Ti – W (Titanium – Tungsten)

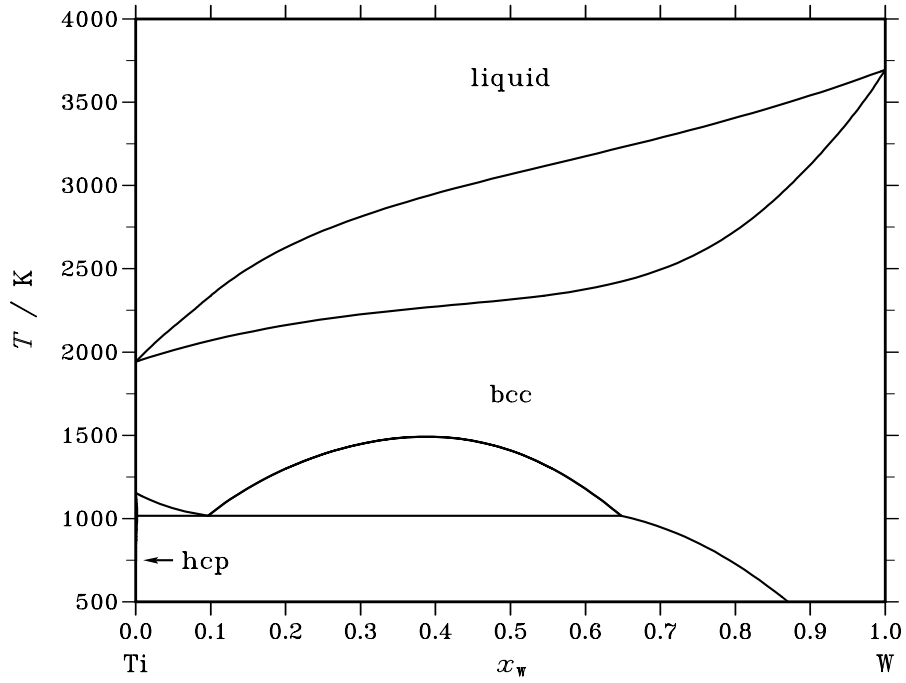

Fig. 1. Calculated phase diagram for the system Ti-W.

Titanium and tungsten are important additions to many alloys, such as superalloys and refractory alloys. The Ti-W system is fairly simple with only three condensed stable phases, liquid, bcc and hcp. Experimental evidence indicates the existence of a monotectoid reaction and a miscibility gap in the bcc phase. Based on results of first principles calculations, [95Rub] doubts the existence of such a miscibility gap. According to the critical evaluation of [87Mur], the solid/solid phase boundaries, as well as the monotectoid reaction temperature, are not well established due to their sluggish reaction rates. A number of thermodynamic descriptions for this system has been developed. The most recent descriptions [93Jin, 96Jon, 98Sau] reproduce the experimental data very well. The major difference between these descriptions is the number of parameters used to describe the excess Gibbs energies of the liquid and bcc phases. The description of [96Jon] used the least number of parameters, thus is recommended.

Table I. Phases, structures and models.

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

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_W			$\Delta_r H$ / (J/mol)
bcc $\rightleftharpoons$ bcc′ + bcc″	critical	1489.9	0.388	0.388	0.388	0
bcc′ $\rightleftharpoons$ hcp + bcc″	monotectoid	1017.8	0.097	0.002	0.648	−5031

Table IIIa. Integral quantities for the liquid phase at 3800 K.

x_{W}	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	−7978	2293	2.703	2293	0.000	0.000
0.200	−11733	4077	4.161	4077	0.000	0.000
0.300	−13949	5351	5.079	5351	0.000	0.000
0.400	−15149	6115	5.596	6115	0.000	0.000
0.500	−15530	6370	5.763	6370	0.000	0.000
0.600	−15149	6115	5.596	6115	0.000	0.000
0.700	−13949	5351	5.079	5351	0.000	0.000
0.800	−11733	4077	4.161	4077	0.000	0.000
0.900	−7978	2293	2.703	2293	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Ti(liquid), W(liquid)

Table IIIb. Partial quantities for Ti in the liquid phase at 3800 K.

