Ta – Zr (Tantalum – Zirconium)

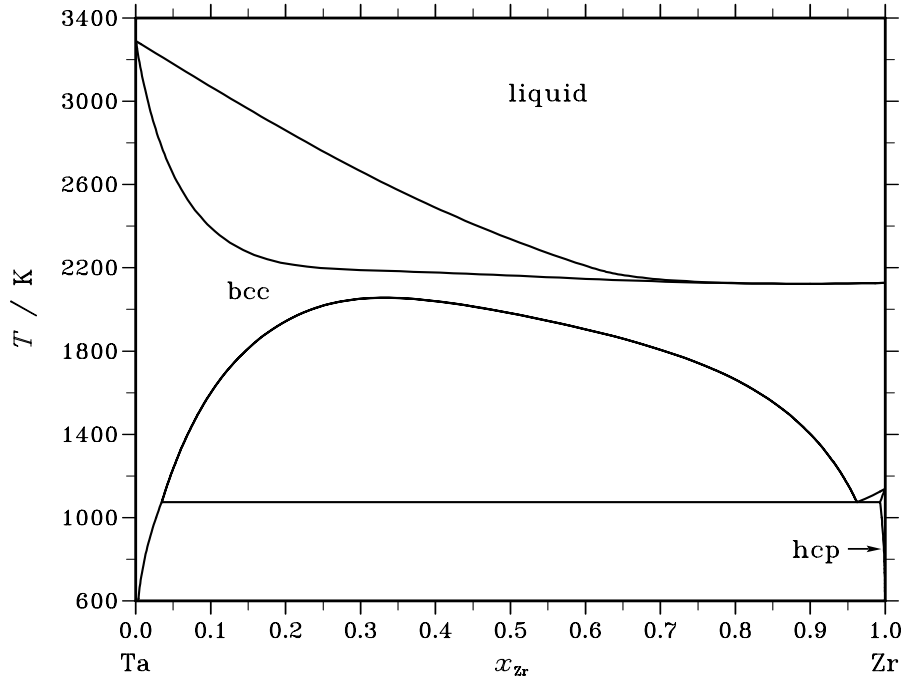

Fig. 1. Calculated phase diagram for the system Ta-Zr.

Tantalum and zirconium are important additions to many alloys, such as superalloys and refractory alloys. The Ta-Zr phase diagram has been subject to a number of experimental investigations which show it to be fairly simple with only three condensed stable phases, liquid, bcc and hcp. The melting curve is very flat over a wide composition range and the bcc phase forms a miscibility gap at temperatures below 2060 K. Data on the excess enthalpies of the phases have been determined with theoretical studies. The available data were critically evaluated by [95Fer] who also derived a thermodynamic description of the system. The calculated phase boundaries reproduce the experimental data well and are in qualitative agreement with the theoretical enthalpy data.

Table I. Phases, structures and models.

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

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Zr}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ bcc	congruent	2123.1	0.891	0.891		−21273
bcc $\rightleftharpoons$ bcc′ + bcc″	critical	2054.4	0.333	0.333	0.333	0
bcc″ $\rightleftharpoons$ bcc′ + hcp	monotectoid	1074.0	0.962	0.035	0.993	−5056

Table IIIa. Integral quantities for the liquid phase at 3300 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	−8190	730	2.703	730	0.000	0.000
0.200	−12203	1527	4.161	1527	0.000	0.000
0.300	−14457	2304	5.079	2304	0.000	0.000
0.400	−15490	2977	5.596	2977	0.000	0.000
0.500	−15561	3458	5.763	3458	0.000	0.000
0.600	−14803	3663	5.596	3663	0.000	0.000
0.700	−13256	3505	5.079	3505	0.000	0.000
0.800	−10830	2900	4.161	2900	0.000	0.000
0.900	−7160	1760	2.703	1760	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Ta in the liquid phase at 3300 K.

