Pd – Rh (Palladium – Rhodium)

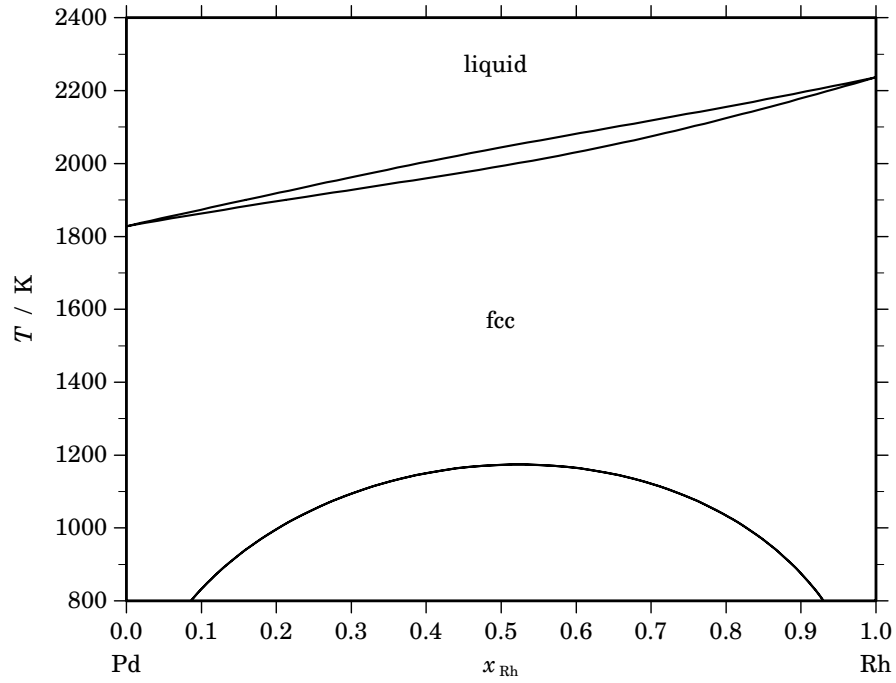

Fig. 1. Calculated phase diagram for the system Pd-Rh.

The system Pd-Rh is characterised by two solution phases, liquid and fcc with continuous miscibility at higher temperatures and a broad miscibility gap opening in the fcc phase at lower temperatures [1959Rau2, 1987Shi]. The melting range is experimentally ill defined [1994Oka]. The thermodynamic assessment of the Pd-Rh system was carried out by Korb [2004Kor]. The calculated miscibility gap agrees well with [1959Rau2] and [1959Rau1] in the Pd-rich region and with [1987Shi] near the critical point. The calculated liquidus and solidus must be seen as a result of the thermodynamic calculations, see [1994Oka].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Pd,Rh)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Pd,Rh)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Rh}			$\Delta_{\mathrm{r}}H$ / (J/mol)
fcc $\rightleftharpoons$ fcc′ + fcc″	critical	1173.6	0.523	0.523	0.523	0

Table IIIa. Integral quantities for the liquid phase at 2250 K.

x_{Rh}	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	−4468	1613	2.703	1613	0.000	0.000
0.200	−6493	2868	4.161	2868	0.000	0.000
0.300	−7663	3765	5.079	3765	0.000	0.000
0.400	−8288	4303	5.596	4303	0.000	0.000
0.500	−8485	4482	5.763	4482	0.000	0.000
0.600	−8288	4303	5.596	4303	0.000	0.000
0.700	−7663	3765	5.079	3765	0.000	0.000
0.800	−6493	2868	4.161	2868	0.000	0.000
0.900	−4468	1613	2.703	1613	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Pd in the liquid phase at 2250 K.

