Eu – Pd (Europium – Palladium)

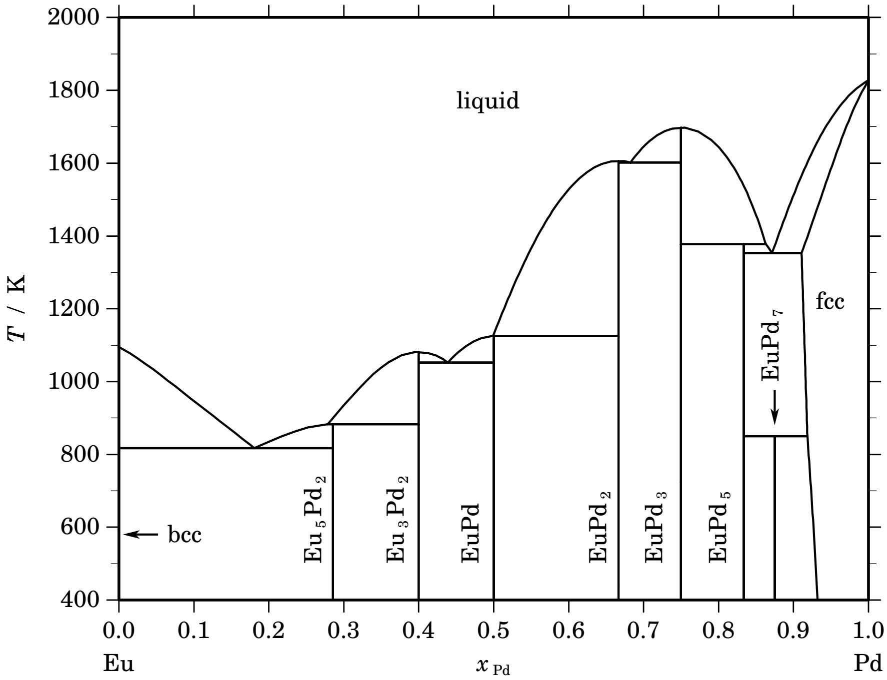

Fig. 1. Calculated phase diagram for the system Eu-Pd.

Intermetallic compounds of palladium with rare earth metals are of interest due to their potential use in hydrogen diffusion membranes for purification and isotope enrichment. A review of the Eu-Pd system and a thermodynamic assessment has been given by [2001Du]. The optimisation is based on data on the the phase diagram which have been reported in [1974Ian] for equilibria with the liquid across the whole composition range and in addition results for equilibria involving the compound $EuPd_7$ which have been reported by [1990Tak]. No thermodynamic data have been available for the melt or the intermetallic compounds. Due to the close chemical relationships among the rare earth metals, [2001Du] have considered in the optimisation of the intermetallic compounds the corresponding enthalpies of formation in the systems Gd-Pd and Pd-Sm which have been available in the literature. The dataset should not be used at too high temperatures because an artificial inverse miscibility gap opens in the liquid above 3550 K.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Eu,Pd)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Eu,Pd)_1$
Eu_5Pd_2	$\cdots$	Mn_5C_2	$mC28$	$C2/c$	EU5PD2	Eu_5Pd_2
Eu_3Pd_2	$\cdots$	Er_3Ni_2	$hR15$	$R\overline{3}$	EU3PD2	Eu_3Pd_2
EuPd	$B33$	CrB	$oC8$	$Cmcm$	EUPD	Eu_1Pd_1
$EuPd_2$	$C15$	$MgCu_2$	$cF24$	$Fd\overline{3}m$	EUPD2	Eu_1Pd_2
$EuPd_3$	$L1_2$	$AuCu_3$	$cP4$	$Pm\overline{3}m$	EUPD3	Eu_1Pd_3
$EuPd_5$	$\cdots$	$\cdots$	$o*72$	$\cdots$	EUPD5	Eu_1Pd_5
$EuPd_7$	$\cdots$	$\cdots$	$c**$	$\cdots$	EUPD7	Eu_1Pd_7
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Eu,Pd)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Pd}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid ⇌ $EuPd_3$	congruent	1697.8	0.750	0.750		−33450
liquid ⇌ $EuPd_2$	congruent	1606.7	0.667	0.667		−36671
liquid ⇌ $EuPd_2$ + $EuPd_3$	eutectic	1602.1	0.683	0.667	0.750	−35350
$EuPd_3$ + liquid ⇌ $EuPd_5$	peritectic	1377.4	0.750	0.863	0.833	−10688
liquid ⇌ $EuPd_5$ + fcc	eutectic	1353.1	0.871	0.833	0.911	−12830
liquid + $EuPd_2$ ⇌ EuPd	peritectic	1125.2	0.499	0.667	0.500	−18832
liquid ⇌ Eu_3Pd_2	congruent	1081.6	0.400	0.400		−17263
liquid ⇌ Eu_3Pd_2 + EuPd	eutectic	1052.4	0.439	0.400	0.500	−17403
liquid + Eu_3Pd_2 ⇌ Eu_5Pd_2	peritectic	882.9	0.278	0.400	0.286	−17452
$EuPd_5$ + fcc ⇌ $EuPd_7$	peritectoid	850.1	0.833	0.918	0.875	−1004
liquid ⇌ bcc + Eu_5Pd_2	eutectic	817.4	0.181	0.000	0.286	−19097

