Co – Pd (Cobalt – Palladium)

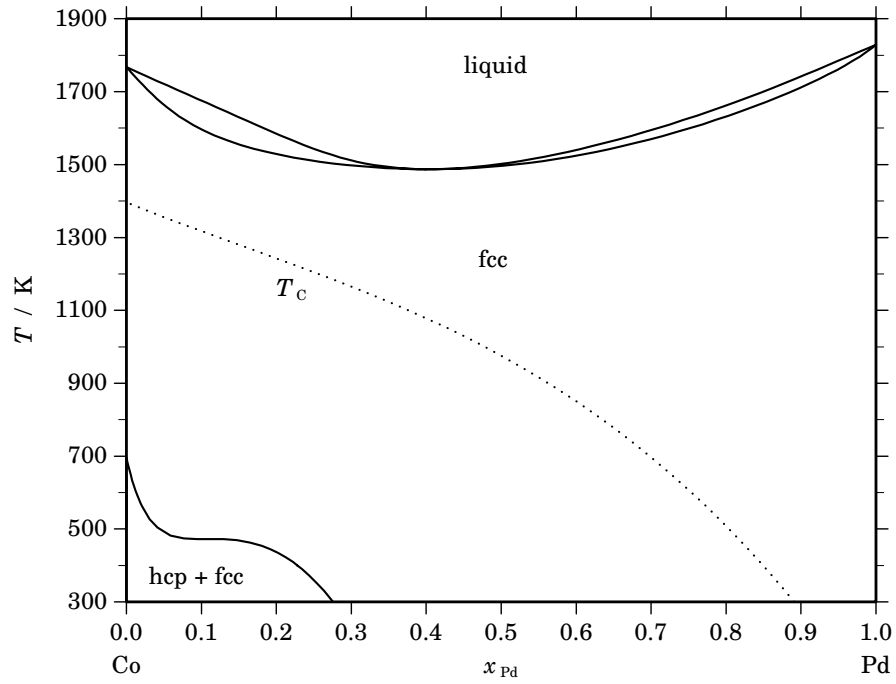

Fig. 1. Calculated phase diagram for the system Co-Pd.

The Co-Pd phase diagram is quite simple, consisting only of the melt, a broad fcc solution phase and at lower temperature the Co-based hcp phase. The present thermochemical optimisation of the Co-Pd system has been done by [2004Fra]. The phase diagram of the Co-Pd system and the T_C curve of fcc alloys have been determined essentially by Grube and Kästner [1936Gru]. The mixing enthalpy in the melt has been measured calorimetrically at 1873 K [1977Vat] and the excess properties of mixing have been determined by Knudsen mass spectrometry for the melt [1994Tom] as well as for solid solutions [1995Wan]. The activity of Co in fcc solid solutions has been measured in gas equilibration experiments [1965Sch] and by EMF methods [1965Sch, 1970Bid]. The experimental results of Vatolin and Kozlov [1977Vat] are in conflict with the results of Tomiska *et al.* [1994Tom]. [1977Vat] obtained slightly positive mixing enthalpies in the liquid whereas [1994Tom] found considerable negative mixing enthalpies. However, the same group investigated also the solid solutions [1995Wan] and both of their datasets are in accord with the phase diagram. Therefore, the results of [1977Vat] have been excluded from the present assessment. Another assessment for Co-Pd has been reported in [1999Gho] but the results of [1977Vat] have been adopted and the dataset predicts the presence of a miscibility gap in the fcc phase below 846 K at 17 at.% Pd which is not supported by experiments.

References

[1936Gru] G. Grube, H. Kästner: Z. Elektrochem. **42** (1936) 156–160.
[1965Sch] K. Schwerdtfeger, A. Muan: Acta Metall. **13** (1965) 509–515.
[1970Bid] L.R. Bidwell, F.E. Rizzo, J.V. Smith: Acta Metall. **18** (1970) 1013–1019.
[1977Vat] N.A. Vatolin, Yu.S. Kozlov: Russ. Metall., No. 1, (1977) 67–71.
[1994Tom] J. Tomiska, M.S. Belegratis, H. Wang: Ber. Bunsenges. Phys. Chem. **98** (1994) 1091–1095.
[1995Wan] H. Wang, M.S. Belegratis, J. Theiner, J. Tomiska: J. Alloys Comp. **220** (1995) 32–38.
[1999Gho] G. Ghosh, C. Kantner, G.B. Olsen: J. Phase Equilibria **20** (1999) 295–308.
[2004Fra] P. Franke, unpublished work, 2004.

Table I. Phases, structures and models.

