Fe – Nb (Iron – Niobium)

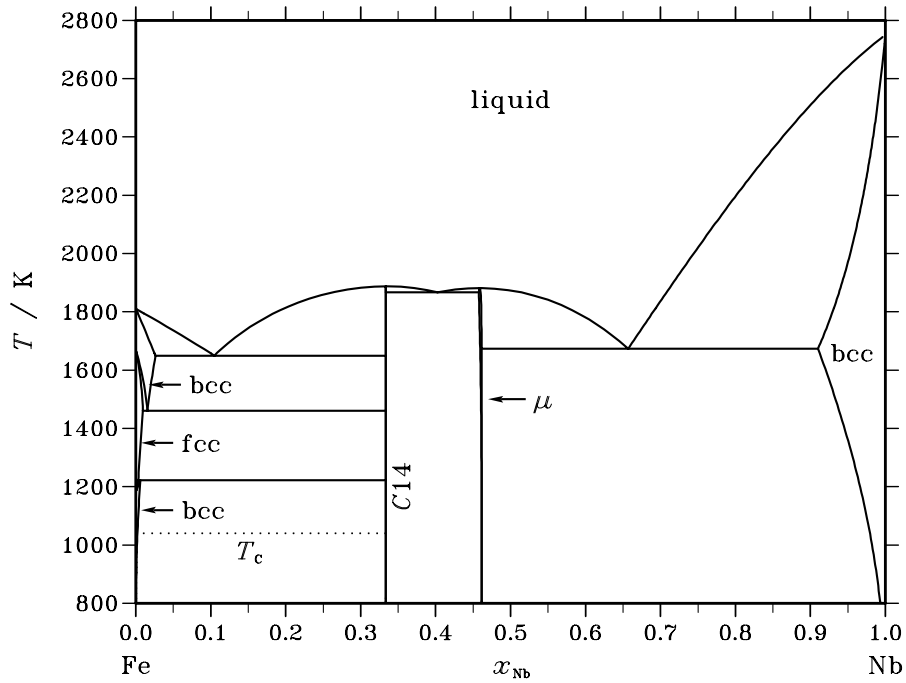

Fig. 1. Calculated phase diagram for the system Fe-Nb.

There are two intermetallic phases, a Laves phase ($C14$) and a μ-phase ($D8_5$), both almost stoichiometric. Nb stabilises bcc but the solubility in Fe is low in both fcc and bcc phases. The assessment presented here [90Hua] is quite old and modelling of the Laves and μ phases is not according to the most recent standards. Nb is also a carbide former and for this reason added to steels.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Fe,Nb)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Fe,Nb)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Fe,Nb)_1$
$C14$	$C14$	$MgZn_2$	$hP12$	$P6_3/mmc$	LAVES_C14	Fe_2Nb_1
μ	$D8_5$	Fe_7W_6	$hR13$	$R\overline{3}m$	D85_MUPHASE	$Fe_7Nb_2(Fe,Nb)_4$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Nb}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons C14$	congruent	1887.6	0.333	0.333		−26460
liquid $\rightleftharpoons \mu$	congruent	1881.0	0.459	0.459		−26351
liquid $\rightleftharpoons C14 + \mu$	eutectic	1867.2	0.402	0.333	0.458	−26100
liquid $\rightleftharpoons \mu$ + bcc	eutectic	1673.7	0.657	0.461	0.910	−21214
liquid $\rightleftharpoons$ bcc + $C14$	eutectic	1649.7	0.105	0.026	0.333	−15455
bcc $\rightleftharpoons$ fcc + $C14$	eutectoid	1460.1	0.015	0.009	0.333	−528
fcc + $C14 \rightleftharpoons$ bcc	peritectoid	1222.4	0.003	0.333	0.006	−599

Table IIIa. Integral quantities for the liquid phase at 2800 K.

x_{Nb}	ΔG_{m} [J/mol]	ΔH_{m} [J/mol]	ΔS_{m} [J/(mol·K)]	$G_{\mathrm{m}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{m}}^{\mathrm{E}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−8964	−4125	1.728	−1396	−0.975	0.000
0.200	−14561	−7762	2.428	−2911	−1.732	0.000
0.300	−18605	−10751	2.805	−4384	−2.274	0.000
0.400	−21321	−12930	2.997	−5653	−2.599	0.000
0.500	−22696	−14138	3.056	−6559	−2.707	0.000
0.600	−22608	−14216	2.997	−6940	−2.599	0.000
0.700	−20856	−13002	2.805	−6635	−2.274	0.000
0.800	−17134	−10335	2.428	−5484	−1.732	0.000
0.900	−10894	−6055	1.728	−3326	−0.975	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Fe in the liquid phase at 2800 K.

