Ta – V (Tantalum – Vanadium)

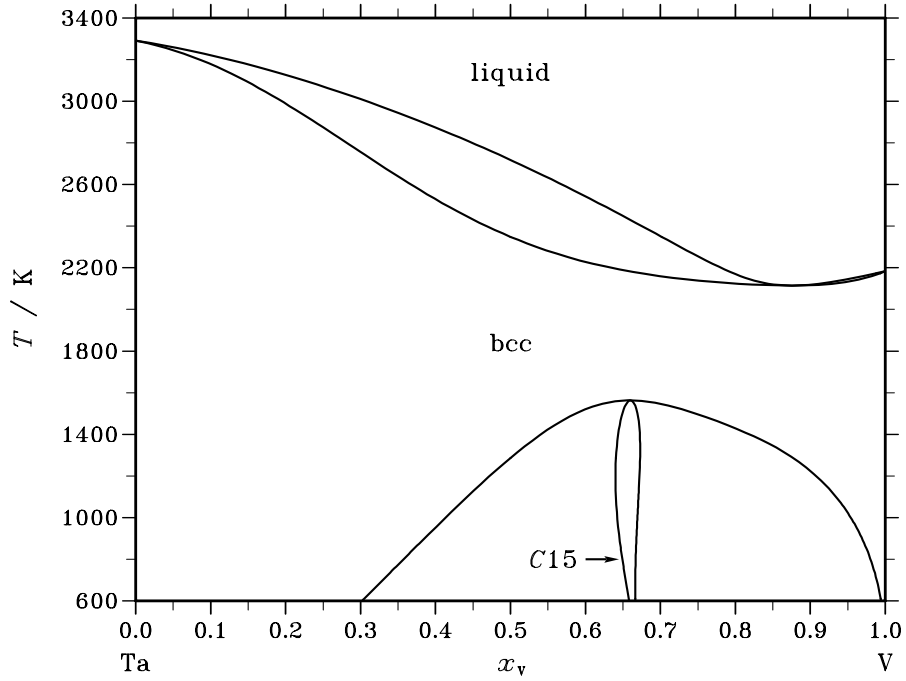

Fig. 1. Calculated phase diagram for the system Ta-V.

Tantalum and vanadium are important additions to many alloys, such as superalloys and refractory alloys. The system has been reviewed by [83Smi] and [04Dan] and in addition, the latter work provides also a complete thermodynamic assessment. The system is characterised by complete miscibility of the components in the liquid and the bcc-phase. At lower temperatures, a cubic Laves phase with a small homogeneity range forms.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Ta,V)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Ta,W)_1$
$C15$	$C15$	Cu_2Mg	$cF24$	$Fd\overline{3}m$	TAV2	Ta_1V_2

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_V		$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ bcc	congruent	2114.4	0.875	0.875	−20475
bcc $\rightleftharpoons$ $C15$	congruent	1563.3	0.660	0.660	−1357

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

x_{V}	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	−9300	−510	2.664	−380	−0.039	0.000
0.200	−14406	−906	4.091	−676	−0.070	0.000
0.300	−17648	−1189	4.988	−887	−0.091	0.000
0.400	−19480	−1359	5.491	−1014	−0.104	0.000
0.500	−20075	−1415	5.654	−1056	−0.109	0.000
0.600	−19480	−1359	5.491	−1014	−0.104	0.000
0.700	−17648	−1189	4.988	−887	−0.091	0.000
0.800	−14406	−906	4.091	−676	−0.070	0.000
0.900	−9300	−510	2.664	−380	−0.039	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Ta(liquid), V(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	−2933	−57	0.872	−42	−0.004	0.899	0.998
0.800	−6292	−226	1.838	−169	−0.017	0.795	0.994
0.700	−10167	−510	2.926	−380	−0.039	0.690	0.986
0.600	−14692	−906	4.178	−676	−0.070	0.585	0.976
0.500	−20075	−1415	5.654	−1056	−0.109	0.481	0.962
0.400	−26662	−2038	7.462	−1521	−0.157	0.378	0.946
0.300	−35105	−2774	9.797	−2071	−0.213	0.278	0.927
0.200	−46864	−3623	13.103	−2705	−0.278	0.181	0.906
0.100	−66601	−4586	18.792	−3423	−0.352	0.088	0.883
0.000	$-\infty$	−5661	∞	−4226	−0.435	0.000	0.857

