure; Experimental)

64Ray: A.E. Ray, K. Strnat, and D. Feldmann, "Preparation and Thermomagnetic Analyses of Compounds of Ce, Pr and Nd with Fe having the Approximate Composition RFe_7," Proc. 3rd Conf. Rare Earth Res., 443-457 (1964). (Equi Diagram, Crys Structure, Magnetism; Experimental)

64Wei: H. Weik, P. Fischer, W. Halg, and E. Stoll, "Investigations of the Structure and Magnetic Behavior of Peritectic Pr-Fe and Nd-Fe Compounds of the Type RFe_7 by means of Neutron Diffraction," Proc. 4th Conf. Rare Earth Res., Vol. I, 1-9 (1964). (Meta Phases, Experimental)

65Ray: A.E. Ray, "The Crystal Structures of $CeFe_7$, $PrFe_7$, $NdFe_7$ and $SmFe_7$," Proc. 5th Conf. Rare Earth Res., Vol. 5, 45 (1965). (Equi Diagram, Crys Structure; Experimental)

***65Ter:** V.F. Terekhova, E.V. Maslava, and Y.M. Savilsky, "Phase Diagram of Fe-Nd Alloy System," *Russ. Metall. 3,* 50 (1965). (Equi Diagram, Crys Structure; Experimental; #)

66Ray: A.E. Ray, "The Crystal Structure of $CeFe_7$, $PrFe_7$, $NdFe_7$ and $SmFe_7$," *Acta Crystallogr., 21,* 426 (1966). (Equi Diagram, Crys Structure; Experimental)

77Bar: I. Barin, O. Knacke, O. Kubaschewski, *Thermochemical Properties of Inorganic Substances,* Vol. 2, Springer-Verlag, Berlin, 448 (1977). (Thermo; Review)

Table 4 Elemental Phase Stabilities for Fe-Nd
$G(T) = A - BT + CT(1 - \ln T) - DT^2/2 - E/2T - FT^3/6$ J/mol

Phase	A	B	C	$D \times 10^{-3}$	$E \times 10^{+5}$	$F \times 10^{-6}$
Fe(bcc)(a)	1 224.8	−100.620	23.514	8.795	−1.5472	0.3536
Fe(fcc)(a)	− 237.6	−107.752	24.664	7.715	−1.5412	0.3536
Fe(L)(a)	−10 839.7	−245.302	46.0	0	0	0
Nd(cph)(b)	−8 006.9	−77.443	25.819	2.188	−0.2636	13.9450
Nd(bcc)(b)	−18 029.7	−195.118	44.560	0	0	0
Nd(L)(b)	−16 333.2	−219.838	48.785	0	0	0

From [87Sch]. (a) Referring to bcc phase at 298.15 K, 1 bar. (b) Referring to cph phase at 298.15 K, 1 bar.

Table 5 Excess Terms for the Fe-Nd Liquid
$\Delta G^{ex} = X_{Fe}X_{Nd}\ \Sigma(X_{Fe} - X_{Nd})^v (A_v - B_vT)$ J/mol

v	A_v	B_v
0	41 218.6	84.049
1	58 077.6	8.813
2	147 412.6	85.472

***82Her:** J.F. Herbst, J.J. Croat, and R.W. Lee, "Neutron Diffraction Studies of $Nd_2(Co_xFe_{1-x})_{17}$ Alloys: Preferential Site Occupation and Magnetic Structure," *J. Appl. Phys., 53*(1), 250 (1982). (Crys Structure, Magnetism; Experimental)

82Kub: O. Kubaschewski, *Iron—Binary Phase Diagrams,* Springer-Verlag, New York (1982). (Equi Diagram, Crys Structure; Review; #)

85Bus: K.H.J. Buschow, D.B. De Mooij, and H.M. Van Noort, "The Fe-rich Isothermal Section of Nd-Fe-B at 900 °C," *Philips J. Res. 40,* 227 (1985). (Crys Structure; Experimental)

85Gui: A. Fernandez Guillermet and P. Gustafson, "An Assessment of the Thermodynamic Properties and the (P,T) Phase Diagram of Iron," *High Temp.-High Press. 16,* 591 (1985). (Thermo; Equi Diagram)

85He: Y. He, X.R. Chang, Z.Z. Tian, C.M. Hsiao, M.H. Wang, H.B. Lu, Y.Y. Wang, and N.Q. Liu, "Positron Annihilation Study on the Solid Solubility Limit of Neodymium in Pure Iron," *Scr. Metallurgica, 19,* 79 (1985). (Equi Diagram; Review)

***86Bus:** K.H.J. Buschow, D.B. De Mooij, and H.M. Van Noort, "Properties of Metastable Ternary Compounds and Amorphous Alloys in the Nd-Fe-B System," *J. Less-Common Met., 125,* 135 (1986). (Magnetism; Experimental)

86Gsc: K.A. Gschneidner, Jr. and F.W. Calderwood, "Intra Rare Earth Binary Alloys: Phase Relationships, Lattice Parameters and Systematics," *Handbook on the Physics and Chemistry of Rare Earths,* Vol. 8, K.A. Gschneidner, Jr. and L. Eyring, Ed., North-Holland Physics Publishing, Amsterdam, 1-161 (1986). (Equi Diagram, Crys Structure; Compilation)

86Sch: G. Schneider, E.T. Henig, G. Petzow, and H.H. Stadelmaier, "Phase Relations in the System Fe-Nd-B," *Z. Metallkd., 77*(11), 755 (1986). (Meta Phases; Experimental)

***86Sta:** H.H. Stadelmaier, G. Schneider, and M. Ellner, "$ACaCu_5$-Type Iron-Neodymium Phase Stabilized by Rapid Solidification," *J. Less-Common Met., 115,* L11 (1986). (Meta Phases, Crys Structure; Experimental)

***87Sch:** G. Schneider, E.T. Henig, G. Petzow, and H.H. Stadelmaier, "The Binary System Iron-Neodymium," *Z. Metallkd., 78*(10), 694-696 (1987). (Equi Diagram, Thermo, Experimental)

87Wan: Y.Y. Wang, N.Q. Liu, Z.Z. Tian, and X.R. Chang, "Determination of the Solubility of Neodymium in Iron by Positron Annihilation," *Acta Metall. Sin. (China), 23*(3), B149-151 (1987) in Chinese. (Equi Diagram; Experimental)

87Zha: W. Zhang, X. Li, G. Liu, and S. Pan, "Determination of the Solubility of Nd, Ce, Sm in Iron by Diffusion Couple Method," unpublished research (1987). (Equi Diagram; Experimental)

* Indicates key paper.
# Indicates presence of a phase diagram.

Fe-Nd evaluation, by **W. Zhang, G. Liu,** and **K. Han,** Department of Materials Science and and Engineering, University of Science and Technology Beijing, Beijing 100083, People's Republic of China.

This work was supported by the National Natural Science Foundation of China (NSFC). Literature searched through 1987. Professor Zhang is the Alloy Phase Diagram Program Contributing Editor for binary iron-rare earth alloys.