Fe – Pt (Iron – Platinum)

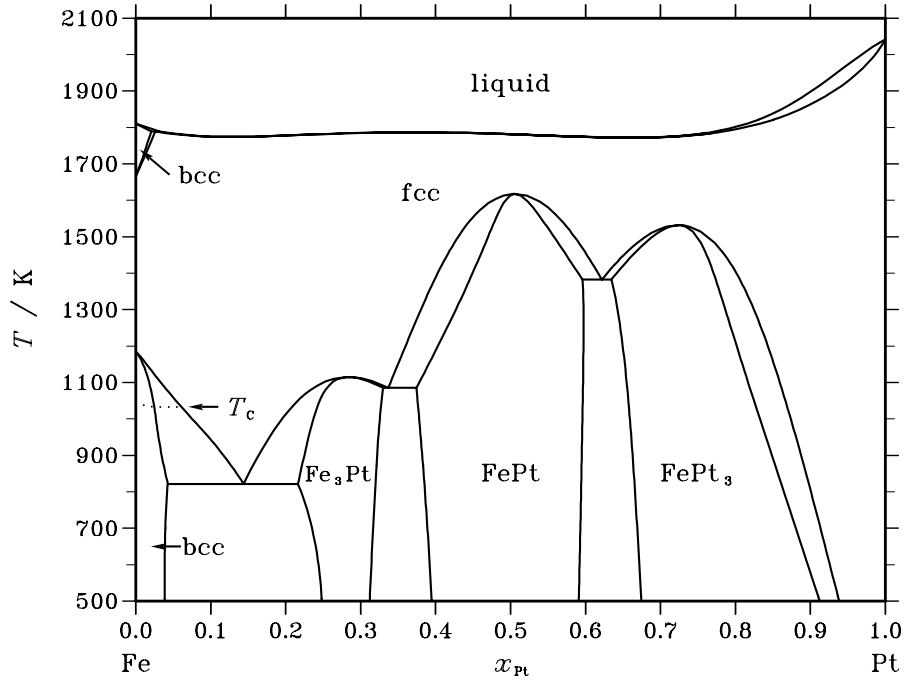

Fig. 1. Calculated phase diagram for the system Fe-Pt.

The interest in Fe-Pt alloys is due to their magnetic properties, especially the Invar effect. In addition, the use of Pt as material for laboratory crucibles demands for the knowlege of its reactivity with other materials, including iron. The Fe-Pt system has been reviewed by [93Oka] and a thermodynamic assessment has been given by [01Fre1]. The optimization is based on literature data for the phase diagram and for thermodynamic properties of liquid and solid alloys. In addition, new data obtained from EMF [01Fre2] and DTA [04Fre] experiments are included. The liquid and the iron-rich bcc-phases have been described by substitutional models while an ambitious 4-sublattice model has been selected for the fcc phase which transforms into the $L1_0$ and $L1_2$ super-structures at lower temperatures.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Fe,Pt)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_L102	$(Fe,Pt)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Fe,Pt)_1$
Fe_3Pt, $FePt_3$	$L1_2$	Cu_3Au	$cP4$	$Pm\overline{3}m$	FCC_L102	$3(Fe,Pt)_1$ $1(FePt)_1$
FePt	$L1_0$	AuCu	$tP4$	$P4/mmm$	FCC_L102	$2(Fe,Pt)_1$ $2(Fe,Pt)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Pt}			$\Delta_{\mathrm{r}}H$ / (J/mol)
bcc + liquid ⇌ fcc	peritectic	1788.8	0.021	0.032	0.026	−7713
liquid ⇌ fcc	congruent	1786.4	0.369	0.369		−22286
liquid ⇌ fcc	congruent	1774.2	0.125	0.125		−15649
liquid ⇌ fcc	congruent	1772.0	0.661	0.661		−22868
fcc ⇌ FePt	congruent	1617.9	0.506	0.506		−7230
fcc ⇌ $FePt_3$	congruent	1531.7	0.723	0.723		−4601
fcc ⇌ FePt + $FePt_3$	eutectoid	1382.5	0.622	0.596	0.634	−3053
fcc ⇌ Fe_3Pt	congruent	1114.9	0.283	0.283		−3485
fcc ⇌ Fe_3Pt + FePt	eutectoid	1085.4	0.337	0.330	0.374	−2630
fcc ⇌ bcc + Fe_3Pt	eutectoid	821.6	0.144	0.043	0.216	−3595

Table IIIa. Integral quantities for the liquid phase at 2050 K.

