Fe – Nd (Iron – Neodymium)

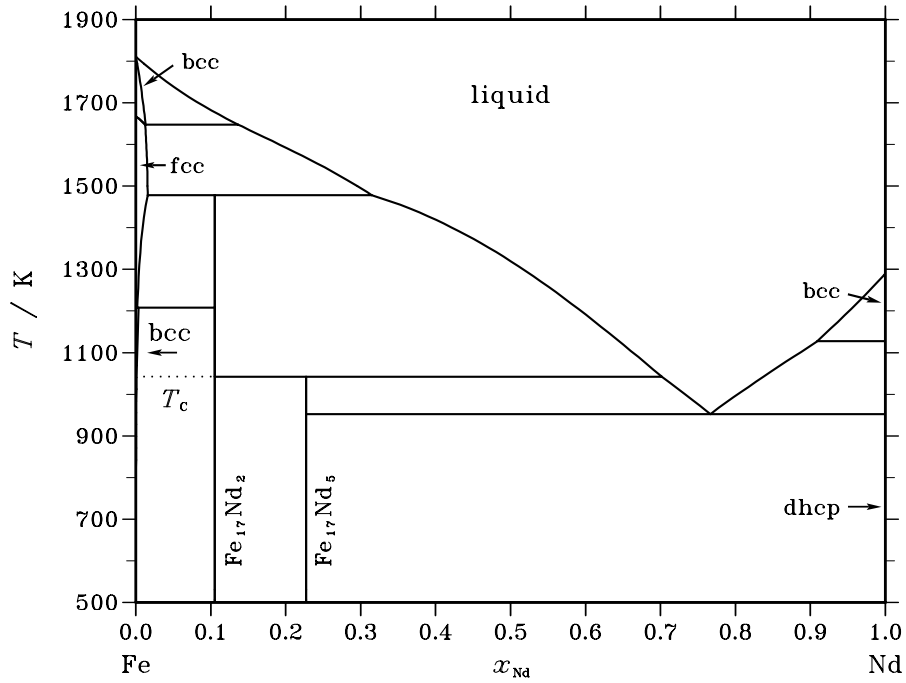

Fig. 1. Calculated phase diagram for the system Fe-Nd.

The Fe–Nd system is of considerable interest because of the the superior magnetic properties of the intermetallic compound $Fe_{14}Nd_2B$. In several publications the system has been reviewed and thermochemical assessments have been prepared [82Kub, 87Sch, 92Zha, 93Hen, 95Hal]. The optimisation of [95Hal] is recommended here because it provides a good description of the binary system and it has been used in the assessment of the ternary system Fe–Nd–B [95Hal].
The assessment is based mainly on phase equilibrium data from the phase diagram throughout the whole composition range and temperatures between about 900 K and the liquidus. Data for the Gibbs energies of $Fe_{17}Nd_2$ and $Fe_{17}Nd_5$ have been determined by EMF measurements in [93Hen].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Fe,Nd)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Fe,Nd)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Fe,Nd)_1$
$Fe_{17}Nd_2$	$\cdots$	Th_2Zn_{17}	$hR19$	$R\overline{3}m$	FE17ND2	$Fe_{17}Nd_2$
$Fe_{17}Nd_5$	$\cdots$	$\cdots$	$h*$	$\cdots$	FE17ND5	$Fe_{17}Nd_5$
dhcp	$A3'$	αLa	$hP4$	$P6_3/mmc$	DHCP	Nd_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Nd}			$\Delta_{\mathrm{r}}H$ / (J/mol)
bcc $\rightleftharpoons$ fcc + liquid	metatectic	1647.7	0.013	0.012	0.136	−424
fcc + liquid $\rightleftharpoons$ $Fe_{17}Nd_2$	peritectic	1478.4	0.016	0.315	0.105	−10861
fcc + $Fe_{17}Nd_2$ $\rightleftharpoons$ bcc	peritectoid	1207.8	0.002	0.105	0.004	−720
bcc $\rightleftharpoons$ liquid + dhcp	degenerate	1128.0	1.000	0.909	1.000	−3029
$Fe_{17}Nd_2$ + liquid $\rightleftharpoons$ $Fe_{17}Nd_5$	peritectic	1041.9	0.105	0.702	0.227	−2465
liquid $\rightleftharpoons$ $Fe_{17}Nd_5$ + dhcp	eutectic	952.7	0.766	0.227	1.000	−11518

Table IIIa. Integral quantities for the liquid phase at 1900 K.

