Ta – Ti (Tantalum – Titanium)

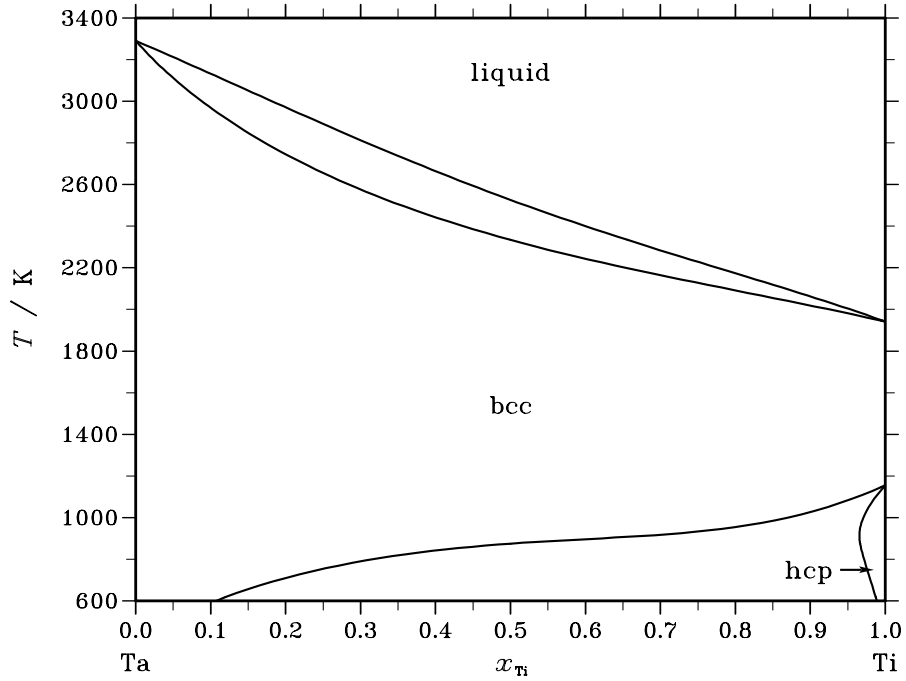

Fig. 1. Calculated phase diagram for the system Ta-Ti.

Tantalum and titanium are important additions to many alloys, such as superalloys and refractory alloys. The Ta-Ti system is fairly simple with only three condensed stable phases, liquid, bcc and hcp. According to the critical evaluation of [87Mur], the phase boundaries are only poorly established by experiments. Several of thermodynamic descriptions for this systems have been developed. The assessment of [98Sau] reproduces the solid/solid phase boundaries proposed by [87Mur] and the highest solidus temperatures observed in experiments. Therefore, this description is recommended.

Table I. Phases, structures and models.

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

Table IIa. Integral quantities for the liquid phase at 3300 K.

x_{Ti}	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	−9334	−414	2.703	−414	0.000	0.000
0.200	−14242	−512	4.161	−512	0.000	0.000
0.300	−17139	−378	5.079	−378	0.000	0.000
0.400	−18562	−96	5.596	−96	0.000	0.000
0.500	−18769	250	5.763	250	0.000	0.000
0.600	−17890	576	5.596	576	0.000	0.000
0.700	−15963	798	5.079	798	0.000	0.000
0.800	−12898	832	4.161	832	0.000	0.000
0.900	−8326	594	2.703	594	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIb. 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	−3063	−172	0.876	−172	0.000	0.894	0.994
0.800	−6699	−576	1.855	−576	0.000	0.783	0.979
0.700	−10830	−1044	2.966	−1044	0.000	0.674	0.963
0.600	−15424	−1408	4.247	−1408	0.000	0.570	0.950
0.500	−20519	−1500	5.763	−1500	0.000	0.473	0.947
0.400	−26293	−1152	7.619	−1152	0.000	0.384	0.959
0.300	−33231	−196	10.010	−196	0.000	0.298	0.993
0.200	−42624	1536	13.382	1536	0.000	0.212	1.058
0.100	−58966	4212	19.145	4212	0.000	0.117	1.166
0.000	$-\infty$	8000	∞	8000	0.000	0.000	1.339

Reference state: Ta(liquid)

Table IIc. Partial quantities for Ti in the liquid phase at 3300 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}
0.000	$-\infty$	−6000	∞	−6000	0.000	0.000	0.804
0.100	−65770	−2592	19.145	−2592	0.000	0.091	0.910
0.200	−44416	−256	13.382	−256	0.000	0.198	0.991
0.300	−31859	1176	10.010	1176	0.000	0.313	1.044
0.400	−23269	1872	7.619	1872	0.000	0.428	1.071
0.500	−17019	2000	5.763	2000	0.000	0.538	1.076
0.600	−12288	1728	4.247	1728	0.000	0.639	1.065
0.700	−8562	1224	2.966	1224	0.000	0.732	1.046
0.800	−5467	656	1.855	656	0.000	0.819	1.024
0.900	−2699	192	0.876	192	0.000	0.906	1.007
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(liquid)

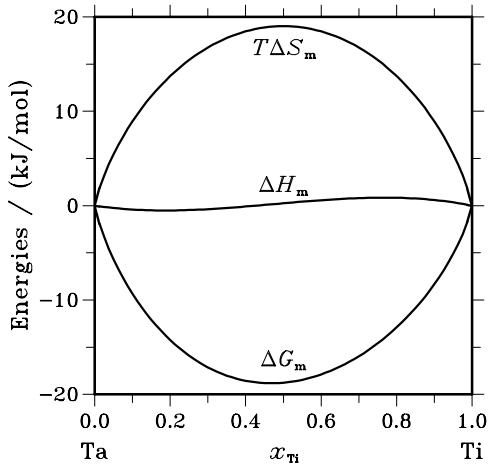

Fig. 2. Integral quantities of the liquid phase at T=3300 K.

