Ni – Pd (Nickel – Palladium)

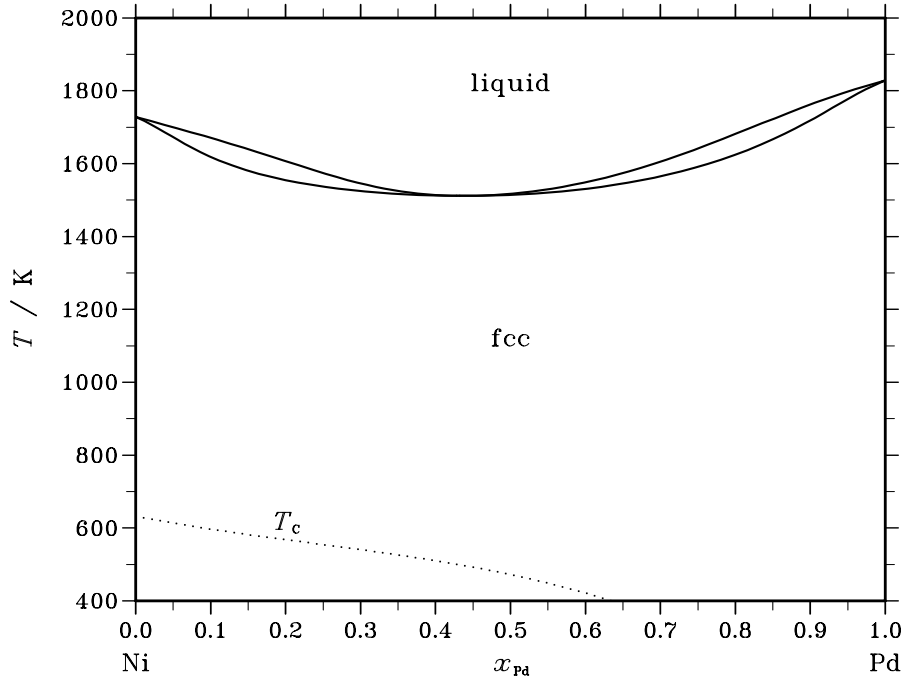

Fig. 1. Calculated phase diagram for the system Ni-Pd.

The Ni-Pd system displays a complete range of liquid and fcc solid solutions. The only feature of the system at lower temperatures is the magnetic transition, which extends across the system from pure Ni at a temperature of 627.5 K to the approximate composition of 76 at.% Pd at room temperature [91Nas]. The assessed thermodynamic parameters for the system reported by Ghosh *et al.* [99Gho] reproduce the liquidus/solidus boundaries well. The calculated enthalpy of mixing and the activity of Pd in the fcc solution phase display moderate negative departures from ideality, while the Ni activity shows small positive departure from ideality in Ni-rich alloys and slight negative departure for Pd-rich concentrations. The component activities in the liquid phase are analogous to those in the solid, whereas the calculated enthalpies of mixing are positive.

Table I. Phases, structures and models.

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

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Pd}		$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ fcc	congruent	1511.5	0.440	0.440	−21975

Table IIIa. Integral quantities for the liquid phase at 1873 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)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−6209	523	3.594	−1146	0.891	0.000
0.200	−10385	1176	6.172	−2592	2.012	0.000
0.300	−13522	1769	8.164	−4009	3.085	0.000
0.400	−15616	2168	9.495	−5135	3.899	0.000
0.500	−16576	2295	10.075	−5782	4.312	0.000
0.600	−16308	2127	9.843	−5827	4.247	0.000
0.700	−14733	1698	8.772	−5220	3.693	0.000
0.800	−11769	1094	6.868	−3976	2.707	0.000
0.900	−7247	462	4.116	−2184	1.413	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Ni in the liquid phase at 1873 K.