x_{Nd}	ΔG_{m} [J/mol]	ΔH_{m} [J/mol]	ΔS_{m} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{m}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{m}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−4120	1015	2.703	1015	0.000	0.000
0.200	−6515	1390	4.161	1390	0.000	0.000
0.300	−8289	1361	5.079	1361	0.000	0.000
0.400	−9514	1118	5.596	1118	0.000	0.000
0.500	−10145	805	5.763	805	0.000	0.000
0.600	−10111	521	5.596	521	0.000	0.000
0.700	−9334	316	5.079	316	0.000	0.000
0.800	−7709	197	4.161	197	0.000	0.000
0.900	−5015	120	2.703	120	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Fe(liquid), Nd(liquid)

Table IIIb. Partial quantities for Fe in the liquid phase at 1900 K.

x_{Fe}	ΔG_{Fe} [J/mol]	ΔH_{Fe} [J/mol]	ΔS_{Fe} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Fe}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Fe}}$ [J/(mol·K)]	a_{Fe}	γ_{Fe}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1301	364	0.876	364	0.000	0.921	1.023
0.800	−2409	1116	1.855	1116	0.000	0.859	1.073
0.700	−3782	1853	2.966	1853	0.000	0.787	1.124
0.600	−5761	2309	4.247	2309	0.000	0.694	1.157
0.500	−8591	2359	5.763	2359	0.000	0.581	1.161
0.400	−12459	2016	7.619	2016	0.000	0.454	1.136
0.300	−17589	1431	10.010	1431	0.000	0.328	1.095
0.200	−24530	895	13.382	895	0.000	0.212	1.058
0.100	−35536	839	19.145	839	0.000	0.105	1.055
0.000	$-\infty$	1831	∞	1831	0.000	0.000	1.123

Reference state: Fe(liquid)

Table IIIc. Partial quantities for Nd in the liquid phase at 1900 K.

x_{Nd}	ΔG_{Nd} [J/mol]	ΔH_{Nd} [J/mol]	ΔS_{Nd} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Nd}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Nd}}$ [J/(mol·K)]	a_{Nd}	γ_{Nd}
0.000	$-\infty$	14263	∞	14263	0.000	0.000	2.467
0.100	−29494	6881	19.145	6881	0.000	0.155	1.546
0.200	−22939	2486	13.382	2486	0.000	0.234	1.170
0.300	−18807	212	10.010	212	0.000	0.304	1.014
0.400	−15145	−670	7.619	−670	0.000	0.383	0.959
0.500	−11699	−749	5.763	−749	0.000	0.477	0.954
0.600	−8545	−476	4.247	−476	0.000	0.582	0.970
0.700	−5796	−161	2.966	−161	0.000	0.693	0.990
0.800	−3503	22	1.855	22	0.000	0.801	1.001
0.900	−1624	40	0.876	40	0.000	0.902	1.003
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Nd(liquid)

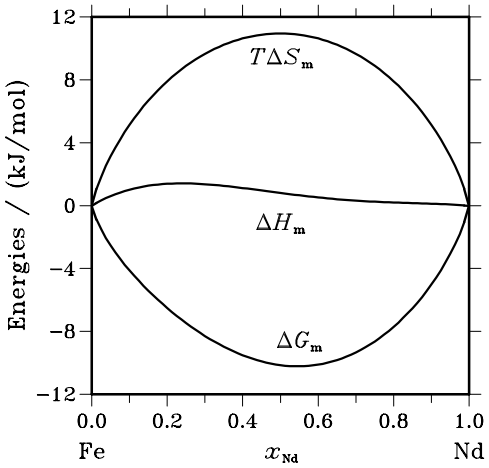

Fig. 2. Integral quantities of the liquid phase at T=1900 K.

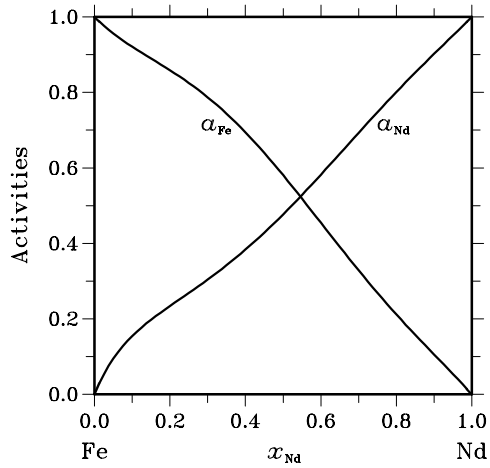

Fig. 3. Activities in the liquid phase at T=1900 K.

Table IV. Standard reaction quantities at 298.15 K for the compounds per mole of atoms.

Compound	x_{Nd}	$\Delta_{\mathrm{f}}G^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}H^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}S^{\circ}$ / (J/(mol·K))	$\Delta_{\mathrm{f}}C^{\circ}_{P}$ / (J/(mol·K))
$Fe_{17}Nd_2$	0.105	−918	−708	0.705	19.440
$Fe_{17}Nd_5$	0.227	−1952	−3076	−3.769	4.071

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