Cd – Y (Cadmium – Yttrium)

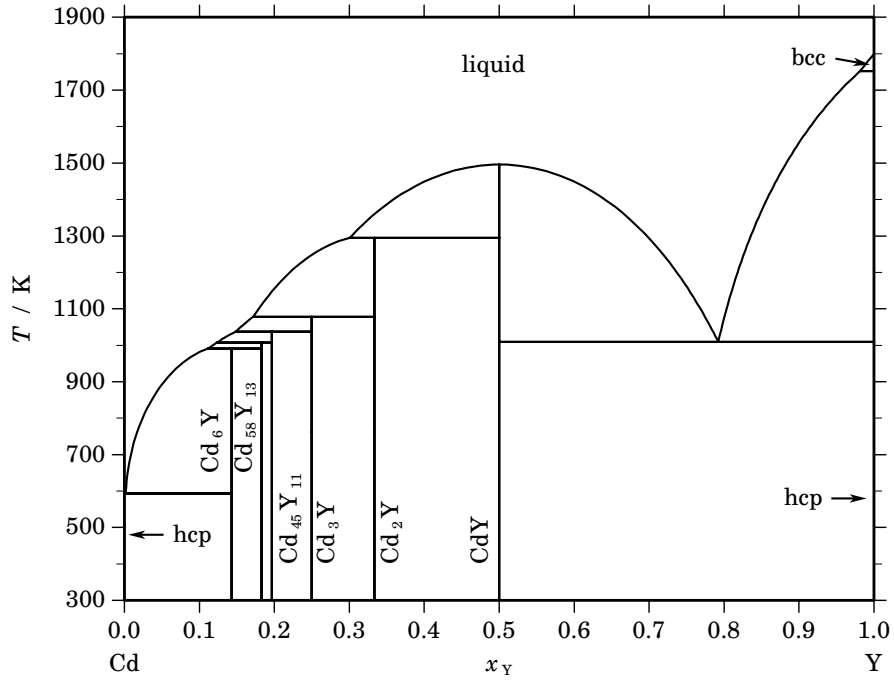

Fig. 1. Calculated phase diagram for the system Cd-Y.

The design of pyrometallurgically reprocessing for recycling nuclear reactor fuels needs thermodynamic information on multicomponent systems of actinides and rare earths solute with cadmium.
The experimental data for the Cd-Y system are relatively limited. There are no information on the mutual solubility of cadmium and yttrium in the solid state. Only the partial phase diagram covering the range 63 to 100 at.% Cd was reported by [1969Ryb]. Phase boundaries were determined by differential thermal analysis, metallography and x-ray diffraction methods. The Cd-richest compound is Cd_6Y which decomposes peritectically. [1988Gsc] reviewed this system. [1995Sak] determined the activity of yttrium using electromotive force measurements. The thermodynamic assessment of the Cd-Y system is from [2001Kur]. The liquid phase was described by a substitutional solution model using the Redlich-Kister equation. The intermetallic compounds Cd_6Y, $Cd_{58}Y_{13}$, $Cd_{45}Y_{11}$, Cd_3Y, Cd_2Y and CdY are treated as stoichiometric compounds. The calculated phase diagram presents slight differences with experimental data. These differences may be due to a lack of experimental solubility data. The activities are well reproduced.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Cd,Y)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Cd,Y)_1$
Cd_6Y	$\cdots$	Cd_6Y	$cI168$	$Im\overline{3}$	CD6Y	Cd_6Y_1
$Cd_{58}Y_{13}$	$\cdots$	$Pu_{13}Zn_{58}$	$hp142$	$P6_3/mmc$	CD58Y13	$Cd_{58}Y_{13}$
$Cd_{45}Y_{11}$	$\cdots$	$Cd_{45}Sm_{11}$	$cF448$	$F\overline{4}3m$	CD45Y11	$Cd_{45}Y_{11}$
Cd_3Y	$\cdots$	Cd_3Er	$oC16$	$Cmcm$	CD3Y	Cd_3Y_1
Cd_2Y	$C6$	CdI_2	$hP3$	$P\overline{3}m1$	CD2Y	Cd_2Y_1
CdY	$B2$	CsCl	$cP2$	$Pm\overline{3}m$	CDY	Cd_1Y_1
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	Y_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Y}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid + bcc $\rightleftharpoons$ hcp	peritectic	1752.0	0.981	1.000	1.000	−4995
liquid $\rightleftharpoons$ CdY	congruent	1496.0	0.500	0.500		−29146
liquid + CdY $\rightleftharpoons$ Cd_2Y	peritectic	1294.9	0.301	0.500	0.333	−12898
liquid + Cd_2Y $\rightleftharpoons$ Cd_3Y	peritectic	1078.2	0.172	0.333	0.250	−6733
liquid + Cd_3Y $\rightleftharpoons$ $Cd_{45}Y_{11}$	peritectic	1036.9	0.148	0.250	0.196	−6945
liquid $\rightleftharpoons$ CdY + hcp	eutectic	1009.5	0.792	0.500	1.000	−9786
liquid + $Cd_{45}Y_{11}$ $\rightleftharpoons$ $Cd_{58}Y_{13}$	peritectic	1007.6	0.124	0.196	0.183	−2237
liquid + $Cd_{58}Y_{13}$ $\rightleftharpoons$ Cd_6Y	peritectic	990.7	0.112	0.183	0.143	−6087
liquid $\rightleftharpoons$ hcp + Cd_6Y	eutectic	593.4	0.002	0.000	0.143	−6219