x_{Ni}	ΔG_{Ni} [J/mol]	ΔH_{Ni} [J/mol]	ΔS_{Ni} [J/(mol·K)]	$G_{\mathrm{Ni}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Ni}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Ni}	γ_{Ni}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1430	−101	0.710	210	−0.166	0.912	1.014
0.800	−3107	−124	1.593	368	−0.263	0.819	1.024
0.700	−5636	227	3.131	−82	0.165	0.696	0.995
0.600	−9440	1082	5.618	−1485	1.370	0.545	0.909
0.500	−14774	2401	9.170	−3980	3.407	0.387	0.774
0.400	−21767	3981	13.747	−7497	6.128	0.247	0.618
0.300	−30508	5448	19.197	−11759	9.187	0.141	0.470
0.200	−41343	6266	25.419	−16279	12.037	0.070	0.352
0.100	−56223	5728	33.076	−20365	13.931	0.027	0.270
0.000	$-\infty$	2962	∞	−23113	13.921	0.000	0.227

Reference state: Ni(liquid)

Table IIIc. Partial quantities for Pd in the liquid phase at 1873 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}
0.000	$-\infty$	3810	∞	−8697	6.678	0.000	0.572
0.100	−49217	6140	29.555	−13358	10.410	0.042	0.424
0.200	−39498	6375	24.491	−14434	11.110	0.079	0.396
0.300	−31921	5365	19.907	−13172	9.897	0.129	0.429
0.400	−24881	3797	15.311	−10611	7.693	0.202	0.506
0.500	−18378	2189	10.981	−7584	5.218	0.307	0.614
0.600	−12669	892	7.240	−4714	2.993	0.443	0.739
0.700	−7972	90	4.304	−2417	1.339	0.599	0.856
0.800	−4376	−199	2.230	−901	0.375	0.755	0.944
0.900	−1805	−123	0.898	−164	0.022	0.891	0.989
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Pd(liquid)

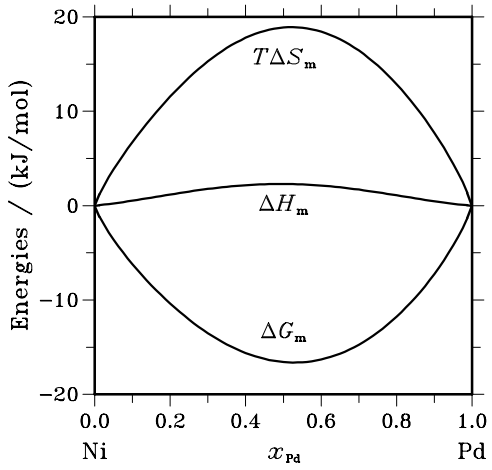

Fig. 2. Integral quantities of the liquid phase at T=1873 K.

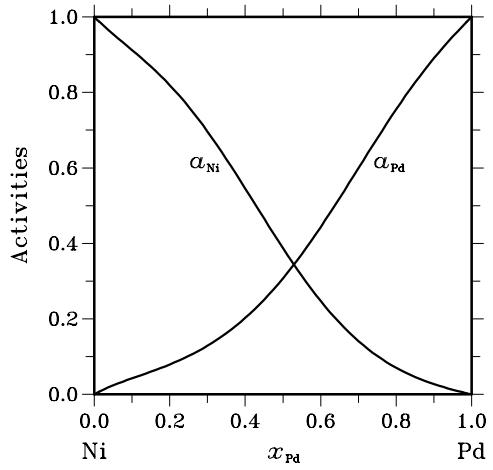

Fig. 3. Activities in the liquid phase at T=1873 K.

Table IVa. Integral quantities for the stable phases at 1273 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	−3572	−350	2.531	−131	−0.172	−0.014
	0.200	−5847	−1332	3.546	−550	−0.615	−0.020
	0.300	−7579	−2477	4.008	−1113	−1.071	−0.021
	0.400	−8815	−3432	4.229	−1692	−1.367	−0.023
	0.500	−9507	−3959	4.358	−2170	−1.405	−0.024
	0.600	−9570	−3938	4.425	−2447	−1.171	−0.025
	0.700	−8901	−3363	4.350	−2435	−0.729	−0.023
	0.800	−7357	−2346	3.936	−2061	−0.224	−0.017
	0.900	−4705	−1112	2.823	−1265	0.120	−0.009
	1.000	0	0	0.000	0	0.000	0.000

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

Table IVb. Partial quantities for Ni in the stable phases at 1273 K.