x_{Pd}	ΔG_{Pd} [J/mol]	ΔH_{Pd} [J/mol]	ΔS_{Pd} [J/(mol·K)]	$G_{\mathrm{Pd}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Pd}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Pd}	γ_{Pd}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1792	179	0.876	179	0.000	0.909	1.010
0.800	−3457	717	1.855	717	0.000	0.831	1.039
0.700	−5059	1613	2.966	1613	0.000	0.763	1.090
0.600	−6688	2868	4.247	2868	0.000	0.699	1.166
0.500	−8485	4482	5.763	4482	0.000	0.635	1.271
0.400	−10688	6454	7.619	6454	0.000	0.565	1.412
0.300	−13739	8784	10.010	8784	0.000	0.480	1.599
0.200	−18635	11474	13.382	11474	0.000	0.369	1.847
0.100	−28555	14521	19.145	14521	0.000	0.217	2.173
0.000	$-\infty$	17928	∞	17928	0.000	0.000	2.607

Reference state: Pd(liquid)

Table IIIc. Partial quantities for Rh in the liquid phase at 2250 K.

x_{Rh}	ΔG_{Rh} [J/mol]	ΔH_{Rh} [J/mol]	ΔS_{Rh} [J/(mol·K)]	$G_{\mathrm{Rh}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Rh}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Rh}	γ_{Rh}
0.000	$-\infty$	17928	∞	17928	0.000	0.000	2.607
0.100	−28555	14521	19.145	14521	0.000	0.217	2.173
0.200	−18635	11474	13.382	11474	0.000	0.369	1.847
0.300	−13739	8784	10.010	8784	0.000	0.480	1.599
0.400	−10688	6454	7.619	6454	0.000	0.565	1.412
0.500	−8485	4482	5.763	4482	0.000	0.635	1.271
0.600	−6688	2868	4.247	2868	0.000	0.699	1.166
0.700	−5059	1613	2.966	1613	0.000	0.763	1.090
0.800	−3457	717	1.855	717	0.000	0.831	1.039
0.900	−1792	179	0.876	179	0.000	0.909	1.010
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Rh(liquid)

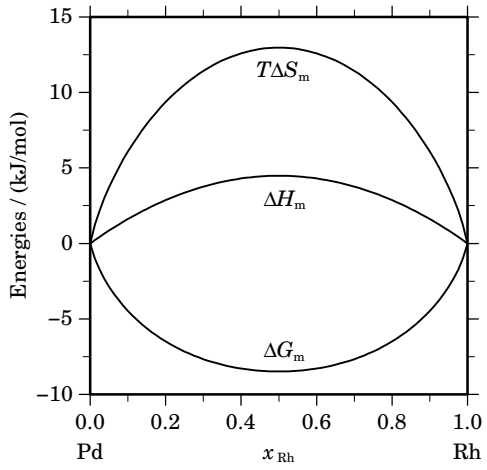

Fig. 2. Integral quantities of the liquid phase at T=2250 K.

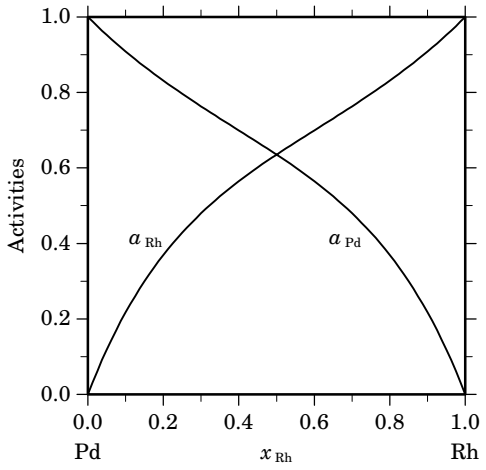

Fig. 3. Activities in the liquid phase at T=2250 K.

Table IVa. Integral quantities for the stable phases at 1575 K.