x_{Fe}	ΔG_{Fe} [J/mol]	ΔH_{Fe} [J/mol]	ΔS_{Fe} [J/(mol·K)]	$G_{\mathrm{Fe}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Fe}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Fe}	γ_{Fe}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2367	−217	0.768	86	−0.108	0.903	1.004
0.800	−5065	−1083	1.422	130	−0.433	0.804	1.006
0.700	−8494	−2919	1.991	−190	−0.975	0.694	0.992
0.600	−13088	−6047	2.515	−1196	−1.732	0.570	0.950
0.500	−19346	−10788	3.056	−3209	−2.707	0.436	0.871
0.400	−27882	−17465	3.720	−6550	−3.898	0.302	0.755
0.300	−39571	−26398	4.705	−11542	−5.306	0.183	0.609
0.200	−55974	−37909	6.452	−18505	−6.930	0.090	0.452
0.100	−81368	−52320	10.374	−27762	−8.771	0.030	0.303
0.000	$-\infty$	−69953	∞	−39635	−10.828	0.000	0.182

Reference state: Fe(liquid)

Table IIIc. Partial quantities for Nb in the liquid phase at 2800 K.

x_{Nb}	ΔG_{Nb} [J/mol]	ΔH_{Nb} [J/mol]	ΔS_{Nb} [J/(mol·K)]	$G_{\mathrm{Nb}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Nb}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Nb}	γ_{Nb}
0.000	$-\infty$	−43153	∞	−12835	−10.828	0.000	0.576
0.100	−68343	−39296	10.374	−14738	−8.771	0.053	0.531
0.200	−52544	−34479	6.452	−15075	−6.930	0.105	0.523
0.300	−42197	−29024	4.705	−14168	−5.306	0.163	0.544
0.400	−33671	−23254	3.720	−12339	−3.898	0.235	0.589
0.500	−26046	−17488	3.056	−9909	−2.707	0.327	0.653
0.600	−19092	−12050	2.515	−7199	−1.732	0.440	0.734
0.700	−12836	−7261	1.991	−4532	−0.975	0.576	0.823
0.800	−7424	−3441	1.422	−2229	−0.433	0.727	0.909
0.900	−3064	−914	0.768	−611	−0.108	0.877	0.974
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Nb(liquid)

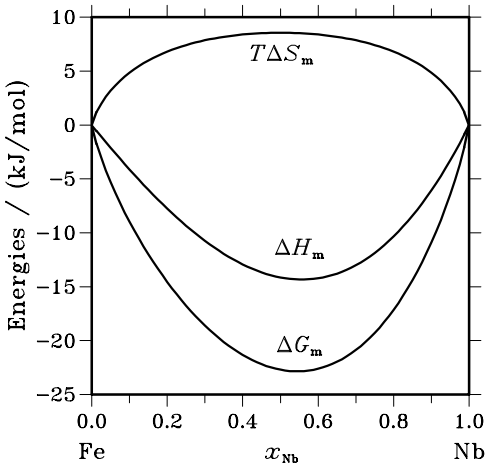

Fig. 2. Integral quantities of the liquid phase at T=2800 K.

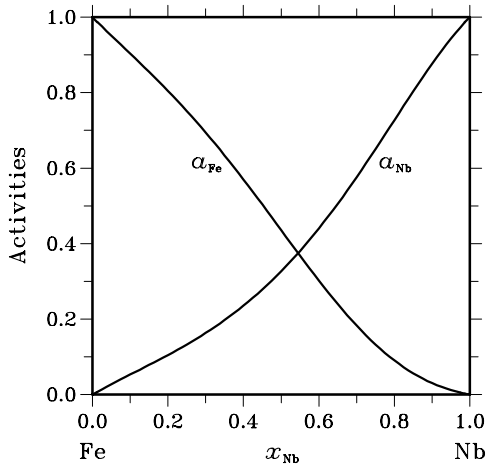

Fig. 3. Activities in the liquid phase at T=2800 K.

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

Compound	x_{Nb}	$\Delta_{\mathrm{f}}G^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}H^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}S^{\circ}$ / (J/(mol·K))	$\Delta_{\mathrm{f}}C_P^{\circ}$ / (J/(mol·K))
$C14$	0.333	−13722	−12559	3.901	0.234
μ	0.462	−15024	−14099	3.104	0.189

References

[90Hua] W. Huang: Z. Metallkd. **81** (1990) 397–404.