Fe – Pd (Iron – Palladium)

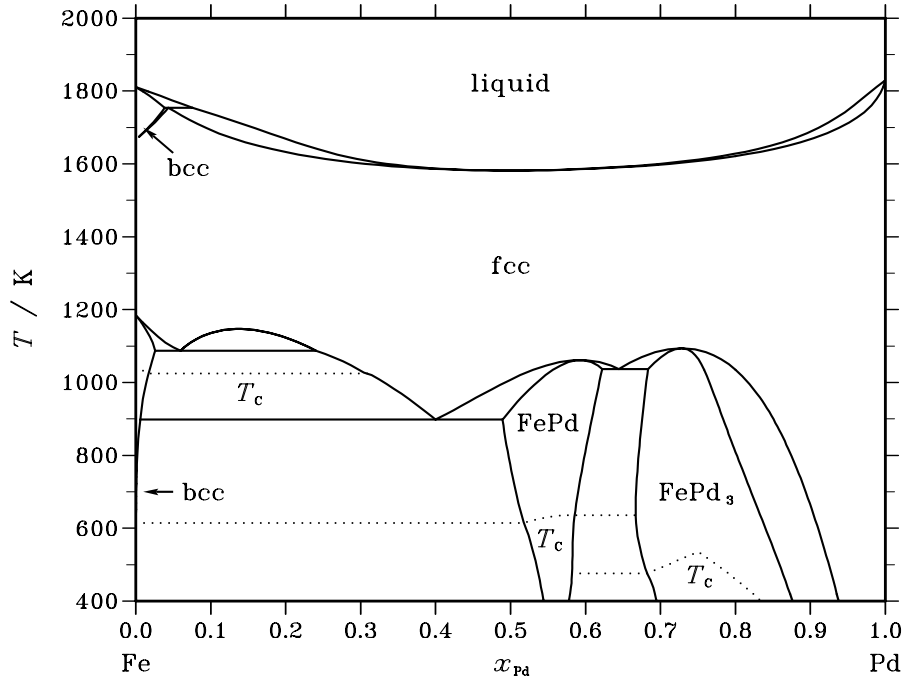

Fig. 1. Calculated phase diagram for the system Fe-Pd.

Alloys of Fe and Pd form a complete range of liquid and fcc solid solutions. The narrow liquidus/solidus boundary displays a minimum at about 1577 K and 54.9 at.% Pd. While there is some disagreement with respect to the lower-temperature phase equilibria in the system, ordering of the fcc phase is known to occur at temperatures below about 1093 K on the Pd-rich side of the system. This results in formation of the FePd and $FePd_3$ phases. The small miscibility gap in the fcc phase in Fe-rich alloys at temperatures between ca. 1073 and 1173 K is not well-defined. The thermodynamic assessment of the system by Ghosh *et al.* [99Gho] provides parameters which allow calculation of all the above-mentioned phase diagram features. Consistent with these features, enthalpies of formation of fcc alloys show small positive deviations from ideality at Fe-rich compositions and are strongly exothermic in the Pd-rich region of the system.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Fe,Pd)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Fe,Pd)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Fe,Pd)_1$
FePd	$L1_0$	AuCu	$tP2$	$P4/mmm$	B2_FEPD	$(Fe,Pd)_1(Fe,Pd)_1$
$FePd_3$	$L1_2$	$AuCu_3$	$cP4$	$Pm\overline{3}m$	L12_FEPD3	$(Fe,Pd)_1(Fe,Pd)_3$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Pd}			$\Delta_{\mathrm{r}}H$ / (J/mol)
bcc + liquid ⇌ fcc	peritectic	1753.5	0.039	0.076	0.043	−2715
liquid ⇌ fcc	congruent	1581.8	0.498	0.498		−26493
fcc ⇌ fcc′ + fcc″	critical	1144.4	0.138	0.138	0.138	0
fcc ⇌ $FePd_3$	congruent	1094.2	0.728	0.728		−7787
fcc′ ⇌ bcc + fcc″	monotectoid	1087.4	0.060	0.026	0.240	−2009
fcc ⇌ FePd	congruent	1061.4	0.593	0.593		−5075
fcc ⇌ FePd + $FePd_3$	eutectoid	1037.1	0.644	0.622	0.683	−5507
fcc ⇌ bcc + FePd	eutectoid	898.0	0.400	0.006	0.489	−6942

Table IIIa. Integral quantities for the liquid phase at 1873 K.

