Fe – Pr (Iron – Praseodymium)

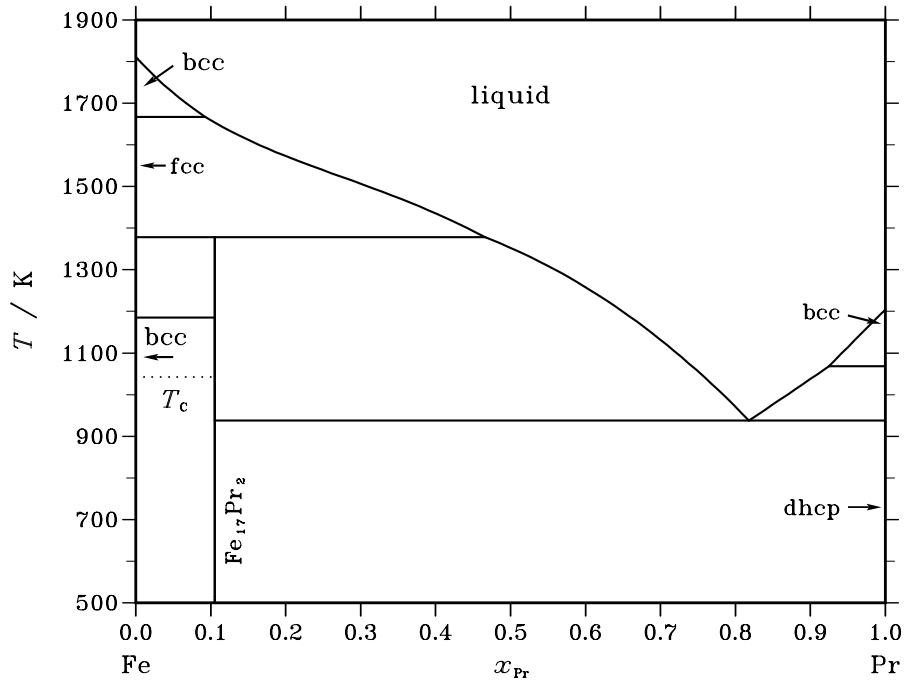

Fig. 1. Calculated phase diagram for the system Fe-Pr.

The binary Fe-Pr system is an important constituent of the Fe-Pr-B ternary to develop hard magnetic materials. Bär and Schaller [95Bae] studied this system experimentally by differential thermal analysis, X-ray diffraction and EMF measurements. On the basis of their results and phase diagram information from Ray [69Ray] and Tian *et al.* [87Tia] they performed a thermodynamic assessment of the system which has been accepted. The system is characterised by a stoichiometric intermetallic compound $Fe_{17}Pr_2$ which forms peritectically at 1378 K. The agreement between the experimental data and the calculated values is very good.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Fe,Pr)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Fe,Pr)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Fe,Pr)_1$
$Fe_{17}Pr_2$	$\cdots$	Th_2Zn_{17}	$hR19$	$R\overline{3}m$	FE17PR2	$Fe_{17}Pr_2$
dhcp	$A3'$	αLa	$hP4$	$P6_3/mmc$	DHCP	Pr_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Pr}			$\Delta_r H$ / (J/mol)
bcc $\rightleftharpoons$ fcc + liquid	degenerate	1667.2	0.000	0.000	0.093	−823
fcc + liquid $\rightleftharpoons$ $Fe_{17}Pr_2$	peritectic	1377.7	0.000	0.466	0.105	−4976
fcc + $Fe_{17}Pr_2$ $\rightleftharpoons$ bcc	degenerate	1185.0	0.000	0.105	0.000	−1011
bcc $\rightleftharpoons$ liquid + dhcp	degenerate	1068.0	1.000	0.925	1.000	−3166
liquid $\rightleftharpoons$ $Fe_{17}Pr_2$ + dhcp	eutectic	938.0	0.818	0.105	1.000	−11573