x_{Pt}	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	−11157	−18900	−3.777	−5616	−6.480	0.000
0.200	−19729	−34816	−7.359	−11200	−11.520	0.000
0.300	−26624	−47208	−10.041	−16212	−15.120	0.000
0.400	−31631	−55584	−11.684	−20160	−17.280	0.000
0.500	−34415	−59500	−12.237	−22600	−18.000	0.000
0.600	−34607	−58560	−11.684	−23136	−17.280	0.000
0.700	−31832	−52416	−10.041	−21420	−15.120	0.000
0.800	−25681	−40768	−7.359	−17152	−11.520	0.000
0.900	−15621	−23364	−3.777	−10080	−6.480	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Fe in the liquid phase at 2050 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	−1718	−1398	0.156	78	−0.720	0.904	1.005
0.800	−4235	−6336	−1.025	−432	−2.880	0.780	0.975
0.700	−8617	−15822	−3.514	−2538	−6.480	0.603	0.862
0.600	−15811	−30720	−7.273	−7104	−11.520	0.395	0.659
0.500	−26665	−51750	−12.237	−14850	−18.000	0.209	0.418
0.400	−41970	−79488	−18.302	−26352	−25.920	0.085	0.213
0.300	−62563	−114366	−25.270	−42042	−35.280	0.025	0.085
0.200	−89641	−156672	−32.698	−62208	−46.080	0.005	0.026
0.100	−126241	−206550	−39.175	−86994	−58.320	0.001	0.006
0.000	$-\infty$	−264000	∞	−116400	−72.000	0.000	0.001

Reference state: Fe(liquid)

Table IIIc. Partial quantities for Pt in the liquid phase at 2050 K.

x_{Pt}	ΔG_{Pt} [J/mol]	ΔH_{Pt} [J/mol]	ΔS_{Pt} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Pt}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Pt}}$ [J/(mol·K)]	a_{Pt}	γ_{Pt}
0.000	$-\infty$	−202000	∞	−54400	−72.000	0.000	0.041
0.100	−96109	−176418	−39.175	−56862	−58.320	0.004	0.036
0.200	−81705	−148736	−32.698	−54272	−46.080	0.008	0.041
0.300	−68639	−120442	−25.270	−48118	−35.280	0.018	0.059
0.400	−55362	−92880	−18.302	−39744	−25.920	0.039	0.097
0.500	−42165	−67250	−12.237	−30350	−18.000	0.084	0.169
0.600	−29699	−44608	−7.273	−20992	−11.520	0.175	0.292
0.700	−18661	−25866	−3.514	−12582	−6.480	0.335	0.478
0.800	−9691	−11792	−1.025	−5888	−2.880	0.566	0.708
0.900	−3330	−3010	0.156	−1534	−0.720	0.823	0.914
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Pt(liquid)

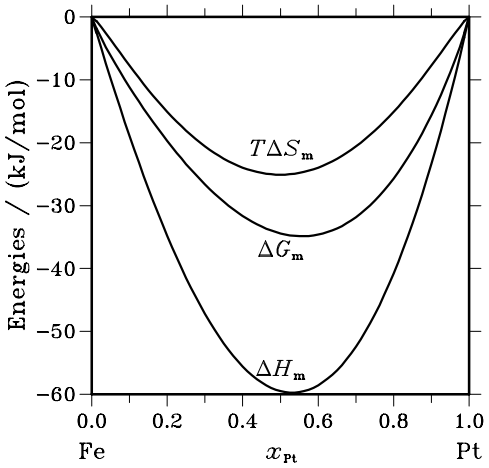

Fig. 2. Integral quantities of the liquid phase at T=2050 K.

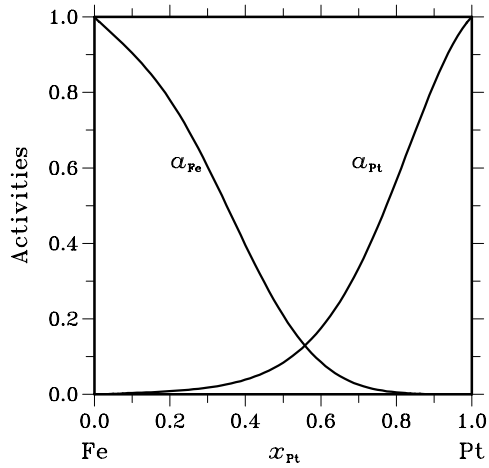

Fig. 3. Activities in the liquid phase at T=2050 K.

Table IVa. Integral quantities for the stable phases at 1650 K.