Reference state: Ta(liquid)

Table IIIc. Partial quantities for V in the liquid phase at 3300 K.

x_{V}	ΔG_{V} [J/mol]	ΔH_{V} [J/mol]	ΔS_{V} [J/(mol·K)]	$G_{\mathrm{V}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{V}}^{\mathrm{E}}$ [J/(mol·K)]	a_{V}	γ_{V}
0.000	$-\infty$	−5661	∞	−4226	−0.435	0.000	0.857
0.100	−66601	−4586	18.792	−3423	−0.352	0.088	0.883
0.200	−46864	−3623	13.103	−2705	−0.278	0.181	0.906
0.300	−35105	−2774	9.797	−2071	−0.213	0.278	0.927
0.400	−26662	−2038	7.462	−1521	−0.157	0.378	0.946
0.500	−20075	−1415	5.654	−1056	−0.109	0.481	0.962
0.600	−14692	−906	4.178	−676	−0.070	0.585	0.976
0.700	−10167	−510	2.926	−380	−0.039	0.690	0.986
0.800	−6292	−226	1.838	−169	−0.017	0.795	0.994
0.900	−2933	−57	0.872	−42	−0.004	0.899	0.998
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: V(liquid)

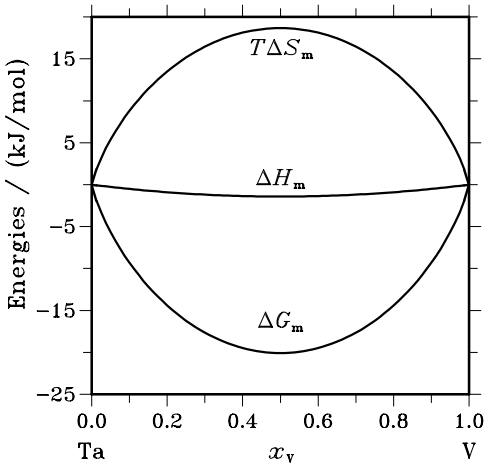

Fig. 2. Integral quantities of the liquid phase at T=3300 K.

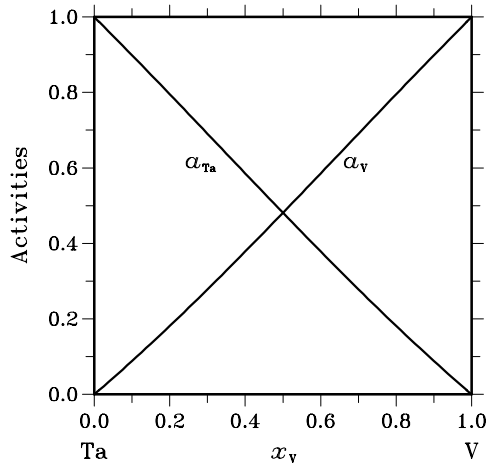

Fig. 3. Activities in the liquid phase at T=3300 K.

Table IVa. Integral quantities for the stable phases at 1800 K.

Phase	x_V	ΔG_m [J/mol]	ΔH_m [J/mol]	ΔS_m [J/(mol·K)]	G_m^E [J/mol]	S_m^E [J/(mol·K)]	ΔC_P [J/(mol·K)]
bcc	0.000	0	0	0.000	0	0.000	0.000
	0.100	−5405	−540	2.703	−540	0.000	0.000
	0.200	−8018	−529	4.161	−529	0.000	0.000
	0.300	−9271	−129	5.079	−129	0.000	0.000
	0.400	−9573	499	5.596	499	0.000	0.000
	0.500	−9180	1193	5.763	1193	0.000	0.000
	0.600	−8280	1792	5.596	1792	0.000	0.000
	0.700	−7008	2134	5.079	2134	0.000	0.000
	0.800	−5432	2057	4.161	2057	0.000	0.000
	0.900	−3466	1399	2.703	1399	0.000	0.000
	1.000	0	0	0.000	0	0.000	0.000

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

Table IVb. Partial quantities for Ta in the stable phases at 1800 K.

