Si – Ta (Silicon – Tantalum)

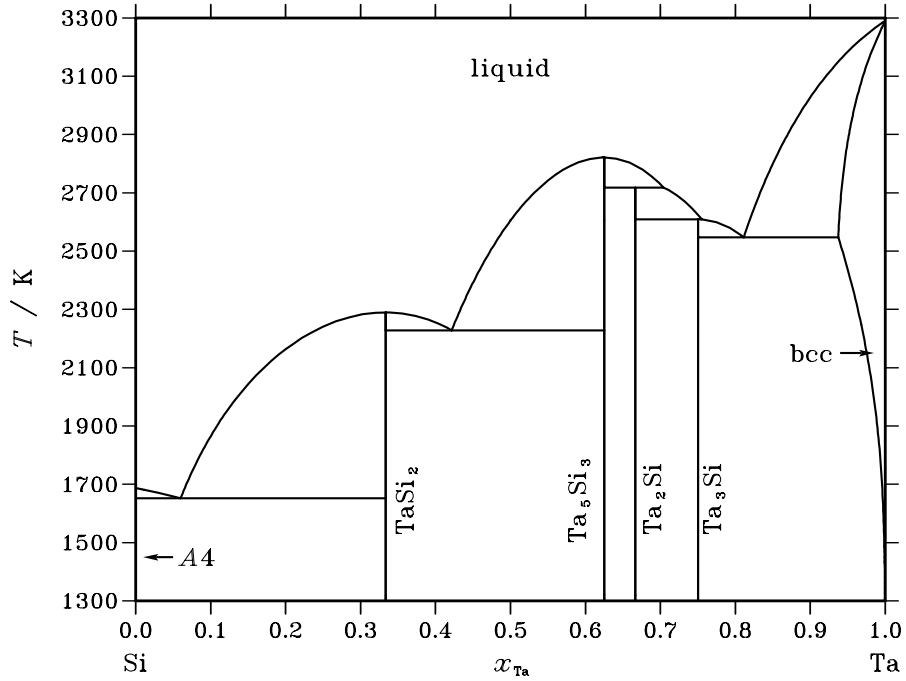

Fig. 1. Calculated phase diagram for the system Si-Ta.

The Si-Ta system has been assessed by [89Vah] and it was later revised by [03Che]. The phase diagram presents complete mutual solubility in the liquid state, a negligible solubility of Ta in crystalline Si, and of Si in bcc-Ta. There are four compounds in the system, $TaSi_2$, Ta_5Si_3, Ta_2Si and Ta_3Si, all considered as stoichiometric. The solution phases were modelled with a simple substitutional model, either sub-regular (liquid) or regular (bcc). The thermodynamic properties of the intermetallic compounds have been determined in various experimental investigations which are reviewed in [89Vah]. The calculated phase diagram is in good agreement with the experimental one. The enthalpy of mixing in the liquid has been determined only at 1950 K for Ta-concentrations less than 10 at.% [88Sud]. Further experimental work would be necessary to assess the liquid enthalpy of mixing and the variation of activity with temperature, which is important for extrapolation of data at high temperatures.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Si,Ta)_1$
$A4$	$A4$	C(diamond)	$cF8$	$Fd\overline{3}m$	DIAMOND_A4	Si_1
$TaSi_2$	$C40$	$CrSi_2$	$hP9$	$P6_222$	TASI2	Ta_1Si_2
βTa_5Si_3	$D8_m$	W_5Si_3	$tI32$	$I4/mcm$	TA5SI3	Ta_5Si_3
αTa_5Si_3	$D8_l$	Cr_5B_3	$tI32$	$I4/mcm$	TA5SI3	Ta_5Si_3
Ta_2Si	$C16$	Al_2Cu	$tI12$	$I4/mcm$	TA2SI	Ta_2Si_1
Ta_3Si	$\cdots$	Ti_3P	$tP32$	$P4_2/n$	TA3SI	Ta_3Si_1
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Si,Ta)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ta}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons$ Ta_5Si_3	congruent	2821.3	0.625	0.625		−28242
Ta_5Si_3 + liquid $\rightleftharpoons$ Ta_2Si	peritectic	2717.7	0.625	0.704	0.667	−16933
Ta_2Si + liquid $\rightleftharpoons$ Ta_3Si	peritectic	2608.6	0.667	0.755	0.750	−31045
liquid $\rightleftharpoons$ Ta_3Si + bcc	eutectic	2547.3	0.811	0.750	0.937	−27058
liquid $\rightleftharpoons$ $TaSi_2$	congruent	2290.0	0.333	0.333		−36397
liquid $\rightleftharpoons$ $TaSi_2$ + Ta_5Si_3	eutectic	2228.4	0.422	0.333	0.625	−29923
liquid $\rightleftharpoons$ $A4$ + $TaSi_2$	eutectic	1652.1	0.060	0.000	0.333	−45318