Phase	x_{Ni}	ΔG_{Ni} [J/mol]	ΔH_{Ni} [J/mol]	ΔS_{Ni} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ni}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ni}}$ [J/(mol·K)]	a_{Ni}	γ_{Ni}
fcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−946	404	1.061	169	0.185	0.914	1.016
	0.800	−1884	932	2.212	478	0.357	0.837	1.046
	0.700	−3115	819	3.090	660	0.125	0.745	1.064
	0.600	−4913	−350	3.585	494	−0.663	0.629	1.048
	0.500	−7540	−2642	3.848	−203	−1.915	0.490	0.981
	0.400	−11270	−5777	4.315	−1572	−3.304	0.345	0.862
	0.300	−16452	−9130	5.752	−3709	−4.258	0.211	0.704
	0.200	−23708	−11731	9.409	−6673	−3.973	0.106	0.532
	0.100	−34852	−12268	17.741	−10480	−1.404	0.037	0.372
	0.000	$-\infty$	−9076	∞	−15105	4.736	0.000	0.240

Reference state: Ni(fcc)

Table IVc. Partial quantities for Pd in the stable phases at 1273 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	0.000	$-\infty$	1518	∞	640	0.690	0.000	1.062
	0.100	−27204	−7138	15.762	−2832	−3.383	0.077	0.765
	0.200	−21696	−10390	8.881	−4661	−4.501	0.129	0.644
	0.300	−17996	−10170	6.148	−5252	−3.863	0.183	0.609
	0.400	−14669	−8055	5.195	−4970	−2.423	0.250	0.625
	0.500	−11473	−5276	4.868	−4137	−0.895	0.338	0.676
	0.600	−8437	−2712	4.498	−3031	0.251	0.451	0.751
	0.700	−5665	−892	3.749	−1889	0.783	0.586	0.837
	0.800	−3270	0	2.568	−908	0.713	0.734	0.918
	0.900	−1356	128	1.166	−241	0.289	0.880	0.978
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Pd(fcc)

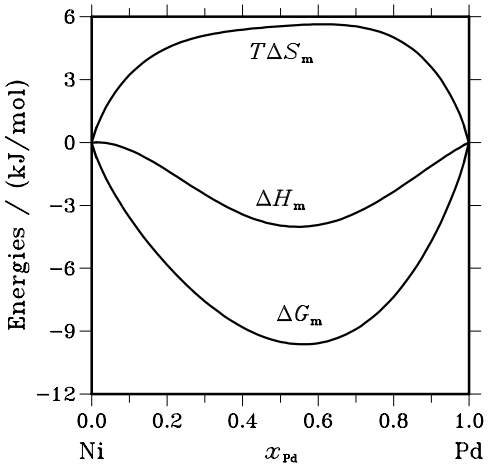

Fig. 4. Integral quantities of the stable phases at T=1273 K.

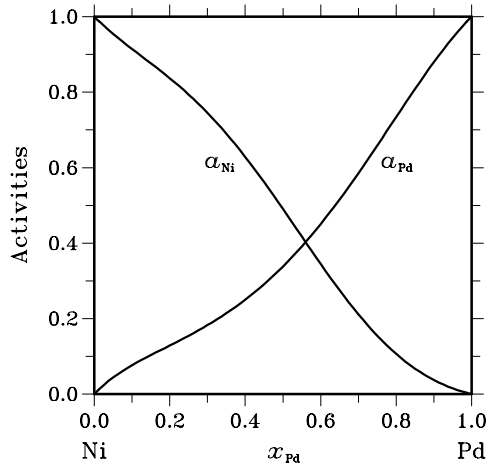

Fig. 5. Activities in the stable phases at T=1273 K.

References

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[99Gho] G. Ghosh, C. Kantner, G.B. Olson: J. Phase Equilibria **20** (1999) 295–308.