Nb – Zr (Niobium – Zirconium)

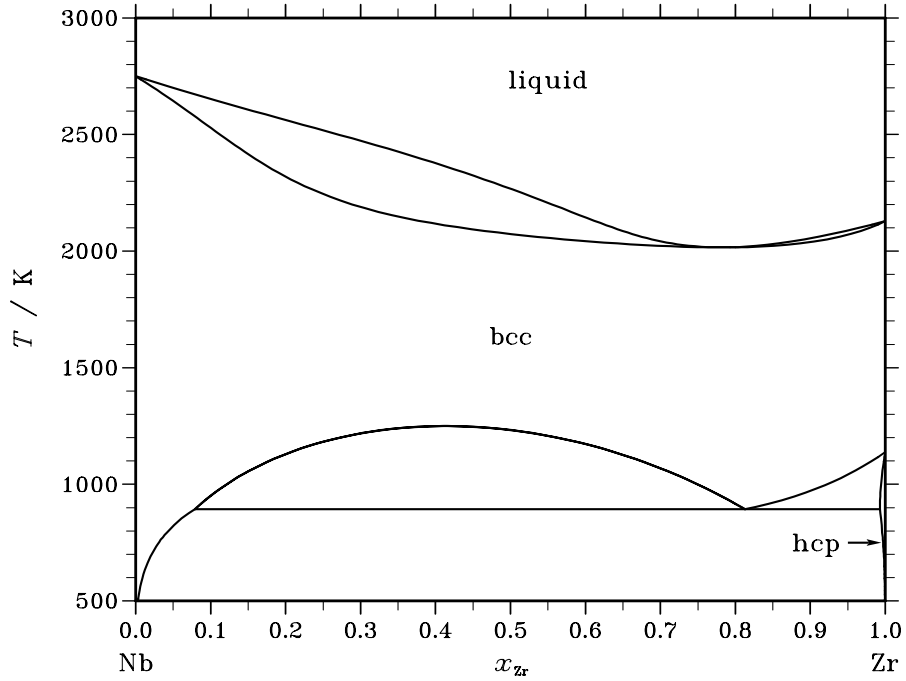

Fig. 1. Calculated phase diagram for the system Nb-Zr.

Niobium and zirconium are important additions to many alloys, such as superalloys and refractory alloys. The Nb-Zr system is fairly simple with only three condensed stable phases, liquid, bcc and hcp. An asymmetric miscibility gap of the bcc phase is well established. This asymmetry cannot be reproduced by the strict regular solution model description of [75Kau]. In the recommended assessment of [91Fer], a quasi-subregular model description was used for the bcc phase to reproduce the experimental data. Selected liquidus, solidus and solvus data were used to determine the model parameters. The calculated enthalpies of formation of the solid and liquid phases compare well with those from first principles and semi-empirical predictions.

Table I. Phases, structures and models.

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

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Zr}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ bcc	congruent	2016.1	0.783	0.783		−21134
bcc $\rightleftharpoons$ bcc′ + bcc″	critical	1249.1	0.413	0.413	0.413	0
bcc″ $\rightleftharpoons$ bcc′ + hcp	monotectoid	893.0	0.813	0.079	0.993	−5968

Table IIIa. Integral quantities for the liquid phase at 2800 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	−6157	1411	2.703	1411	0.000	0.000
0.200	−9356	2294	4.161	2294	0.000	0.000
0.300	−11492	2729	5.079	2729	0.000	0.000
0.400	−12872	2797	5.596	2797	0.000	0.000
0.500	−13559	2578	5.763	2578	0.000	0.000
0.600	−13516	2153	5.596	2153	0.000	0.000
0.700	−12620	1602	5.079	1602	0.000	0.000
0.800	−10644	1006	4.161	1006	0.000	0.000
0.900	−7123	445	2.703	445	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Nb in the liquid phase at 2800 K.