x_{Ta}	ΔG_{Ta} [J/mol]	ΔH_{Ta} [J/mol]	ΔS_{Ta} [J/(mol·K)]	$G_{\mathrm{Ta}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Ta}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Ta}	γ_{Ta}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2938	−48	0.876	−48	0.000	0.898	0.998
0.800	−6199	−76	1.855	−76	0.000	0.798	0.997
0.700	−9700	87	2.966	87	0.000	0.702	1.003
0.600	−13404	612	4.247	612	0.000	0.614	1.023
0.500	−17348	1671	5.763	1671	0.000	0.531	1.063
0.400	−21706	3435	7.619	3435	0.000	0.453	1.133
0.300	−26957	6077	10.010	6077	0.000	0.374	1.248
0.200	−34392	9768	13.382	9768	0.000	0.286	1.428
0.100	−48499	14679	19.145	14679	0.000	0.171	1.707
0.000	$-\infty$	20982	∞	20982	0.000	0.000	2.148

Reference state: Ta(liquid)

Table IIIc. Partial quantities for Zr in the liquid phase at 3300 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	$-\infty$	6682	∞	6682	0.000	0.000	1.276
0.100	−55449	7729	19.145	7729	0.000	0.133	1.325
0.200	−36222	7937	13.382	7937	0.000	0.267	1.335
0.300	−25556	7478	10.010	7478	0.000	0.394	1.313
0.400	−18617	6524	7.619	6524	0.000	0.507	1.268
0.500	−13773	5246	5.763	5246	0.000	0.605	1.211
0.600	−10201	3815	4.247	3815	0.000	0.689	1.149
0.700	−7383	2403	2.966	2403	0.000	0.764	1.092
0.800	−4940	1182	1.855	1182	0.000	0.835	1.044
0.900	−2567	324	0.876	324	0.000	0.911	1.012
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Zr(liquid)

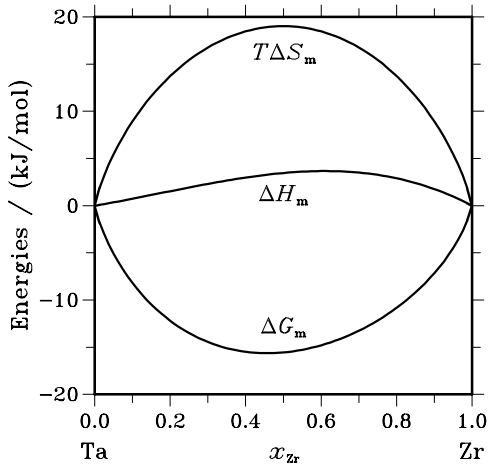

Fig. 2. Integral quantities of the liquid phase at T=3300 K.

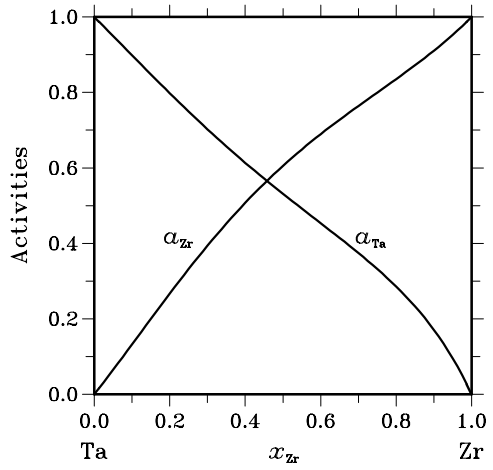

Fig. 3. Activities in the liquid phase at T=3300 K.

Table IVa. Integral quantities for the stable phases at 2100 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	−1935	1972	1.861	3741	−0.842	0.000
	0.200	−2421	3932	3.025	6316	−1.135	0.000
	0.300	−2748	5612	3.981	7918	−1.098	0.000
	0.400	−3051	6808	4.695	8700	−0.901	0.000
	0.500	−3325	7375	5.095	8778	−0.668	0.000
	0.600	−3522	7230	5.120	8229	−0.476	0.000
	0.700	−3572	6351	4.725	7094	−0.354	0.000
	0.800	−3363	4776	3.876	5374	−0.285	0.000
	0.900	−2642	2606	2.499	3034	−0.204	0.000
	1.000	0	0	0.000	0	0.000	0.000

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

Table IVb. Partial quantities for Ta in the stable phases at 2100 K.

