Y – Zr (Yttrium – Zirconium)

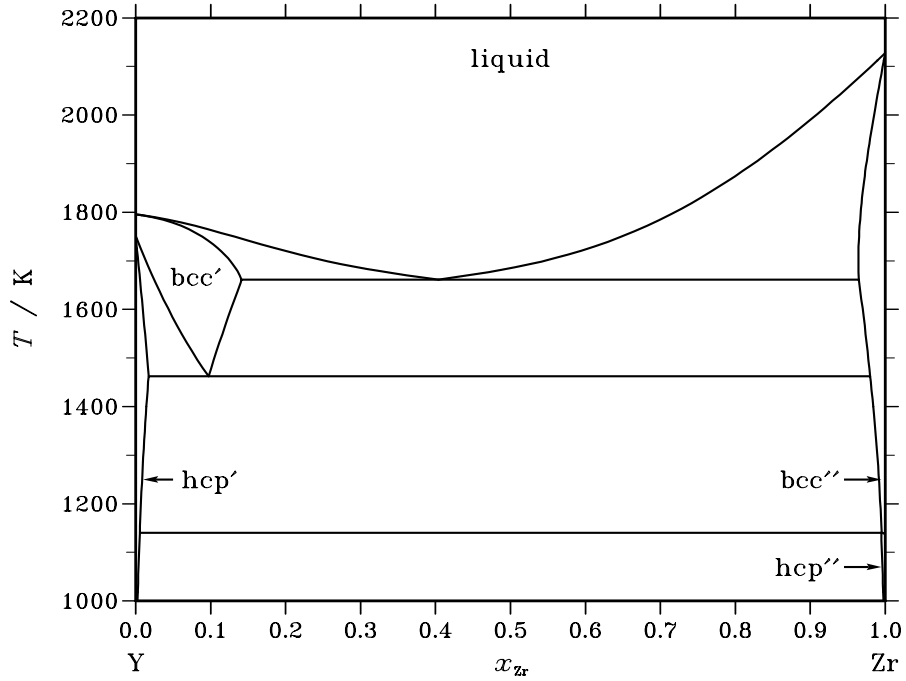

Fig. 1. Calculated phase diagram for the system Y-Zr.

There is complete solubility in the liquid and the solubility of Zr in bcc-Y is large. At higher Zr content there is a miscibility gap between the bcc forms of Y and Zr. At lower temperatures there is also a miscibility gap between the hcp forms of Y and Zr. A thermodynamic assessment of the Y-Zr system has been reported in [97Fla].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Y,Zr)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Y,Zr)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Y,Zr)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Zr}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ bcc′ + bcc′′	eutectic	1660.9	0.404	0.141	0.965	−15906
bcc′ $\rightleftharpoons$ hcp′ + bcc′′	monotectoid	1462.3	0.097	0.017	0.980	−7304
hcp′ + bcc′′ $\rightleftharpoons$ hcp′′	peritectoid	1140.4	0.005	0.995	0.995	−4076

Table IIIa. Integral quantities for the liquid phase at 2200 K.

x_{Zr}	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	−3570	2376	2.703	2376	0.000	0.000
0.200	−5025	4128	4.161	4128	0.000	0.000
0.300	−5882	5292	5.079	5292	0.000	0.000
0.400	−6407	5904	5.596	5904	0.000	0.000
0.500	−6679	6000	5.763	6000	0.000	0.000
0.600	−6695	5616	5.596	5616	0.000	0.000
0.700	−6386	4788	5.079	4788	0.000	0.000
0.800	−5601	3552	4.161	3552	0.000	0.000
0.900	−4002	1944	2.703	1944	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Y in the liquid phase at 2200 K.