x_{Pd}	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	−9055	1332	5.546	−3993	2.843	0.000
0.200	−16131	2203	9.788	−8338	5.628	0.000
0.300	−22084	2674	13.218	−12571	8.139	0.000
0.400	−26707	2808	15.758	−16226	10.163	0.000
0.500	−29634	2667	17.246	−18840	11.482	0.000
0.600	−30427	2312	17.479	−19946	11.883	0.000
0.700	−28593	1806	16.230	−19080	11.151	0.000
0.800	−23570	1210	13.230	−15777	9.070	0.000
0.900	−14635	588	8.127	−9572	5.424	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Fe in the liquid phase at 1873 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	−1387	241	0.869	254	−0.007	0.915	1.016
0.800	−3080	882	2.115	395	0.260	0.821	1.026
0.700	−6060	1798	4.195	−505	1.230	0.678	0.968
0.600	−11333	2865	7.581	−3378	3.333	0.483	0.805
0.500	−19948	3959	12.764	−9153	7.001	0.278	0.556
0.400	−33030	4957	20.281	−18760	12.663	0.120	0.300
0.300	−51878	5733	30.759	−33129	20.749	0.036	0.119
0.200	−78253	6164	45.071	−53189	31.689	0.007	0.033
0.100	−115730	6126	65.059	−79872	45.915	0.001	0.006
0.000	$-\infty$	5495	∞	−114105	63.855	0.000	0.001

Reference state: Fe(liquid)

Table IIIc. Partial quantities for Pd in the liquid phase at 1873 K.

x_{Pd}	ΔG_{Pd} [J/mol]	ΔH_{Pd} [J/mol]	ΔS_{Pd} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Pd}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Pd}}$ [J/(mol·K)]	a_{Pd}	γ_{Pd}
0.000	$-\infty$	15838	∞	−36613	28.003	0.000	0.095
0.100	−78068	11153	47.636	−42210	28.491	0.007	0.067
0.200	−68334	7488	40.482	−43270	27.100	0.012	0.062
0.300	−59473	4720	34.272	−40723	24.262	0.022	0.073
0.400	−49768	2723	28.025	−35499	20.406	0.041	0.102
0.500	−39321	1374	21.727	−28526	15.964	0.080	0.160
0.600	−28692	548	15.611	−20737	11.364	0.158	0.264
0.700	−18614	122	10.003	−13059	7.038	0.303	0.432
0.800	−9899	−28	5.270	−6424	3.415	0.530	0.662
0.900	−3402	−28	1.801	−1761	0.925	0.804	0.893
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Pd(liquid)

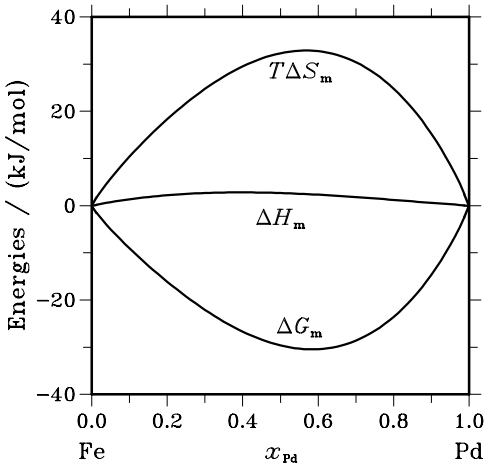

Fig. 2. Integral quantities of the liquid phase at T=1873 K.

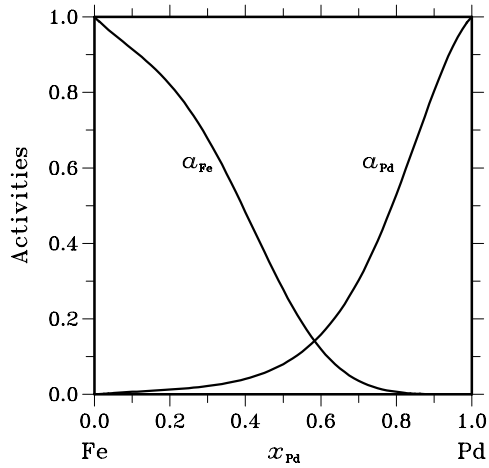

Fig. 3. Activities in the liquid phase at T=1873 K.

Table IVa. Integral quantities for the stable phases at 1273 K.