Table IIIa. Integral quantities for the liquid phase at 1800 K.

x_{Y}	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	−9464	−11889	−1.347	−4599	−4.050	0.000
0.200	−15665	−21136	−3.039	−8176	−7.200	0.000
0.300	−19873	−27741	−4.371	−10731	−9.450	0.000
0.400	−22336	−31704	−5.204	−12264	−10.800	0.000
0.500	−23149	−33025	−5.487	−12775	−11.250	0.000
0.600	−22336	−31704	−5.204	−12264	−10.800	0.000
0.700	−19873	−27741	−4.371	−10731	−9.450	0.000
0.800	−15665	−21136	−3.039	−8176	−7.200	0.000
0.900	−9464	−11889	−1.347	−4599	−4.050	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Cd(liquid), Y(liquid)

Table IIIb. Partial quantities for Cd in the liquid phase at 1800 K.

x_{Cd}	ΔG_{Cd} [J/mol]	ΔH_{Cd} [J/mol]	ΔS_{Cd} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Cd}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Cd}}$ [J/(mol·K)]	a_{Cd}	γ_{Cd}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2088	−1321	0.426	−511	−0.450	0.870	0.966
0.800	−5384	−5284	0.055	−2044	−1.800	0.698	0.872
0.700	−9937	−11889	−1.084	−4599	−4.050	0.515	0.735
0.600	−15821	−21136	−2.953	−8176	−7.200	0.347	0.579
0.500	−23149	−33025	−5.487	−12775	−11.250	0.213	0.426
0.400	−32109	−47556	−8.581	−18396	−16.200	0.117	0.293
0.300	−43058	−64729	−12.040	−25039	−22.050	0.056	0.188
0.200	−56791	−84544	−15.418	−32704	−28.800	0.022	0.112
0.100	−75852	−107001	−17.305	−41391	−36.450	0.006	0.063
0.000	$-\infty$	−132100	∞	−51100	−45.000	0.000	0.033

Reference state: Cd(liquid)

Table IIIc. Partial quantities for Y in the liquid phase at 1800 K.

