Fe – N (Iron – Nitrogen)

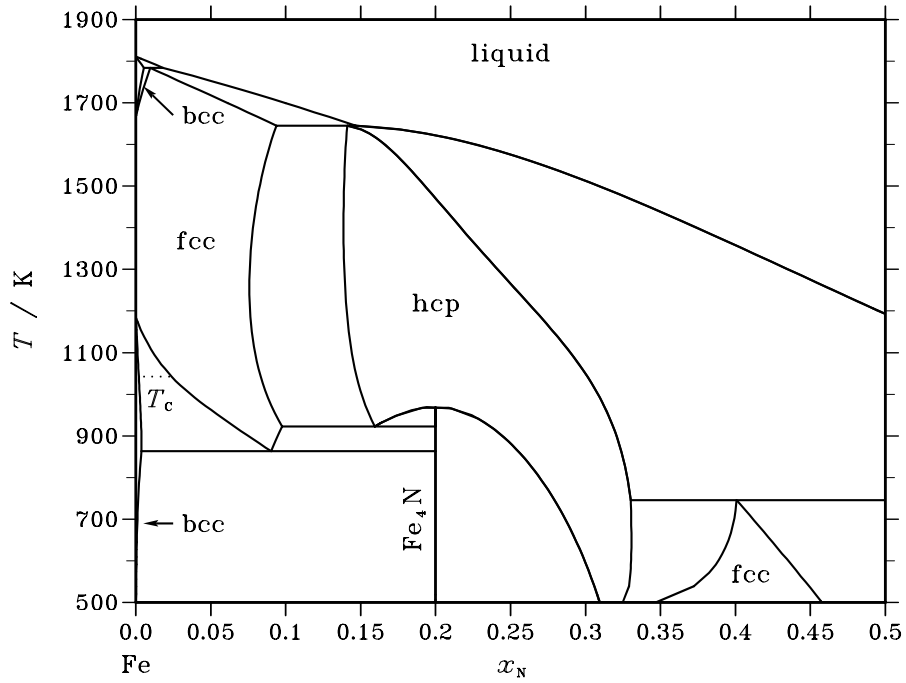

Fig. 1. Calculated phase diagram for the system Fe-N.

The phase diagram presented here is metastable as the gas phase is suspended. In the first diagram the composition is plotted vs. T and in the second the activity of N, with gas as reference state. The solubility of N in Fe is negligible relative to gas but as it is possible to nitride steels with a very high nitrogen activity one may find both the metastable Fe_4N and hexagonal nitride phases at the surface of the steel.
The solubility of N in the fcc phase is quite high and at higher N activities the hexagonal phase becomes stable. According to the assessment by [91Fri] the fcc phase becomes stable again at low temperatures and even higher nitrogen activities but that is an extrapolation from higher temperatures and there are no experimental evidence.
Nitrogen is an important alloying element in steels as it forms hard nitrides but also as fcc stabiliser in stainless steels.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Fe,N)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$Fe_1(N,\Box)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$Fe_1(N,\Box)_3$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$Fe_2(N,\Box)_1$
Fe_4N	$L1'_1$	Fe_4N	$cP5$	$Pm\overline{3}m$	FE4N	Fe_4N_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{N}			$\Delta_{\mathrm{r}}H$ / (J/mol)
bcc + liquid $\rightleftharpoons$ fcc	peritectic	1784.0	0.005	0.018	0.010	−5605
fcc + liquid $\rightleftharpoons$ hcp	peritectic	1644.5	0.094	0.147	0.141	−14047
hcp $\rightleftharpoons$ Fe_4N	congruent	970.1	0.200	0.200		−3735
hcp $\rightleftharpoons$ fcc + Fe_4N	eutectoid	922.8	0.159	0.098	0.200	−3074
fcc $\rightleftharpoons$ bcc + Fe_4N	eutectoid	863.0	0.090	0.004	0.200	−3834
hcp + liquid $\rightleftharpoons$ fcc	peritectic	745.7	0.330	0.771	0.401	−4324

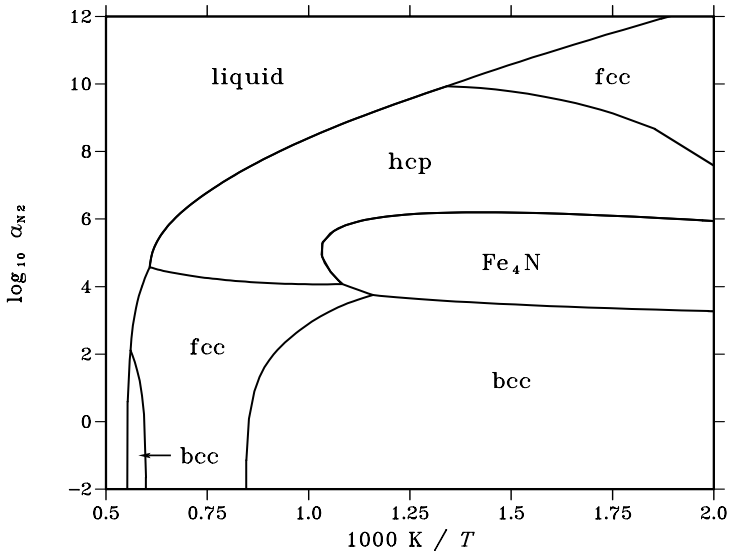

Fig. 2. Calculated temperature-activity phase diagram. Reference state: $\frac{1}{2}N_2$(gas, 0.1 MPa).

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

Compound	x_{N}	$\Delta_{\mathrm{f}}G^\circ$ / (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))
Fe_4N_1	0.200	1672	−429	−7.048	−0.334

References

[91Fri] K. Frisk: Calphad **15** (1991) 79–106.