C – Pd (Carbon – Palladium)

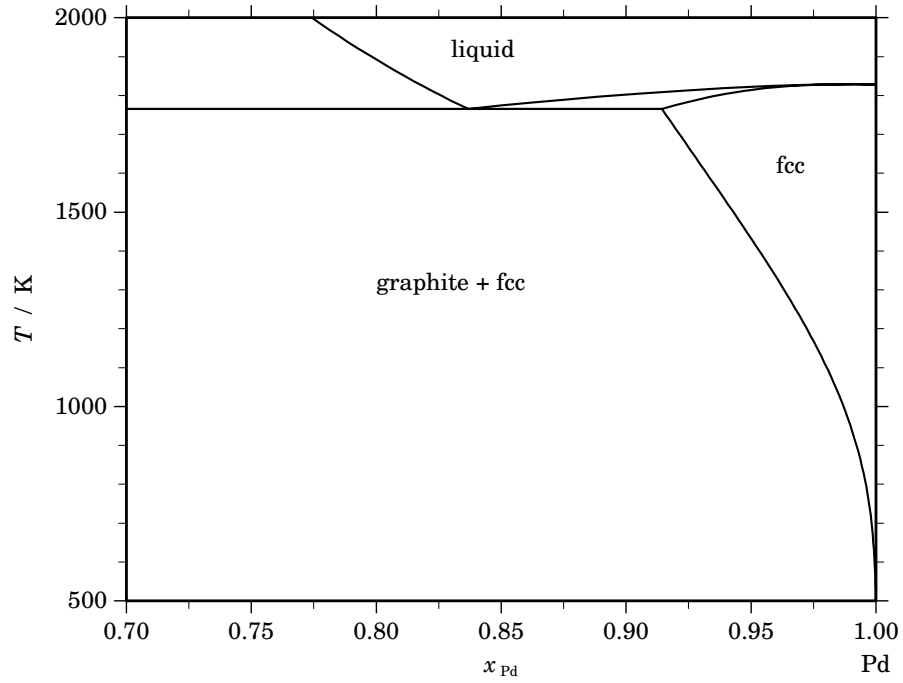

Fig. 1. Calculated phase diagram for the system C-Pd.

The C-Pd phase diagram is eutectic and includes the liquid phase, the fcc phase based on Pd and graphite [1990Mas]. Experimental data on the C-Pd system are limited and as the basis for the optimisation the phase diagram data given by [1996Mas, 2004Din] are used. The solid solubility of C in Pd was determined by Siller and Oates [1968Sil] in the temperature range 1173 to 1473 K. The eutectic reaction was studied by different authors using various methods. Nadler and Kempter [1960Nad] reported the eutectic temperature at about 1777 K, Bhatt and Venkataramani [1987Bha] at about 1783 K. Later investigations carried out by Dinsdale [2004Din] pointed out the temperature 1765 K, which has been used for the data assessment. The thermodynamic assessment of the C-Pd system was carried out by Korb [2004Kor]. The most recent experimental [2004Din] and the calculated invariant equilibria agree well.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(C,Pd)_1$
graphite	$A9$	C(graphite)	$hP4$	$P6_3/mmc$	GRAPHITE	C_1
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$Pd_1(C,\Box)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Pd}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ fcc	congruent	1828.8	0.989	0.989		−16895
liquid $\rightleftharpoons$ graphite + fcc	eutectic	1765.2	0.837	0.000	0.914	−19546

Table IIIa. Integral quantities for the liquid phase at 1900 K.

x_{Pd}	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)]
0.798	−2452	10441	6.786	5494	2.604	0.000
0.800	−2458	10367	6.750	5447	2.589	0.000
0.900	−2205	5990	4.313	2930	1.611	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: C(graphite), Pd(liquid)

Table IIIb. Partial quantities for C in the liquid phase at 1900 K.

x_{C}	ΔG_{C} [J/mol]	ΔH_{C} [J/mol]	ΔS_{C} [J/(mol·K)]	$G_{\mathrm{C}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{C}}^{\mathrm{E}}$ [J/(mol·K)]	a_{C}	γ_{C}
0.202	0	41741	21.969	25276	8.666	1.000	4.953
0.200	−163	41820	22.096	25263	8.714	0.990	4.949
0.100	−9681	51016	31.946	26694	12.801	0.542	5.418
0.000	$-\infty$	71579	∞	33028	20.290	0.000	8.090

Reference state: C(graphite)

Table IIIc. Partial quantities for Pd in the liquid phase at 1900 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}
0.798	−3073	2523	2.945	490	1.070	0.823	1.031
0.800	−3032	2504	2.913	493	1.058	0.825	1.032
0.900	−1375	987	1.243	290	0.367	0.917	1.018
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Pd(liquid)

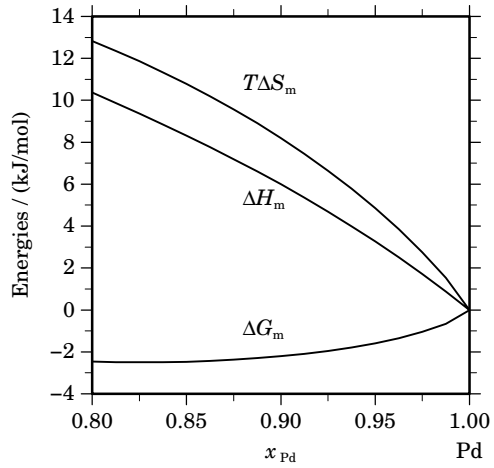

Fig. 2. Integral quantities of the liquid phase at T=1900 K.

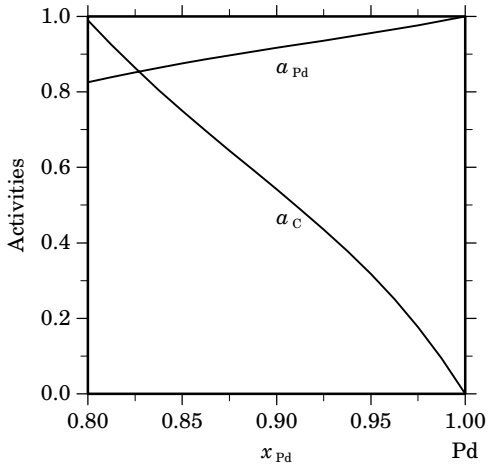

Fig. 3. Activities in the liquid phase at T=1900 K.

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