Pd – Ru (Palladium – Ruthenium)

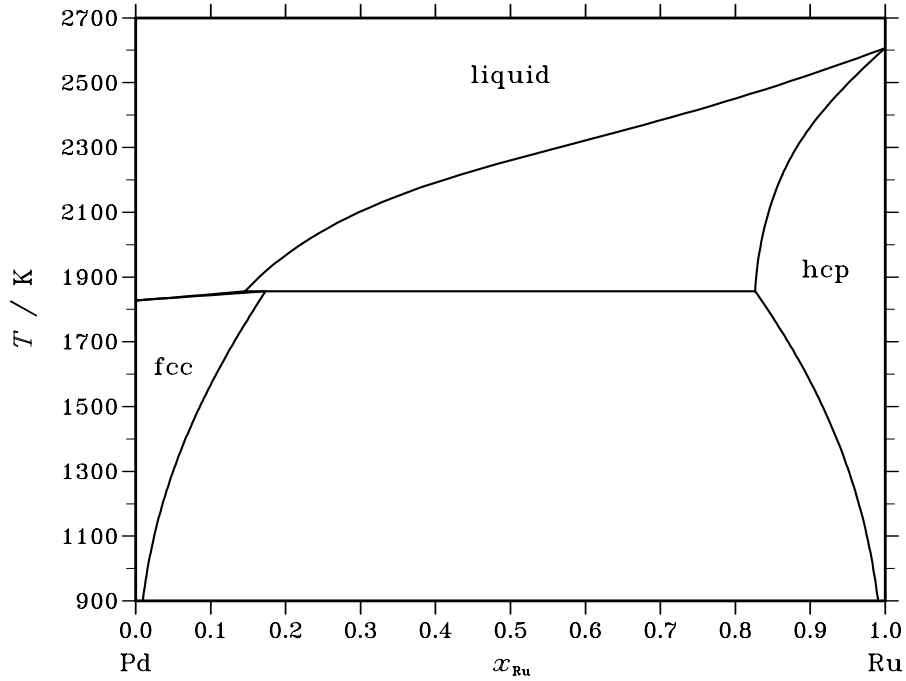

Fig. 1. Calculated phase diagram for the system Pd-Ru.

The phase diagram of the Pd-Ru system is only moderately well established, with most of the experimental information pertaining to Pd-rich alloys. The solidus and liquidus boundaries at higher Ru contents are uncertain [86Mas, 93Tri]. Nevertheless, those presented by Massalski [86Mas], as well as the boundary of the Ru-rich solid solution, have been given preference over the updated assessed diagram due to Tripathi *et al.* [93Tri] in Spencer's thermodynamic assessment of the system [98Spe]. The latter allows calculation of the Pd-rich solid solution boundary in good accord with published experimental measurements and reproduces the peritectic temperature well. Calculated thermodynamic properties of solid and liquid alloys show positive departure from ideality.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Pd,Ru)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Pd,Ru)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Pd,Ru)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ru}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid + hcp $\rightleftharpoons$ fcc	peritectic	1856.2	0.146	0.827	0.173	−15780

Table IIIa. Integral quantities for the liquid phase at 2700 K.

x_{Ru}	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	−5156	2142	2.703	2142	0.000	0.000
0.200	−7426	3808	4.161	3808	0.000	0.000
0.300	−8715	4998	5.079	4998	0.000	0.000
0.400	−9397	5712	5.596	5712	0.000	0.000
0.500	−9611	5950	5.763	5950	0.000	0.000
0.600	−9397	5712	5.596	5712	0.000	0.000
0.700	−8715	4998	5.079	4998	0.000	0.000
0.800	−7426	3808	4.161	3808	0.000	0.000
0.900	−5156	2142	2.703	2142	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Pd in the liquid phase at 2700 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	−2127	238	0.876	238	0.000	0.910	1.011
0.800	−4057	952	1.855	952	0.000	0.835	1.043
0.700	−5865	2142	2.966	2142	0.000	0.770	1.100
0.600	−7660	3808	4.247	3808	0.000	0.711	1.185
0.500	−9611	5950	5.763	5950	0.000	0.652	1.303
0.400	−12002	8568	7.619	8568	0.000	0.586	1.465
0.300	−15366	11662	10.010	11662	0.000	0.504	1.681
0.200	−20899	15232	13.382	15232	0.000	0.394	1.971
0.100	−32413	19278	19.145	19278	0.000	0.236	2.360
0.000	$-\infty$	23800	∞	23800	0.000	0.000	2.887

Reference state: Pd(liquid)

Table IIIc. Partial quantities for Ru in the liquid phase at 2700 K.

x_{Ru}	ΔG_{Ru} [J/mol]	ΔH_{Ru} [J/mol]	ΔS_{Ru} [J/(mol·K)]	$G_{\mathrm{Ru}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Ru}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Ru}	γ_{Ru}
0.000	$-\infty$	23800	∞	23800	0.000	0.000	2.887
0.100	−32413	19278	19.145	19278	0.000	0.236	2.360
0.200	−20899	15232	13.382	15232	0.000	0.394	1.971
0.300	−15366	11662	10.010	11662	0.000	0.504	1.681
0.400	−12002	8568	7.619	8568	0.000	0.586	1.465
0.500	−9611	5950	5.763	5950	0.000	0.652	1.303
0.600	−7660	3808	4.247	3808	0.000	0.711	1.185
0.700	−5865	2142	2.966	2142	0.000	0.770	1.100
0.800	−4057	952	1.855	952	0.000	0.835	1.043
0.900	−2127	238	0.876	238	0.000	0.910	1.011
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ru(liquid)