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

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Pd}		$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons$ fcc	congruent	1487.2	0.405	0.405	−13821

Table IIIa. Integral quantities for the liquid phase at 1850 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	−6109	−3427	1.450	−1109	−1.253	0.000
0.200	−10037	−6430	1.949	−2339	−2.211	0.000
0.300	−12949	−8883	2.198	−3553	−2.881	0.000
0.400	−14965	−10660	2.327	−4613	−3.269	0.000
0.500	−16041	−11633	2.383	−5380	−3.380	0.000
0.600	−16068	−11675	2.375	−5716	−3.221	0.000
0.700	−14881	−10659	2.282	−5484	−2.797	0.000
0.800	−12244	−8460	2.045	−4546	−2.115	0.000
0.900	−7765	−4949	1.522	−2764	−1.181	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Co in the liquid phase at 1850 K.

x_{Co}	ΔG_{Co} [J/mol]	ΔH_{Co} [J/mol]	ΔS_{Co} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Co}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Co}}$ [J/(mol·K)]	a_{Co}	γ_{Co}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1537	−190	0.728	84	−0.148	0.905	1.005
0.800	−3282	−931	1.271	151	−0.585	0.808	1.010
0.700	−5561	−2475	1.668	−74	−1.298	0.697	0.995
0.600	−8725	−5077	1.972	−868	−2.275	0.567	0.945
0.500	−13168	−8990	2.258	−2506	−3.505	0.425	0.850
0.400	−19358	−14468	2.643	−5264	−4.975	0.284	0.710
0.300	−27937	−21764	3.337	−9417	−6.674	0.163	0.542
0.200	−39999	−31132	4.793	−15243	−8.589	0.074	0.371
0.100	−58434	−42826	8.437	−23016	−10.708	0.022	0.224
0.000	$-\infty$	−57100	∞	−33013	−13.020	0.000	0.117

Reference state: Co(liquid)

Table IIIc. Partial quantities for Pd in the liquid phase at 1850 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	$-\infty$	−35960	∞	−10023	−14.020	0.000	0.521
0.100	−47261	−32552	7.951	−11843	−11.194	0.046	0.463
0.200	−37056	−28426	4.665	−12300	−8.717	0.090	0.449
0.300	−30190	−23836	3.435	−11670	−6.576	0.140	0.468
0.400	−24324	−19034	2.859	−10229	−4.759	0.206	0.514
0.500	−18915	−14275	2.508	−8253	−3.255	0.292	0.585
0.600	−13875	−9812	2.196	−6018	−2.051	0.406	0.676
0.700	−9285	−5900	1.830	−3799	−1.136	0.547	0.781
0.800	−5305	−2791	1.359	−1872	−0.497	0.708	0.885
0.900	−2135	−740	0.754	−514	−0.122	0.870	0.967
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Pd(liquid)

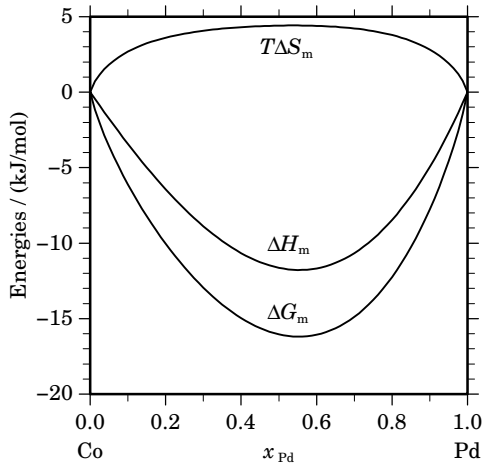

Fig. 2. Integral quantities of the liquid phase at T=1850 K.

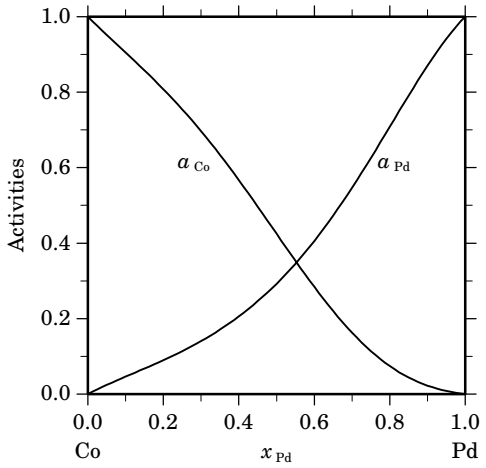

Fig. 3. Activities in the liquid phase at T=1850 K.