x_{Ti}	ΔG_{Ti} [J/mol]	ΔH_{Ti} [J/mol]	ΔS_{Ti} [J/(mol·K)]	$G_{\mathrm{Ti}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Ti}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Ti}	γ_{Ti}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−3074	255	0.876	255	0.000	0.907	1.008
0.800	−6031	1019	1.855	1019	0.000	0.826	1.033
0.700	−8976	2293	2.966	2293	0.000	0.753	1.075
0.600	−12063	4077	4.247	4077	0.000	0.683	1.138
0.500	−15530	6370	5.763	6370	0.000	0.612	1.223
0.400	−19777	9173	7.619	9173	0.000	0.535	1.337
0.300	−25554	12486	10.010	12486	0.000	0.445	1.485
0.200	−34543	16308	13.382	16308	0.000	0.335	1.676
0.100	−52111	20640	19.145	20640	0.000	0.192	1.922
0.000	$-\infty$	25481	∞	25481	0.000	0.000	2.240

Reference state: Ti(liquid)

Table IIIc. Partial quantities for W in the liquid phase at 3800 K.

x_{W}	ΔG_{W} [J/mol]	ΔH_{W} [J/mol]	ΔS_{W} [J/(mol·K)]	$G_{\mathrm{W}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{W}}^{\mathrm{E}}$ [J/(mol·K)]	a_{W}	γ_{W}
0.000	$-\infty$	25481	∞	25481	0.000	0.000	2.240
0.100	−52111	20640	19.145	20640	0.000	0.192	1.922
0.200	−34543	16308	13.382	16308	0.000	0.335	1.676
0.300	−25554	12486	10.010	12486	0.000	0.445	1.485
0.400	−19777	9173	7.619	9173	0.000	0.535	1.337
0.500	−15530	6370	5.763	6370	0.000	0.612	1.223
0.600	−12063	4077	4.247	4077	0.000	0.683	1.138
0.700	−8976	2293	2.966	2293	0.000	0.753	1.075
0.800	−6031	1019	1.855	1019	0.000	0.826	1.033
0.900	−3074	255	0.876	255	0.000	0.907	1.008
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: W(liquid)

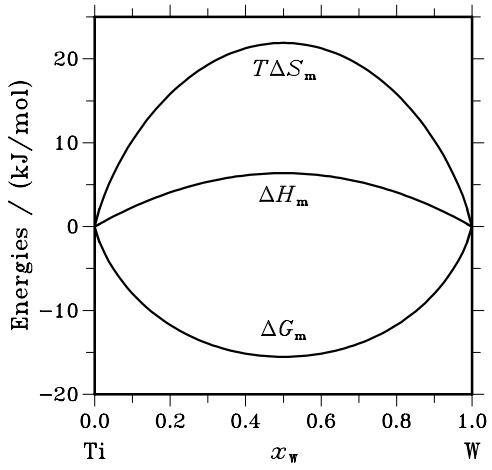

Fig. 2. Integral quantities of the liquid phase at T=3800 K.

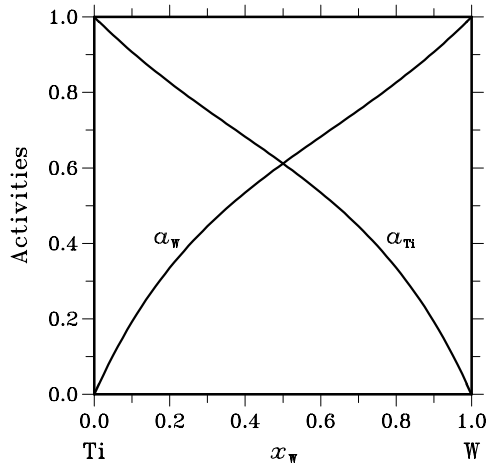

Fig. 3. Activities in the liquid phase at T=3800 K.

Table IVa. Integral quantities for the stable phases at 1600 K.

Phase	x_{W}	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	−1832	1091	1.827	2493	−0.876	0.000
	0.200	−2344	1628	2.482	4313	−1.678	0.000
	0.300	−2621	1726	2.717	5505	−2.362	0.000
	0.400	−2840	1504	2.715	6114	−2.881	0.000
	0.500	−3038	1078	2.573	6183	−3.190	0.000
	0.600	−3196	566	2.351	5757	−3.244	0.000
	0.700	−3245	85	2.081	4882	−2.998	0.000
	0.800	−3056	−248	1.755	3601	−2.405	0.000
	0.900	−2366	−315	1.282	1958	−1.421	0.000
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Ti(bcc), W(bcc)

Table IVb. Partial quantities for Ti in the stable phases at 1600 K.