Phase	x_{Rh}	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	−2547	1710	2.703	1710	0.000	0.000
	0.200	−3494	3059	4.161	3059	0.000	0.000
	0.300	−3959	4041	5.079	4041	0.000	0.000
	0.400	−4166	4647	5.596	4647	0.000	0.000
	0.500	−4206	4871	5.763	4871	0.000	0.000
	0.600	−4108	4705	5.596	4705	0.000	0.000
	0.700	−3857	4142	5.079	4142	0.000	0.000
	0.800	−3377	3176	4.161	3176	0.000	0.000
	0.900	−2460	1797	2.703	1797	0.000	0.000
	1.000	0	0	0.000	0	0.000	0.000

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

Table IVb. Partial quantities for Pd in the stable phases at 1575 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	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1201	179	0.876	179	0.000	0.912	1.014
	0.800	−2196	726	1.855	726	0.000	0.846	1.057
	0.700	−3015	1656	2.966	1656	0.000	0.794	1.135
	0.600	−3707	2982	4.247	2982	0.000	0.753	1.256
	0.500	−4357	4720	5.763	4720	0.000	0.717	1.434
	0.400	−5115	6884	7.619	6884	0.000	0.677	1.692
	0.300	−6278	9488	10.010	9488	0.000	0.619	2.064
	0.200	−8529	12547	13.382	12547	0.000	0.521	2.607
	0.100	−14077	16076	19.145	16076	0.000	0.341	3.413
	0.000	$-\infty$	20089	∞	20089	0.000	0.000	4.637

Reference state: Pd(fcc)

Table IVc. Partial quantities for Rh in the stable phases at 1575 K.

Phase	x_{Rh}	ΔG_{Rh} [J/mol]	ΔH_{Rh} [J/mol]	ΔS_{Rh} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Rh}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Rh}}$ [J/(mol·K)]	a_{Rh}	γ_{Rh}
fcc	0.000	$-\infty$	18879	∞	18879	0.000	0.000	4.228
	0.100	−14665	15488	19.145	15488	0.000	0.326	3.263
	0.200	−8684	12393	13.382	12393	0.000	0.515	2.576
	0.300	−6160	9607	10.010	9607	0.000	0.625	2.083
	0.400	−4854	7145	7.619	7145	0.000	0.690	1.726
	0.500	−4055	5022	5.763	5022	0.000	0.734	1.467
	0.600	−3436	3253	4.247	3253	0.000	0.769	1.282
	0.700	−2819	1852	2.966	1852	0.000	0.806	1.152
	0.800	−2090	833	1.855	833	0.000	0.853	1.066
	0.900	−1169	211	0.876	211	0.000	0.915	1.016
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Rh(fcc)

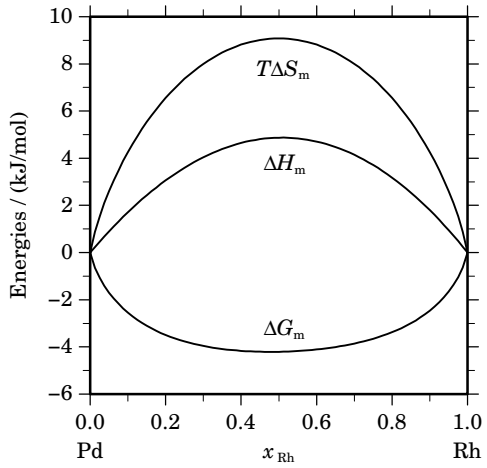

Fig. 4. Integral quantities of the stable phases at T=1575 K.

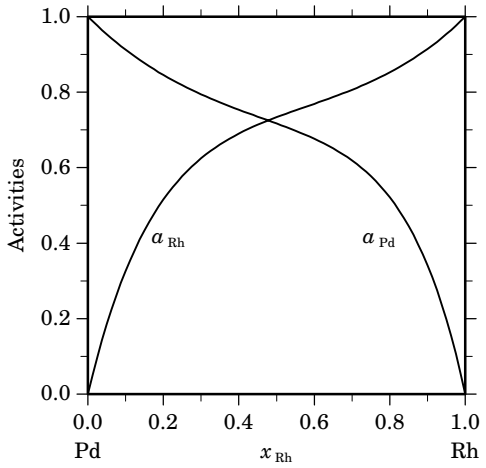

Fig. 5. Activities in the stable phases at T=1575 K.

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