x_{Nb}	ΔG_{Nb} [J/mol]	ΔH_{Nb} [J/mol]	ΔS_{Nb} [J/(mol·K)]	$G_{\mathrm{Nb}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Nb}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Nb}	γ_{Nb}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2175	278	0.876	278	0.000	0.911	1.012
0.800	−4192	1003	1.855	1003	0.000	0.835	1.044
0.700	−6289	2015	2.966	2015	0.000	0.763	1.090
0.600	−8740	3153	4.247	3153	0.000	0.687	1.145
0.500	−11882	4255	5.763	4255	0.000	0.600	1.201
0.400	−16171	5161	7.619	5161	0.000	0.499	1.248
0.300	−22319	5710	10.010	5710	0.000	0.383	1.278
0.200	−31728	5740	13.382	5740	0.000	0.256	1.280
0.100	−48514	5091	19.145	5091	0.000	0.124	1.244
0.000	$-\infty$	3602	∞	3602	0.000	0.000	1.167

Reference state: Nb(liquid)

Table IIIc. Partial quantities for Zr in the liquid phase at 2800 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	$-\infty$	17020	∞	17020	0.000	0.000	2.077
0.100	−41993	11613	19.145	11613	0.000	0.165	1.647
0.200	−30011	7458	13.382	7458	0.000	0.276	1.378
0.300	−23634	4395	10.010	4395	0.000	0.362	1.208
0.400	−19069	2263	7.619	2263	0.000	0.441	1.102
0.500	−15236	901	5.763	901	0.000	0.520	1.039
0.600	−11745	147	4.247	147	0.000	0.604	1.006
0.700	−8462	−159	2.966	−159	0.000	0.695	0.993
0.800	−5373	−178	1.855	−178	0.000	0.794	0.992
0.900	−2524	−71	0.876	−71	0.000	0.897	0.997
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Zr(liquid)

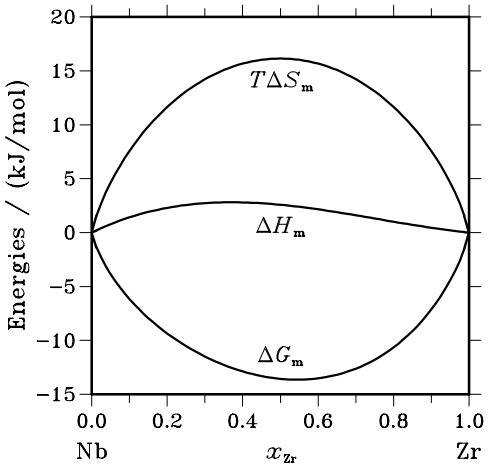

Fig. 2. Integral quantities of the liquid phase at T=2800 K.

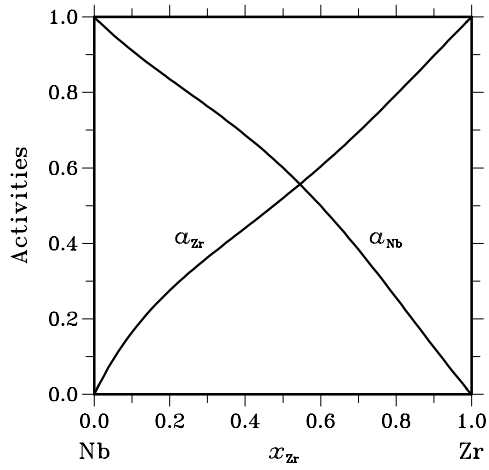

Fig. 3. Activities in the liquid phase at T=2800 K.

Table IVa. Integral quantities for the stable phases at 1500 K.

Phase	x_{Zr}	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)]
bcc	0.000	0	0	0.000	0	0.000	0.000
	0.100	−2006	1714	2.480	2049	−0.223	0.000
	0.200	−2672	2922	3.729	3569	−0.431	0.000
	0.300	−3030	3671	4.467	4588	−0.612	0.000
	0.400	−3259	4007	4.844	5134	−0.752	0.000
	0.500	−3411	3978	4.926	5234	−0.838	0.000
	0.600	−3479	3631	4.739	4915	−0.856	0.000
	0.700	−3414	3012	4.284	4205	−0.795	0.000
	0.800	−3110	2170	3.520	3131	−0.641	0.000
	0.900	−2334	1150	2.323	1720	−0.380	0.000
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Nb(bcc), Zr(bcc)

Table IVb. Partial quantities for Nb in the stable phases at 1500 K.