x_Y	ΔG_Y [J/mol]	ΔH_Y [J/mol]	ΔS_Y [J/(mol·K)]	G_Y^E [J/mol]	S_Y^E [J/(mol·K)]	a_Y	γ_Y
0.000	$-\infty$	−132100	∞	−51100	−45.000	0.000	0.033
0.100	−75852	−107001	−17.305	−41391	−36.450	0.006	0.063
0.200	−56791	−84544	−15.418	−32704	−28.800	0.022	0.112
0.300	−43058	−64729	−12.040	−25039	−22.050	0.056	0.188
0.400	−32109	−47556	−8.581	−18396	−16.200	0.117	0.293
0.500	−23149	−33025	−5.487	−12775	−11.250	0.213	0.426
0.600	−15821	−21136	−2.953	−8176	−7.200	0.347	0.579
0.700	−9937	−11889	−1.084	−4599	−4.050	0.515	0.735
0.800	−5384	−5284	0.055	−2044	−1.800	0.698	0.872
0.900	−2088	−1321	0.426	−511	−0.450	0.870	0.966
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Y(liquid)

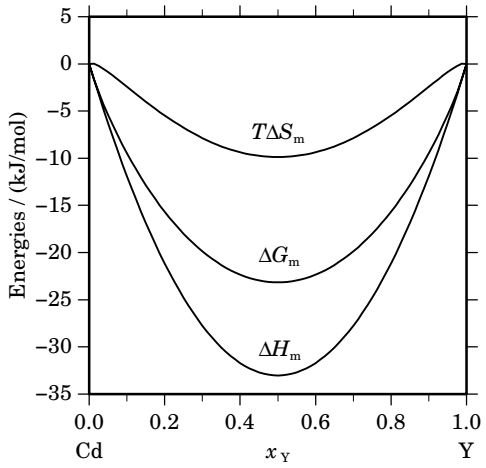

Fig. 2. Integral quantities of the liquid phase at T=1800 K.

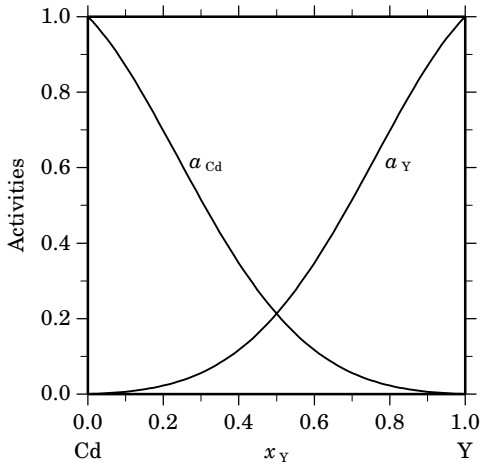

Fig. 3. Activities in the liquid phase at T=1800 K.

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

Compound	x_Y	$\Delta_f G^\circ$ / (J/mol)	$\Delta_f H^\circ$ / (J/mol)	$\Delta_f S^\circ$ / (J/(mol·K))	$\Delta_f C_P^\circ$ / (J/(mol·K))
Cd_6Y_1	0.143	−19674	−20876	−4.031	0.000
$Cd_{58}Y_{13}$	0.183	−23837	−25529	−5.673	0.000
$Cd_{45}Y_{11}$	0.196	−25033	−26825	−6.011	0.000
Cd_3Y_1	0.250	−29083	−31104	−6.777	0.000
Cd_2Y_1	0.333	−35289	−37814	−8.469	0.000
Cd_1Y_1	0.500	−47210	−51936	−15.852	0.000

References

[1969Ryb] E. Ryba, P.K. Kejriwal, R. Elmendorf: J. Less-Common Met. **18** (1969) 419–422.
[1988Gsc] K.A. Gschneidner Jr., F.W. Calderwood: Bull. Alloy Phase Diagrams **9** (1988) 139–140.
[1995Sak] Y. Sakamura, T. Inoue, T.S. Storvick, L.F. Grantham: Proc. Int. Conf. Evaluation of Emerging Nuclear Fuel Cycle Systems, Global 95, Versailles, France, Sept. 11-14, vol. 2, 1185–1192 (1995).
[2001Kur] M. Kurata, Y. Sakamura: J. Phase Equilibria **22** (2001) 232–240.