x_{Y}	ΔG_{Y} [J/mol]	ΔH_{Y} [J/mol]	ΔS_{Y} [J/(mol·K)]	$G_{\mathrm{Y}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Y}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Y}	γ_{Y}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1609	318	0.876	318	0.000	0.916	1.018
0.800	−2858	1224	1.855	1224	0.000	0.855	1.069
0.700	−3878	2646	2.966	2646	0.000	0.809	1.156
0.600	−4832	4512	4.247	4512	0.000	0.768	1.280
0.500	−5929	6750	5.763	6750	0.000	0.723	1.446
0.400	−7473	9288	7.619	9288	0.000	0.665	1.662
0.300	−9969	12054	10.010	12054	0.000	0.580	1.933
0.200	−14464	14976	13.382	14976	0.000	0.454	2.268
0.100	−24137	17982	19.145	17982	0.000	0.267	2.673
0.000	$-\infty$	21000	∞	21000	0.000	0.000	3.152

Reference state: Y(liquid)

Table IIIc. Partial quantities for Zr in the liquid phase at 2200 K.

x_{Zr}	ΔG_{Zr} [J/mol]	ΔH_{Zr} [J/mol]	ΔS_{Zr} [J/(mol·K)]	$G_{\mathrm{Zr}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Zr}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Zr}	γ_{Zr}
0.000	$-\infty$	27000	∞	27000	0.000	0.000	4.376
0.100	−21221	20898	19.145	20898	0.000	0.313	3.135
0.200	−13696	15744	13.382	15744	0.000	0.473	2.365
0.300	−10557	11466	10.010	11466	0.000	0.562	1.872
0.400	−8769	7992	7.619	7992	0.000	0.619	1.548
0.500	−7429	5250	5.763	5250	0.000	0.666	1.332
0.600	−6176	3168	4.247	3168	0.000	0.713	1.189
0.700	−4850	1674	2.966	1674	0.000	0.767	1.096
0.800	−3386	696	1.855	696	0.000	0.831	1.039
0.900	−1765	162	0.876	162	0.000	0.908	1.009
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Zr(liquid)

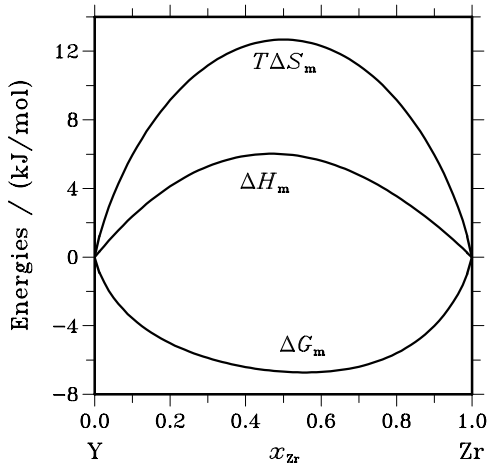

Fig. 2. Integral quantities of the liquid phase at T=2200 K.

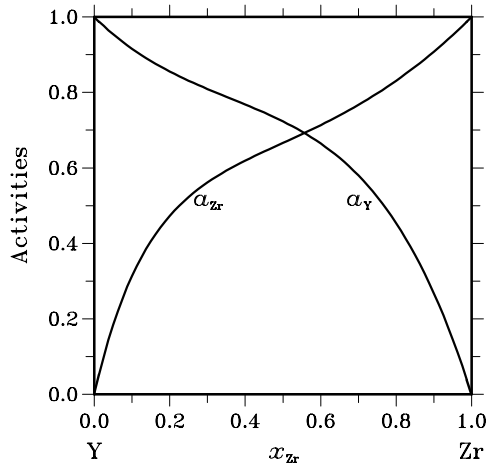

Fig. 3. Activities in the liquid phase at T=2200 K.

References

[97Fla] H. Flandorfer, J. Gröbner, A. Stamou, N. Hassiotis, A. Saccone, P. Rogl, R. Wouters, H. Seifert, D. Maccio, R. Ferro, G. Haidemenopoulos, L. Delaey, G. Effenberg: Z. Metallkd. **88** (1997) 529–538.