Table IVa. Integral quantities for the stable phases at 1473 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	−4321	−1872	1.662	−339	−1.041	−1.600
	0.200	−7231	−4160	2.085	−1102	−2.076	−2.216
	0.300	−9574	−6488	2.095	−2093	−2.984	−2.422
	0.400	−11364	−8544	1.915	−3122	−3.681	−2.425
	0.500	−12497	−10049	1.662	−4008	−4.101	−2.296
	0.600	−12814	−10738	1.409	−4572	−4.186	−2.043
	0.700	−12116	−10353	1.197	−4634	−3.882	−1.657
	0.800	−10144	−8623	1.032	−4016	−3.128	−1.155
	0.900	−6513	−5267	0.846	−2532	−1.857	−0.585
	1.000	0	0	0.000	0	0.000	0.000

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

Table IVb. Partial quantities for Co in the stable phases at 1473 K.

Phase	x_{Co}	ΔG_{Co} [J/mol]	ΔH_{Co} [J/mol]	ΔS_{Co} [J/(mol·K)]	G^{E}_{Co} [J/mol]	S^{E}_{Co} [J/(mol·K)]	a_{Co}	γ_{Co}
fcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1044	278	0.898	246	0.022	0.918	1.020
	0.800	−2018	567	1.755	715	−0.101	0.848	1.060
	0.700	−3339	235	2.427	1029	−0.539	0.761	1.088
	0.600	−5427	−1243	2.841	829	−1.407	0.642	1.070
	0.500	−8724	−4348	2.971	−235	−2.792	0.491	0.981
	0.400	−13735	−9563	2.832	−2513	−4.786	0.326	0.814
	0.300	−21113	−17431	2.500	−6368	−7.511	0.178	0.595
	0.200	−31891	−28584	2.245	−12180	−11.137	0.074	0.370
	0.100	−48529	−43656	3.308	−20329	−15.837	0.019	0.190
	0.000	−∞	−63128	∞	−31164	−21.700	0.000	0.079

Reference state: Co(fcc)

Table IVc. Partial quantities for Pd in the stable phases at 1473 K.

Phase	x_{Pd}	ΔG_{Pd} [J/mol]	ΔH_{Pd} [J/mol]	ΔS_{Pd} [J/(mol·K)]	G^{E}_{Pd} [J/mol]	S^{E}_{Pd} [J/(mol·K)]	a_{Pd}	γ_{Pd}
fcc	0.000	−∞	−15101	∞	−575	−9.862	0.000	0.954
	0.100	−33806	−21225	8.541	−5605	−10.604	0.063	0.633
	0.200	−28083	−23066	3.405	−8371	−9.976	0.101	0.505
	0.300	−24121	−22174	1.322	−9376	−8.688	0.140	0.465
	0.400	−20270	−19496	0.526	−9048	−7.093	0.191	0.478
	0.500	−16270	−15749	0.354	−7781	−5.409	0.265	0.530
	0.600	−12200	−11521	0.461	−5944	−3.786	0.369	0.615
	0.700	−8260	−7319	0.639	−3891	−2.327	0.509	0.728
	0.800	−4707	−3633	0.729	−1974	−1.126	0.681	0.851
	0.900	−1845	−1001	0.573	−554	−0.303	0.860	0.956
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Pd(fcc)

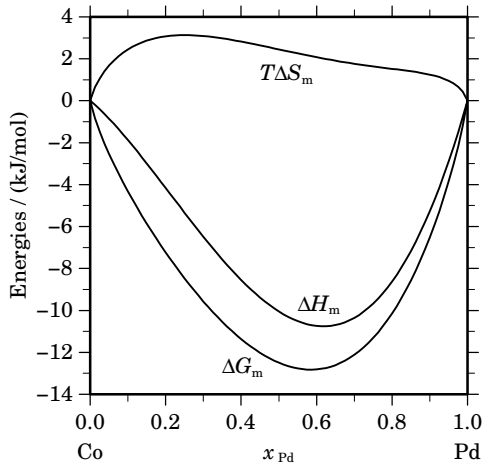

Fig. 4. Integral quantities of the stable phases at T=1473 K.

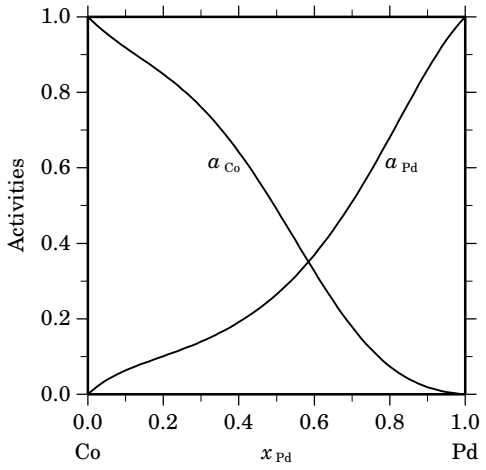

Fig. 5. Activities in the stable phases at T=1473 K.