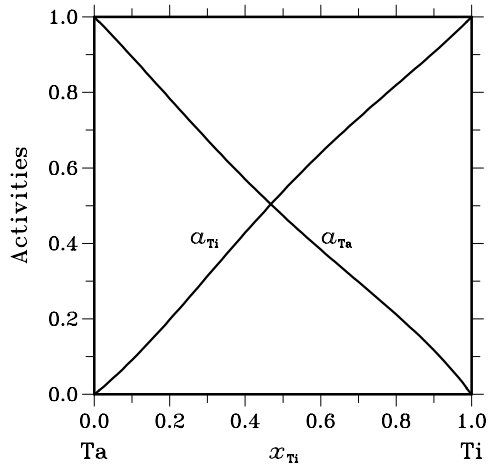

Fig. 3. Activities in the liquid phase at T=3300 K.

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

Phase	x_{Ti}	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	−3154	900	2.703	900	0.000	0.000
	0.200	−4561	1680	4.161	1680	0.000	0.000
	0.300	−5309	2310	5.079	2310	0.000	0.000
	0.400	−5634	2760	5.596	2760	0.000	0.000
	0.500	−5645	3000	5.763	3000	0.000	0.000
	0.600	−5394	3000	5.596	3000	0.000	0.000
	0.700	−4889	2730	5.079	2730	0.000	0.000
	0.800	−4081	2160	4.161	2160	0.000	0.000
	0.900	−2794	1260	2.703	1260	0.000	0.000
	1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Ta in the stable phases at 1500 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	−1259	55	0.876	55	0.000	0.904	1.004
	0.800	−2523	260	1.855	260	0.000	0.817	1.021
	0.700	−3773	675	2.966	675	0.000	0.739	1.056
	0.600	−5011	1360	4.247	1360	0.000	0.669	1.115
	0.500	−6270	2375	5.763	2375	0.000	0.605	1.210
	0.400	−7648	3780	7.619	3780	0.000	0.542	1.354
	0.300	−9381	5635	10.010	5635	0.000	0.471	1.571
	0.200	−12073	8000	13.382	8000	0.000	0.380	1.899
	0.100	−17782	10935	19.145	10935	0.000	0.240	2.403
	0.000	$-\infty$	14500	∞	14500	0.000	0.000	3.198

Reference state: Ta(bcc)

Table IIIc. Partial quantities for Ti in the stable phases at 1500 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	0.000	$-\infty$	9500	∞	9500	0.000	0.000	2.142
	0.100	−20212	8505	19.145	8505	0.000	0.198	1.978
	0.200	−12713	7360	13.382	7360	0.000	0.361	1.804
	0.300	−8891	6125	10.010	6125	0.000	0.490	1.634
	0.400	−6568	4860	7.619	4860	0.000	0.591	1.477
	0.500	−5020	3625	5.763	3625	0.000	0.669	1.337
	0.600	−3891	2480	4.247	2480	0.000	0.732	1.220
	0.700	−2963	1485	2.966	1485	0.000	0.789	1.126
	0.800	−2083	700	1.855	700	0.000	0.846	1.058
	0.900	−1129	185	0.876	185	0.000	0.913	1.015
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(bcc)

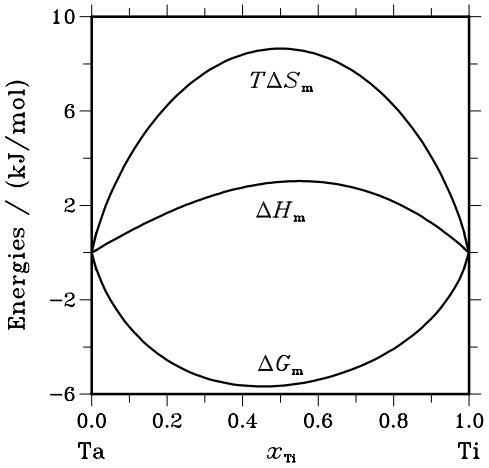

Fig. 4. Integral quantities of the stable phases at T=1500 K.

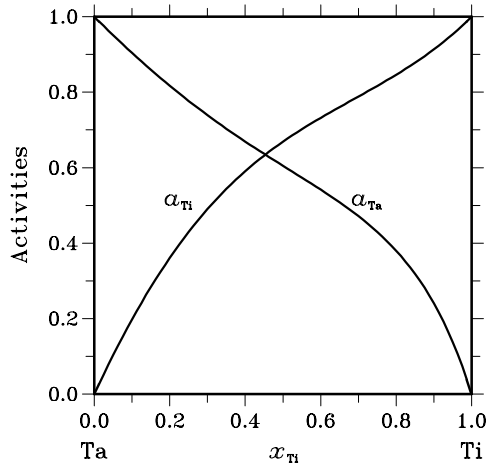

Fig. 5. Activities in the stable phases at T=1500 K.

References

[87Mur] J.L. Murray: in "Phase Diagrams of Binary Titanium Alloys", Ed. J.L. Murray, ASM International, Metals Park, OH, 1987, pp. 302–306.

[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, 293–296.