Phase	x_{Nb}	ΔG_{Nb} [J/mol]	ΔH_{Nb} [J/mol]	ΔS_{Nb} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Nb}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Nb}}$ [J/(mol·K)]	a_{Nb}	γ_{Nb}
bcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1045	261	0.871	269	−0.005	0.920	1.022
	0.800	−1745	981	1.817	1038	−0.038	0.869	1.087
	0.700	−2194	2067	2.841	2254	−0.125	0.839	1.198
	0.600	−2510	3424	3.956	3861	−0.292	0.818	1.363
	0.500	−2840	4958	5.198	5805	−0.565	0.796	1.593
	0.400	−3398	6574	6.648	8030	−0.970	0.762	1.904
	0.300	−4533	8180	8.476	10482	−1.535	0.695	2.317
	0.200	−6966	9681	11.098	13107	−2.284	0.572	2.860
	0.100	−12868	10983	15.901	15849	−3.244	0.356	3.564
	0.000	$-\infty$	11992	∞	18654	−4.441	0.000	4.462

Reference state: Nb(bcc)

Table IVc. Partial quantities for Zr in the stable phases at 1500 K.

Phase	x_{Zr}	ΔG_{Zr} [J/mol]	ΔH_{Zr} [J/mol]	ΔS_{Zr} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Zr}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Zr}}$ [J/(mol·K)]	a_{Zr}	γ_{Zr}
bcc	0.000	$-\infty$	19830	∞	23219	−2.259	0.000	6.435
	0.100	−10650	14793	16.962	18068	−2.183	0.426	4.257
	0.200	−6381	10685	11.377	13691	−2.004	0.599	2.997
	0.300	−4981	7412	8.262	10035	−1.748	0.671	2.236
	0.400	−4384	4881	6.177	7044	−1.442	0.704	1.759
	0.500	−3981	2998	4.653	4663	−1.110	0.727	1.453
	0.600	−3532	1668	3.467	2838	−0.780	0.753	1.256
	0.700	−2934	797	2.487	1514	−0.478	0.790	1.129
	0.800	−2146	292	1.625	637	−0.230	0.842	1.052
	0.900	−1164	57	0.814	150	−0.062	0.911	1.012
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Zr(bcc)

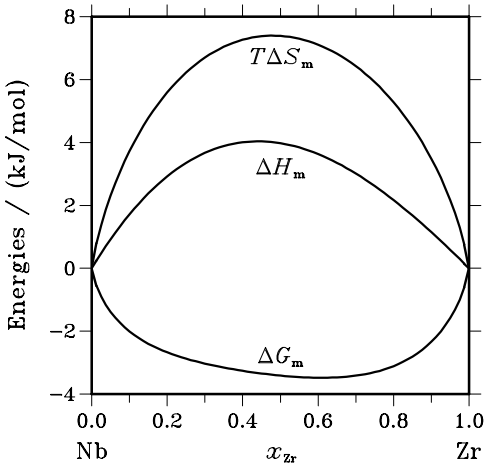

Fig. 4. Integral quantities of the stable phases at T=1500 K.

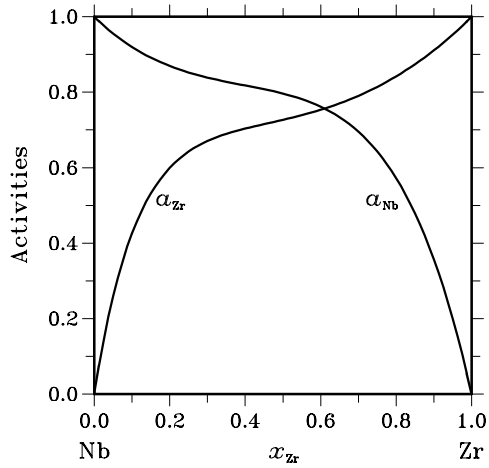

Fig. 5. Activities in the stable phases at T=1500 K.

References

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