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

x_{Pr}	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	−3787	1665	2.869	1349	0.167	0.000
0.200	−5783	2620	4.423	2122	0.262	0.000
0.300	−7211	3011	5.380	2439	0.301	0.000
0.400	−8223	2974	5.893	2409	0.297	0.000
0.500	−8817	2634	6.027	2133	0.263	0.000
0.600	−8927	2104	5.806	1705	0.210	0.000
0.700	−8444	1489	5.228	1206	0.149	0.000
0.800	−7192	881	4.249	713	0.088	0.000
0.900	−4843	361	2.739	292	0.036	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Fe(liquid), Pr(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)]	$G_{\mathrm{Fe}}^{\mathrm{E}}$ [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	−1356	380	0.914	308	0.038	0.918	1.020
0.800	−2455	1321	1.987	1070	0.132	0.856	1.070
0.700	−3573	2545	3.220	2062	0.255	0.798	1.139
0.600	−4985	3808	4.628	3085	0.381	0.729	1.216
0.500	−6982	4899	6.253	3968	0.490	0.643	1.286
0.400	−9910	5636	8.182	4565	0.564	0.534	1.335
0.300	−14262	5874	10.598	4758	0.587	0.405	1.351
0.200	−20973	5497	13.931	4452	0.550	0.265	1.326
0.100	−32793	4422	19.587	3582	0.442	0.125	1.255
0.000	$-\infty$	2600	∞	2106	0.260	0.000	1.143

Reference state: Fe(liquid)

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

x_{Pr}	ΔG_{Pr} [J/mol]	ΔH_{Pr} [J/mol]	ΔS_{Pr} [J/(mol·K)]	$G_{\mathrm{Pr}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Pr}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Pr}	γ_{Pr}
0.000	$-\infty$	20718	∞	16782	2.072	0.000	2.893
0.100	−25661	13227	20.468	10714	1.323	0.197	1.970
0.200	−19095	7816	14.163	6331	0.782	0.299	1.493
0.300	−15700	4098	10.420	3320	0.410	0.370	1.234
0.400	−13080	1723	7.791	1395	0.172	0.437	1.092
0.500	−10651	369	5.800	299	0.037	0.510	1.019
0.600	−8272	−250	4.222	−203	−0.025	0.592	0.987
0.700	−5950	−390	2.927	−316	−0.039	0.686	0.980
0.800	−3746	−273	1.828	−221	−0.027	0.789	0.986
0.900	−1738	−91	0.867	−73	−0.009	0.896	0.995
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Pr(liquid)

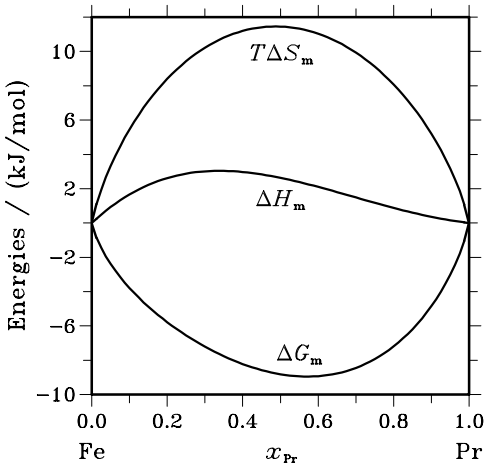

Fig. 2. Integral quantities of the liquid phase at T=1900 K.

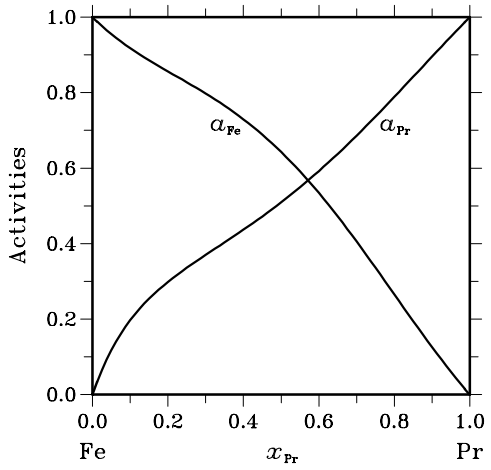

Fig. 3. Activities in the liquid phase at T=1900 K.

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

Compound	x_{Pr}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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))
$Fe_{17}Pr_2$	0.105	−287	−324	−0.126	4.056

References

[69Ray] A.E. Ray: Tech. Rep. AFML-TR-69-239 (1969) 1.
[87Tia] J. Tian, Y. Huang, J. Liang: Sci. Sin. Ser. A **30** (1987) 607–619.
[95Bae] S. Bär, H.-J. Schaller: Z. Metallkd. **86** (1995) 388–394.