Phase	x_{Ta}	ΔG_{Ta} [J/mol]	ΔH_{Ta} [J/mol]	ΔS_{Ta} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ta}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ta}}$ [J/(mol·K)]	a_{Ta}	γ_{Ta}
bcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1222	−43	0.561	618	−0.315	0.932	1.036
	0.800	−1700	214	0.911	2197	−0.944	0.907	1.134
	0.700	−1818	1211	1.442	4410	−1.523	0.901	1.287
	0.600	−1874	3207	2.419	7046	−1.828	0.898	1.497
	0.500	−2098	6276	3.988	10005	−1.776	0.887	1.774
	0.400	−2697	10311	6.194	13302	−1.424	0.857	2.142
	0.300	−3956	15020	9.036	17066	−0.974	0.797	2.658
	0.200	−6562	19930	12.615	21540	−0.766	0.687	3.434
	0.100	−13125	24385	17.862	27079	−1.283	0.472	4.716
	0.000	$-\infty$	27543	∞	34155	−3.149	0.000	7.072

Reference state: Ta(bcc)

Table IVc. Partial quantities for Zr in the stable phases at 2100 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	$-\infty$	18750	∞	43969	−12.009	0.000	12.406
	0.100	−8355	20111	13.555	31849	−5.589	0.620	6.197
	0.200	−5306	18805	11.481	22796	−1.901	0.738	3.690
	0.300	−4918	15882	9.905	16104	−0.106	0.755	2.515
	0.400	−4817	12210	8.108	11182	0.489	0.759	1.897
	0.500	−4552	8474	6.203	7551	0.439	0.771	1.541
	0.600	−4072	5176	4.404	4847	0.157	0.792	1.320
	0.700	−3408	2635	2.878	2820	−0.088	0.823	1.175
	0.800	−2563	987	1.691	1333	−0.165	0.863	1.079
	0.900	−1477	186	0.792	363	−0.084	0.919	1.021
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Zr(bcc)

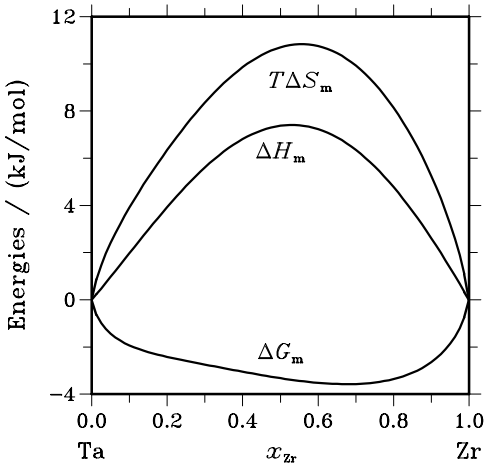

Fig. 4. Integral quantities of the stable phases at T=2100 K.

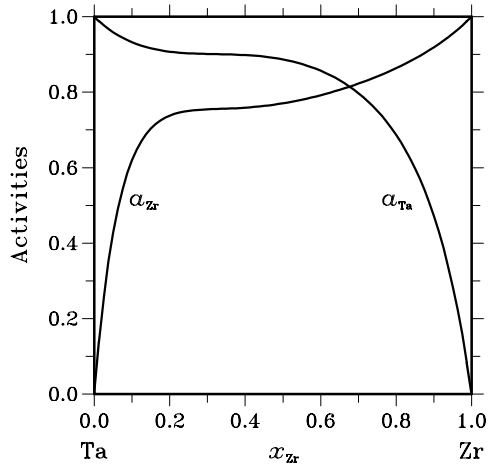

Fig. 5. Activities in the stable phases at T=2100 K.

References

[95Fer] A. Fernández Guillermet: J. Alloys Comp. **226** (1995) 174–184.