Phase	x_{Ti}	ΔG_{Ti} [J/mol]	ΔH_{Ti} [J/mol]	ΔS_{Ti} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ti}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ti}}$ [J/(mol·K)]	a_{Ti}	γ_{Ti}
bcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1058	297	0.847	344	−0.029	0.924	1.026
	0.800	−1653	1032	1.678	1316	−0.177	0.883	1.104
	0.700	−1918	1971	2.430	2827	−0.535	0.866	1.237
	0.600	−2007	2878	3.053	4788	−1.194	0.860	1.433
	0.500	−2110	3520	3.519	7111	−2.244	0.853	1.707
	0.400	−2485	3663	3.842	9705	−3.776	0.830	2.074
	0.300	−3535	3071	4.128	12482	−5.882	0.767	2.556
	0.200	−6058	1510	4.730	15353	−8.652	0.634	3.171
	0.100	−12404	−1254	6.969	18228	−12.176	0.394	3.936
	0.000	$-\infty$	−5455	∞	21019	−16.546	0.000	4.855

Reference state: Ti(bcc)

Table IVc. Partial quantities for W in the stable phases at 1600 K.

Phase	x_W	ΔG_W [J/mol]	ΔH_W [J/mol]	ΔS_W [J/(mol·K)]	G_W^E [J/mol]	S_W^E [J/(mol·K)]	a_W	γ_W
bcc	0.000	$-\infty$	14081	∞	28443	−8.976	0.000	8.483
	0.100	−8796	8241	10.648	21836	−8.497	0.516	5.162
	0.200	−5108	4011	5.699	16303	−7.683	0.681	3.406
	0.300	−4262	1156	3.387	11754	−6.624	0.726	2.420
	0.400	−4088	−557	2.207	8101	−5.412	0.735	1.839
	0.500	−3966	−1364	1.627	5255	−4.136	0.742	1.484
	0.600	−3670	−1498	1.358	3125	−2.890	0.759	1.265
	0.700	−3121	−1194	1.204	1624	−1.762	0.791	1.130
	0.800	−2306	−687	1.012	663	−0.844	0.841	1.051
	0.900	−1251	−211	0.650	151	−0.226	0.910	1.011
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: W(bcc)

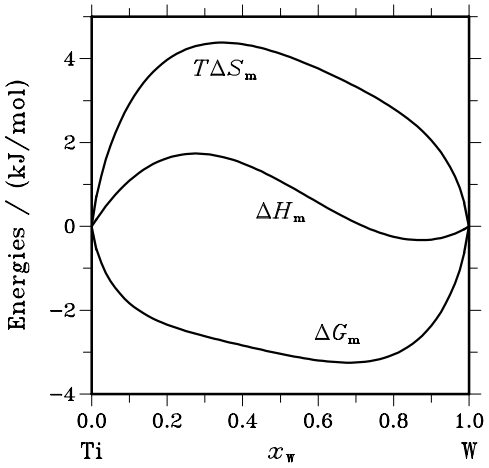

Fig. 4. Integral quantities of the stable phases at T=1600 K.

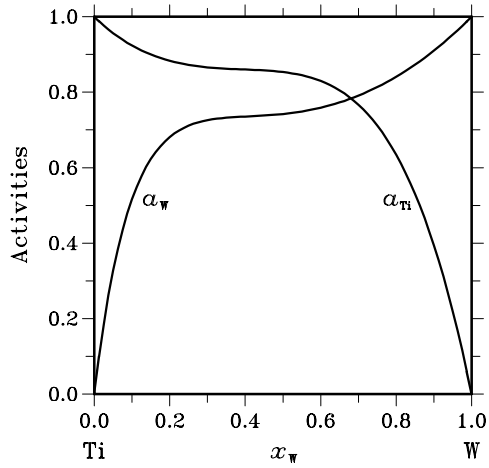

Fig. 5. Activities in the stable phases at T=1600 K.

References

[87Mur] J.L. Murray: in "Phase Diagrams of Binary Titanium Alloys", Ed. J.L. Murray, ASM International, Metals Park, OH, 1987, pp. 328–332.

[93Jin] Z. Jin, C. Qiu: Mater. Sci. Technol. **9** (1993) 378–383.

[95Rub] G. Rubin, A. Finel: J. Phys. Condens. Matter **7** (1995) 3139–3152.

[96Jon] S. Jonsson: Z. Metallkd. **87** (1996) 784–787.

[98Sau] N. Saunders in: I. Ansara, A.T. Dinsdale, M.H. Rand (eds.): COST 507, "Thermochemical database for light metal alloys", Vol. 2, EUR 18499, 1998, 299–302.