Phase	x_{Pt}	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	−12200	−18612	−3.886	−7741	−6.589	0.000
	0.200	−22105	−36253	−8.574	−15240	−12.735	0.000
	0.300	−30056	−50834	−12.593	−21675	−17.672	0.000
	0.400	−35609	−60784	−15.257	−26376	−20.853	0.000
	0.500	−38335	−65044	−16.187	−28826	−21.950	0.000
	0.600	−37896	−63070	−15.257	−28663	−20.853	0.000
	0.700	−34058	−54836	−12.593	−25677	−17.672	0.000
	0.800	−26679	−40826	−8.574	−19814	−12.735	0.000
	0.900	−15631	−22042	−3.886	−11171	−6.589	0.000
	1.000	0	0	0.000	0	0.000	0.000

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

Table IVb. Partial quantities for Fe in the stable phases at 1650 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	−1416	−95	0.801	30	−0.075	0.902	1.002
	0.800	−4118	−3420	0.423	−1057	−1.433	0.741	0.926
	0.700	−9568	−13380	−2.310	−4675	−5.275	0.498	0.711
	0.600	−18790	−31831	−7.904	−11782	−12.151	0.254	0.424
	0.500	−32380	−59089	−16.187	−22871	−21.950	0.094	0.189
	0.400	−50548	−93923	−26.288	−37977	−33.906	0.025	0.063
	0.300	−73191	−133559	−36.587	−56674	−46.597	0.005	0.016
	0.200	−100152	−173679	−44.561	−78073	−57.943	0.001	0.003
	0.100	−132414	−208419	−46.063	−100825	−65.208	0.000	0.001
	0.000	$-\infty$	−230372	∞	−123122	−65.000	0.000	0.000

Reference state: Fe(fcc)

Table IVc. Partial quantities for Pt in the stable phases at 1650 K.

Phase	x_{Pt}	ΔG_{Pt} [J/mol]	ΔH_{Pt} [J/mol]	ΔS_{Pt} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Pt}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Pt}}$ [J/(mol·K)]	a_{Pt}	γ_{Pt}
fcc	0.000	$-\infty$	−182732	∞	−75482	−65.000	0.000	0.004
	0.100	−109261	−185266	−46.063	−77672	−65.208	0.000	0.003
	0.200	−94054	−167581	−44.561	−71975	−57.943	0.001	0.005
	0.300	−77860	−138228	−36.587	−61342	−46.597	0.003	0.011
	0.400	−60838	−104213	−26.288	−48268	−33.906	0.012	0.030
	0.500	−44290	−70999	−16.187	−34781	−21.950	0.040	0.079
	0.600	−29461	−42502	−7.904	−22453	−12.151	0.117	0.195
	0.700	−17286	−21097	−2.310	−12393	−5.275	0.284	0.405
	0.800	−8310	−7613	0.423	−5249	−1.433	0.546	0.682
	0.900	−2655	−1334	0.801	−1209	−0.075	0.824	0.916
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Pt(fcc)

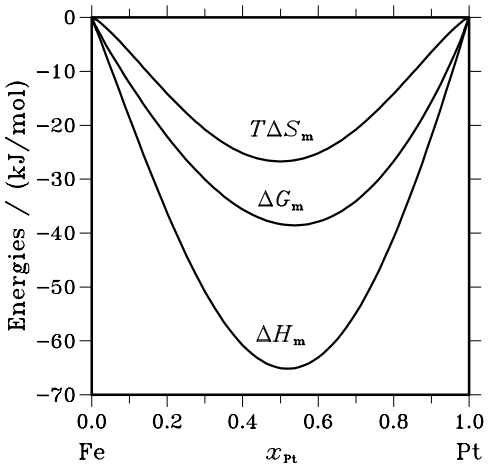

Fig. 4. Integral quantities of the stable phases at T=1650 K.

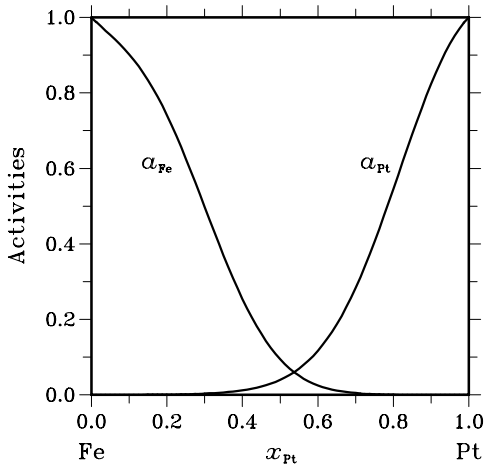

Fig. 5. Activities in the stable phases at T=1650 K.

References

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