Gd – Zr (Gadolinium – Zirconium)

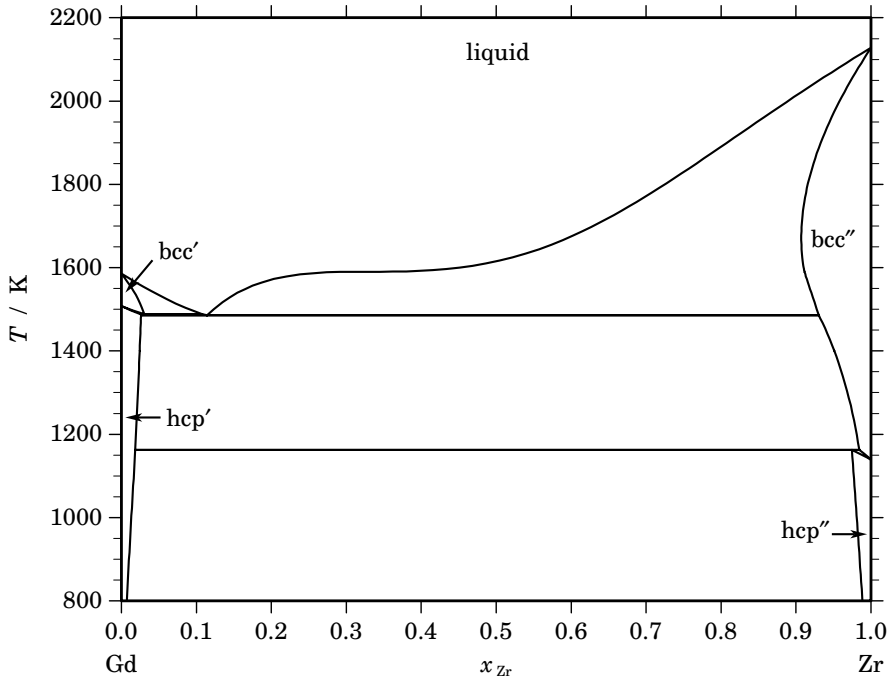

Fig. 1. Calculated phase diagram for the system Gd-Zr.

The interest in the Gd-Zr system is related to ternary and higher systems, e.g.. with iron, where intermetallic compounds with interesting magnetic properties are found. The presence of Zr enables also the formation of metallic glasses. The phase diagram of the Gd-Zr systems is of eutectic type with no intermetallic phases and limited mutual solubility in the terminal phases. The phase diagram has been investigated by Copeland and co-workers [1961Cop, 1964Cop]. No investigations of the thermodynamic mixing properties are known. Based on these limited data, a thermodynamic dataset for Gd-Zr has been optimised by [2001Zin].

Table I. Phases, structures and models.

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

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Zr}			$\Delta_r H$ / (J/mol)
bcc′ ⇌ hcp′ + liquid	metatectic	1488.5	0.030	0.025	0.108	−3894
liquid ⇌ hcp′ + bcc″	eutectic	1485.6	0.114	0.026	0.930	−15380
hcp′ + bcc″ ⇌ hcp″	peritectoid	1162.4	0.019	0.984	0.974	−4346

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	−3302	2265	2.531	2644	−0.172	0.000
0.200	−4695	3785	3.855	4458	−0.306	0.000
0.300	−5641	4649	4.677	5533	−0.402	0.000
0.400	−6352	4949	5.137	5959	−0.459	0.000
0.500	−6851	4777	5.285	5828	−0.478	0.000
0.600	−7079	4222	5.137	5231	−0.459	0.000
0.700	−6915	3376	4.677	4259	−0.402	0.000
0.800	−6151	2329	3.855	3002	−0.306	0.000
0.900	−4394	1174	2.531	1552	−0.172	0.000
1.000	0	0	0.000	0	0.000	0.000

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

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

x_{Gd}	ΔG_{Gd} [J/mol]	ΔH_{Gd} [J/mol]	ΔS_{Gd} [J/(mol·K)]	$G_{\mathrm{Gd}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Gd}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Gd}	γ_{Gd}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1497	388	0.857	430	−0.019	0.921	1.024
0.800	−2482	1431	1.779	1600	−0.076	0.873	1.091
0.700	−3198	2948	2.793	3326	−0.172	0.840	1.199
0.600	−3916	4755	3.941	5428	−0.306	0.807	1.345
0.500	−4955	6672	5.285	7724	−0.478	0.763	1.525
0.400	−6730	8516	6.930	10030	−0.688	0.692	1.730
0.300	−9856	10105	9.073	12167	−0.937	0.583	1.945
0.200	−15490	11258	12.158	13950	−1.224	0.429	2.144
0.100	−26919	11792	17.596	15199	−1.549	0.230	2.295
0.000	$-\infty$	11525	∞	15732	−1.912	0.000	2.363

Reference state: Gd(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	$-\infty$	26688	∞	30895	−1.912	0.000	5.414
0.100	−19550	19161	17.596	22568	−1.549	0.343	3.434
0.200	−13549	13199	12.158	15891	−1.224	0.477	2.384
0.300	−11342	8619	9.073	10681	−0.937	0.538	1.793
0.400	−10006	5241	6.930	6755	−0.688	0.579	1.447
0.500	−8746	2881	5.285	3933	−0.478	0.620	1.240
0.600	−7312	1359	3.941	2032	−0.306	0.670	1.117
0.700	−5654	491	2.793	870	−0.172	0.734	1.049
0.800	−3816	97	1.779	265	−0.076	0.812	1.015
0.900	−1891	−6	0.857	36	−0.019	0.902	1.002
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Zr(liquid)

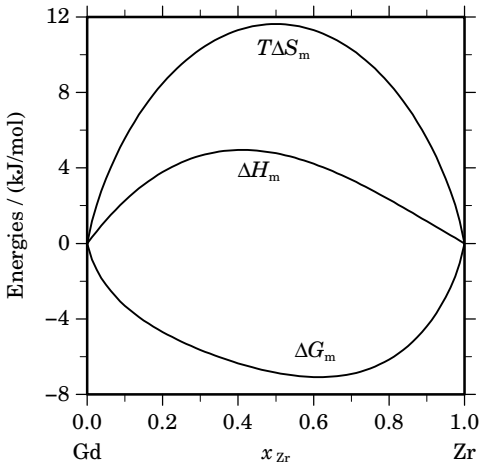

Fig. 2. Integral quantities of the liquid phase at T=2200 K.

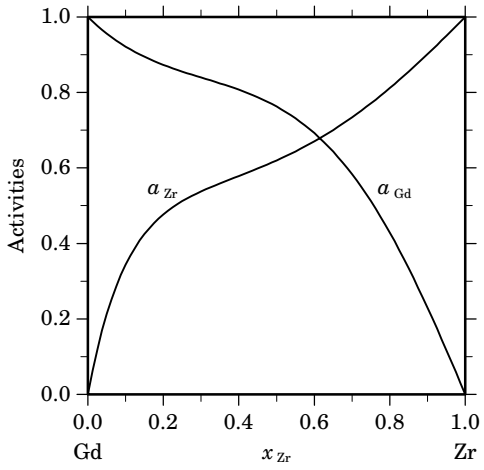

Fig. 3. Activities in the liquid phase at T=2200 K.

References

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[1964Cop] M. Copeland, H. Kato, in: "Physics and Material Problems of Reactor Control Rods", IAEA, Vienna, 1964, 295–317.

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