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)]	$G^{\mathrm{E}}_{\mathrm{m}}$ [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	−40633	−7879	17.239	−35497	14.536	0.000
0.200	−70223	−21784	25.494	−62318	21.334	0.000
0.300	−90408	−38799	27.163	−80758	22.084	0.000
0.400	−101744	−56007	24.072	−91112	18.477	0.000
0.500	−104627	−70492	17.966	−93677	12.203	0.000
0.600	−99380	−79337	10.548	−88748	4.953	0.000
0.700	−86270	−79627	3.496	−76620	−1.583	0.000
0.800	−65494	−68445	−1.554	−57589	−5.714	0.000
0.900	−37086	−42875	−3.047	−31950	−5.750	0.000
1.000	0	0	0.000	0	0.000	0.000

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

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

x_{Eu}	ΔG_{Eu} [J/mol]	ΔH_{Eu} [J/mol]	ΔS_{Eu} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Eu}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Eu}}$ [J/(mol·K)]	a_{Eu}	γ_{Eu}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−6052	3499	5.027	−4388	4.151	0.682	0.757
0.800	−20681	10108	16.205	−17156	14.349	0.270	0.338
0.700	−43349	13994	30.180	−37714	27.215	0.064	0.092
0.600	−73541	9324	43.613	−65471	39.366	0.010	0.016
0.500	−110785	−9735	53.184	−99835	47.421	0.001	0.002
0.400	−154691	−49014	55.619	−140215	48.001	0.000	0.000
0.300	−205041	−114347	47.734	−186021	37.723	0.000	0.000
0.200	−262085	−211566	26.589	−236660	13.207	0.000	0.000
0.100	−327917	−346505	−9.783	−291542	−28.928	0.000	0.000
0.000	$-\infty$	−524995	∞	−350075	−92.063	0.000	0.000

Reference state: Eu(liquid)

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)]	$G^{\mathrm{E}}_{\mathrm{Pd}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Pd}}$ [J/(mol·K)]	a_{Pd}	γ_{Pd}
0.000	$-\infty$	−38939	∞	−399340	189.685	0.000	0.000
0.100	−351860	−110282	127.147	−315485	108.002	0.000	0.000
0.200	−268391	−149351	62.653	−242966	49.271	0.000	0.000
0.300	−200213	−161981	20.122	−181193	10.112	0.000	0.000
0.400	−144049	−154002	−5.238	−129574	−12.857	0.000	0.000
0.500	−98469	−131249	−17.253	−87519	−23.016	0.002	0.004
0.600	−62505	−99553	−19.499	−54436	−23.746	0.019	0.032
0.700	−35368	−64748	−15.463	−29733	−18.429	0.107	0.152
0.800	−16346	−32665	−8.589	−12821	−10.444	0.355	0.444
0.900	−4771	−9138	−2.299	−3107	−3.175	0.739	0.821
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Pd(liquid)

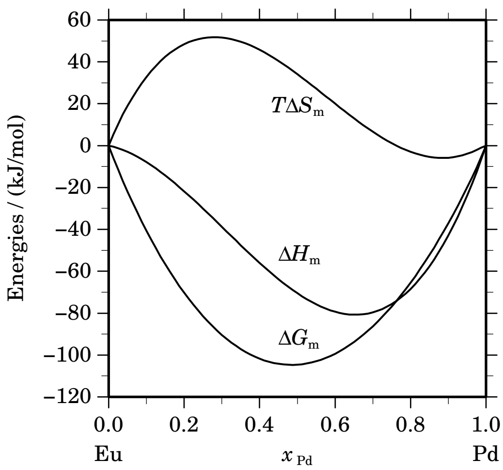

Fig. 2. Integral quantities of the liquid phase at T=1900 K.

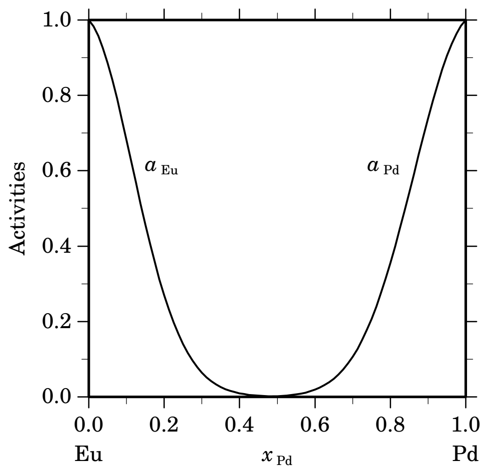

Fig. 3. Activities in the liquid phase at T=1900 K.

Table IV. Standard reaction quantities at 298.15 K for the compounds per mole of atoms.

Compound	x_{Pd}	$\Delta_{\mathrm{f}}G^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}H^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}S^{\circ}$ / (J/(mol·K))	$\Delta_{\mathrm{f}}C^{\circ}_{P}$ / (J/(mol·K))
Eu_5Pd_2	0.286	−48926	−44766	13.953	0.000
Eu_3Pd_2	0.400	−67389	−62722	15.652	0.000
Eu_1Pd_1	0.500	−81068	−78545	8.461	0.000
Eu_1Pd_2	0.667	−101882	−104636	−9.236	0.000
Eu_1Pd_3	0.750	−92103	−95334	−10.836	0.000
Eu_1Pd_5	0.833	−63717	−65892	−7.294	0.000
Eu_1Pd_7	0.875	−49326	−51176	−6.207	0.000

References

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