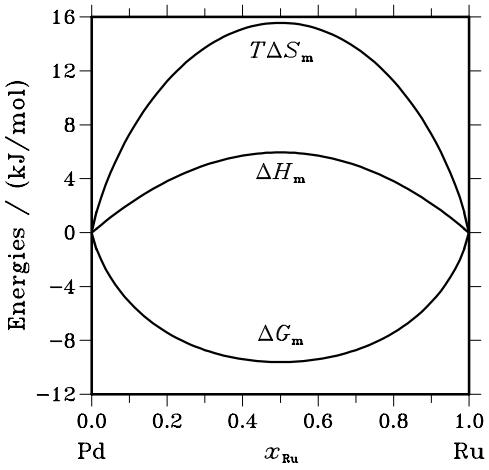

Fig. 2. Integral quantities of the liquid phase at T=2700 K.

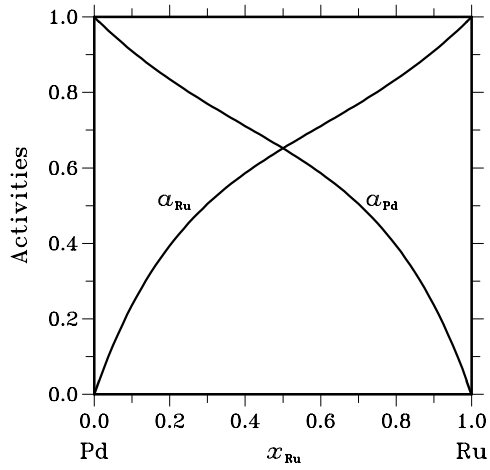

Fig. 3. Activities in the liquid phase at T=2700 K.

Table IVa. Integral quantities for the stable phases at 1800 K.

Phase	x_{Ru}	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	−1798	3504	2.946	3067	0.243	0.000
	0.158	−1914	5296	4.005	4607	0.382	0.000
hcp	0.843	−1771	4721	3.607	4736	−0.008	0.000
	0.900	−1661	3196	2.698	3204	−0.005	0.000
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Pd(fcc), Ru(hcp)

Table IVb. Partial quantities for Pd in the stable phases at 1800 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	−1327	250	0.876	250	0.000	0.915	1.017
	0.842	−1946	622	1.427	621	0.001	0.878	1.042
hcp	0.157	−1946	25648	15.330	25756	−0.060	0.878	5.590
	0.100	−5404	28960	19.091	29057	−0.054	0.697	6.969
	0.000	$-\infty$	35283	∞	35362	−0.044	0.000	10.620

Reference state: Pd(fcc)

Table IVc. Partial quantities for Ru in the stable phases at 1800 K.

Phase	x_{Ru}	ΔG_{Ru} [J/mol]	ΔH_{Ru} [J/mol]	ΔS_{Ru} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ru}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ru}}$ [J/(mol·K)]	a_{Ru}	γ_{Ru}
fcc	0.000	$-\infty$	37546	∞	33169	2.432	0.000	9.173
	0.100	−6040	32787	21.570	28421	2.426	0.668	6.679
	0.158	−1739	30273	17.784	25912	2.422	0.890	5.649
hcp	0.843	−1739	821	1.422	819	0.001	0.890	1.056
	0.900	−1245	333	0.877	332	0.001	0.920	1.022
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ru(hcp)

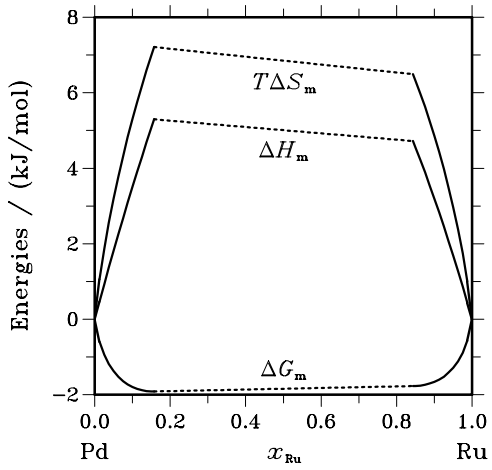

Fig. 4. Integral quantities of the stable phases at T=1800 K.

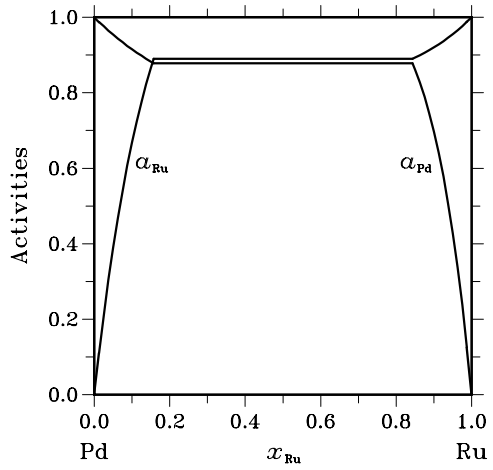

Fig. 5. Activities in the stable phases at T=1800 K.

References

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[93Tri] S.N. Tripathi, S.R. Bharadwaj, S.R. Dharwadkar: J. Phase Equilibria **14** (1993) 638–642.
[98Spe] P.J. Spencer: unpublished work, 1998.