Phase	x_{Ta}	ΔG_{Ta} [J/mol]	ΔH_{Ta} [J/mol]	ΔS_{Ta} [J/(mol·K)]	G_{Ta}^E [J/mol]	S_{Ta}^E [J/(mol·K)]	a_{Ta}	γ_{Ta}
bcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1879	−302	0.876	−302	0.000	0.882	0.980
	0.800	−4334	−994	1.855	−994	0.000	0.749	0.936
	0.700	−7091	−1753	2.966	−1753	0.000	0.623	0.889
	0.600	−9899	−2254	4.247	−2254	0.000	0.516	0.860
	0.500	−12548	−2174	5.763	−2174	0.000	0.432	0.865
	0.400	−14905	−1191	7.619	−1191	0.000	0.369	0.923
	0.300	−17000	1019	10.010	1019	0.000	0.321	1.070
	0.200	−19308	4779	13.382	4779	0.000	0.275	1.376
	0.100	−24048	10413	19.145	10413	0.000	0.201	2.005
	0.000	$-\infty$	18243	∞	18243	0.000	0.000	3.384

Reference state: Ta(bcc)

Table IVc. Partial quantities for V in the stable phases at 1800 K.

Phase	x_{V}	ΔG_{V} [J/mol]	ΔH_{V} [J/mol]	ΔS_{V} [J/(mol·K)]	$G_{\mathrm{V}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{V}}^{\mathrm{E}}$ [J/(mol·K)]	a_{V}	γ_{V}
bcc	0.000	$-\infty$	−8697	∞	−8697	0.000	0.000	0.559
	0.100	−37141	−2680	19.145	−2680	0.000	0.084	0.836
	0.200	−22756	1331	13.382	1331	0.000	0.219	1.093
	0.300	−14360	3659	10.010	3659	0.000	0.383	1.277
	0.400	−9086	4628	7.619	4628	0.000	0.545	1.362
	0.500	−5813	4561	5.763	4561	0.000	0.678	1.356
	0.600	−3864	3781	4.247	3781	0.000	0.772	1.287
	0.700	−2726	2612	2.966	2612	0.000	0.833	1.191
	0.800	−1963	1376	1.855	1376	0.000	0.877	1.096
	0.900	−1179	398	0.876	398	0.000	0.924	1.027
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: V(bcc)

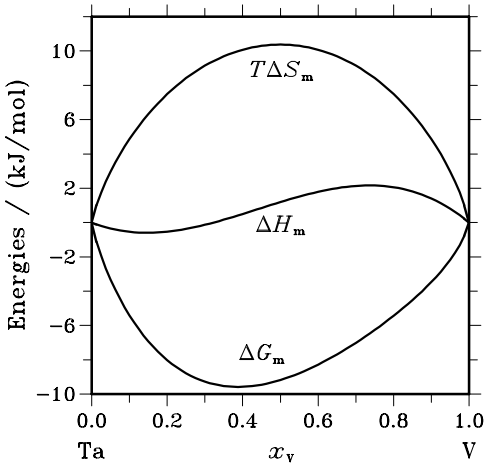

Fig. 4. Integral quantities of the stable phases at T=1800 K.

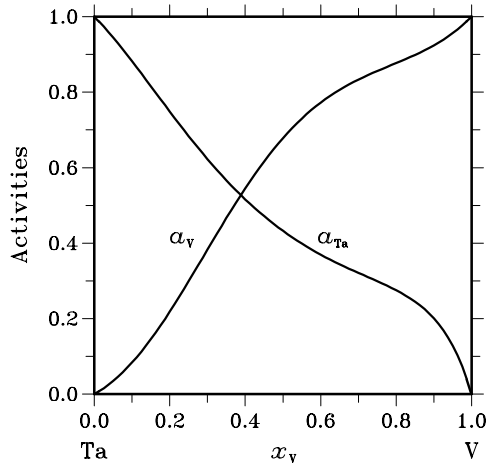

Fig. 5. Activities in the stable phases at T=1800 K.

Table V. Standard reaction quantities at 298.15 K for the compounds per mole of atoms.

Compound	x_{V}	$\Delta_{\mathrm{f}}G^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}H^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}S^{\circ}$ / (J/(mol·K))	$\Delta_{\mathrm{f}}C_P^{\circ}$ / (J/(mol·K))
$C15$	0.666	−1864	−1064	2.685	0.001

References

[83Smi] J.F. Smith, O.N. Carlson: Bull. Alloy Phase Diagrams **4** (1983) 284–289.
[04Dan] C.A. Danon, C. Servant: J. Alloys Comp. **366** (2004) 191–200.