Phase	x_{Pd}	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)]
fcc	0.000	0	0	0.000	0	0.000	0.000
	0.100	−5224	1255	5.089	−1783	2.386	0.000
	0.200	−9706	192	7.776	−4410	3.615	0.004
	0.300	−13880	−2421	9.002	−7414	3.923	0.001
	0.400	−17464	−5860	9.115	−10341	3.519	0.122
	0.500	−20053	−9329	8.424	−12716	2.661	0.256
	0.600	−21191	−12014	7.209	−14067	1.613	0.252
	0.700	−20396	−13157	5.686	−13930	0.607	0.132
	0.800	−17145	−12039	4.010	−11848	−0.150	0.030
	0.900	−10802	−7913	2.269	−7361	−0.434	0.001
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Fe(fcc), Pd(fcc)

Table IVb. Partial quantities for Fe in the stable phases at 1273 K.

Phase	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}
fcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−616	1285	1.494	499	0.618	0.943	1.048
	0.800	−985	4126	4.015	1377	2.159	0.911	1.139
	0.700	−2077	6962	7.100	1698	4.135	0.822	1.174
	0.600	−4826	8506	10.473	581	6.226	0.634	1.056
	0.500	−10344	6713	13.399	−3008	7.636	0.376	0.753
	0.400	−19667	199	15.606	−9969	7.987	0.156	0.390
	0.300	−33907	−12223	17.034	−21163	7.023	0.041	0.135
	0.200	−54538	−31990	17.712	−37503	4.331	0.006	0.029
	0.100	−84347	−60918	18.404	−59976	−0.740	0.000	0.003
	0.000	$-\infty$	−100652	∞	−89534	−8.734	0.000	0.000

Reference state: Fe(fcc)

Table IVc. Partial quantities for Pd in the stable phases at 1273 K.

Phase	x_{Pd}	ΔG_{Pd} [J/mol]	ΔH_{Pd} [J/mol]	ΔS_{Pd} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Pd}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Pd}}$ [J/(mol·K)]	a_{Pd}	γ_{Pd}
fcc	0.000	$-\infty$	26673	∞	−12066	30.431	0.000	0.320
	0.100	−46695	977	37.449	−22323	18.304	0.012	0.121
	0.200	−44593	−15544	22.819	−27558	9.438	0.015	0.074
	0.300	−41421	−24314	13.439	−28678	3.428	0.020	0.067
	0.400	−36421	−27411	7.078	−26723	−0.540	0.032	0.080
	0.500	−29761	−25370	3.449	−22425	−2.314	0.060	0.120
	0.600	−22206	−20156	1.611	−16800	−2.636	0.123	0.204
	0.700	−14605	−13558	0.823	−10830	−2.143	0.252	0.359
	0.800	−7796	−7052	0.585	−5435	−1.270	0.479	0.598
	0.900	−2630	−2024	0.476	−1515	−0.400	0.780	0.867
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Pd(fcc)

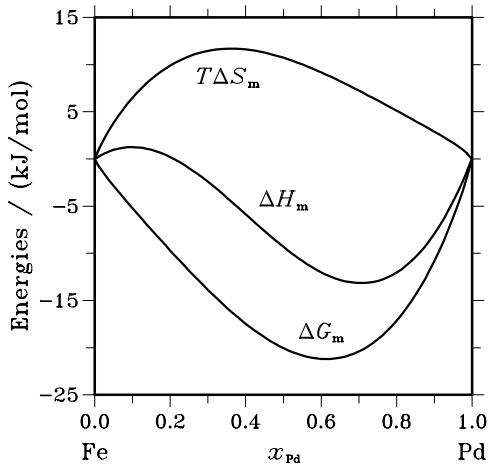

Fig. 4. Integral quantities of the stable phases at T=1273 K.

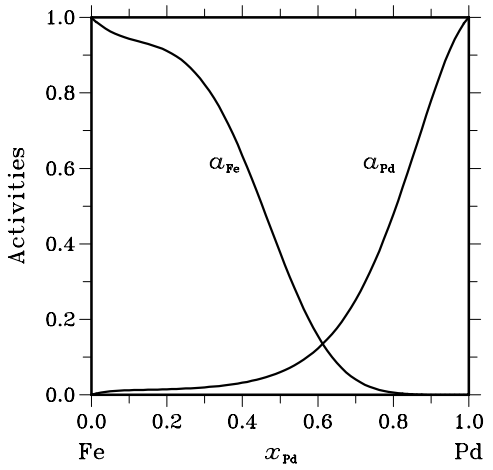

Fig. 5. Activities in the stable phases at T=1273 K.

References

[99Gho] G. Ghosh, C. Kantner, G.B. Olson: J. Phase Equilibria **20** (1999) 295–308.