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

x_{Ta}	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)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−11440	−17597	−1.866	−2520	−4.569	0.000
0.200	−19158	−32232	−3.962	−5428	−8.122	0.000
0.300	−25130	−43549	−5.581	−8369	−10.660	0.000
0.400	−29453	−51193	−6.588	−10987	−12.183	0.000
0.500	−31945	−54807	−6.928	−12927	−12.691	0.000
0.600	−32298	−54037	−6.588	−13832	−12.183	0.000
0.700	−30109	−48527	−5.581	−13348	−10.660	0.000
0.800	−24848	−37922	−3.962	−11118	−8.122	0.000
0.900	−15707	−21864	−1.866	−6787	−4.569	0.000
1.000	0	0	0.000	0	0.000	0.000

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

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

x_{Si}	ΔG_{Si} [J/mol]	ΔH_{Si} [J/mol]	ΔS_{Si} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Si}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Si}}$ [J/(mol·K)]	a_{Si}	γ_{Si}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2637	−1422	0.368	253	−0.508	0.908	1.009
0.800	−5583	−6161	−0.175	539	−2.031	0.816	1.020
0.700	−9639	−14930	−1.603	147	−4.569	0.704	1.005
0.600	−15651	−28439	−3.875	−1635	−8.122	0.565	0.942
0.500	−24537	−47399	−6.928	−5518	−12.691	0.409	0.818
0.400	−37355	−72522	−10.657	−12214	−18.275	0.256	0.641
0.300	−55467	−104518	−14.864	−22433	−24.874	0.132	0.441
0.200	−81046	−144100	−19.107	−36886	−32.489	0.052	0.261
0.100	−119463	−191978	−21.974	−56285	−41.119	0.013	0.129
0.000	$-\infty$	−248863	∞	−81342	−50.764	0.000	0.052

Reference state: Si(liquid)

Table IIIc. 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)]	$G^{\mathrm{E}}_{\mathrm{Ta}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ta}}$ [J/(mol·K)]	a_{Ta}	γ_{Ta}
0.000	$-\infty$	−189595	∞	−22074	−50.764	0.000	0.447
0.100	−90659	−163174	−21.974	−27481	−41.119	0.037	0.367
0.200	−73459	−136514	−19.107	−29300	−32.489	0.069	0.344
0.300	−61275	−110326	−14.864	−28241	−24.874	0.107	0.357
0.400	−50157	−85324	−10.657	−25016	−18.275	0.161	0.402
0.500	−39354	−62216	−6.928	−20335	−12.691	0.238	0.477
0.600	−28927	−41715	−3.875	−14911	−8.122	0.348	0.581
0.700	−19241	−24531	−1.603	−9454	−4.569	0.496	0.709
0.800	−10799	−11377	−0.175	−4676	−2.031	0.675	0.843
0.900	−4178	−2963	0.368	−1288	−0.508	0.859	0.954
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ta(liquid)

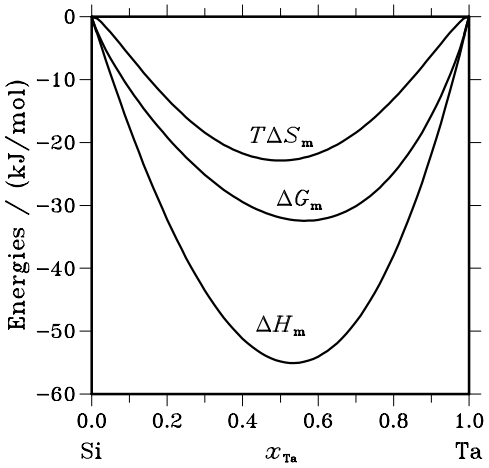

Fig. 2. Integral quantities of the liquid phase at T=3300 K.

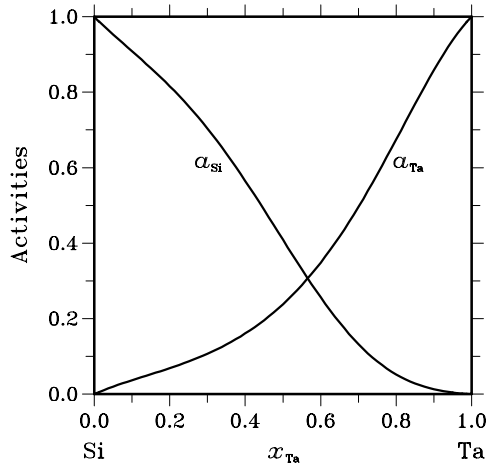

Fig. 3. Activities in the liquid phase at T=3300 K.

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

Compound	x_{Ta}	$\Delta_{\mathrm{f}}G^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}H^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}S^{\circ}$ / (J/(mol·K))	$\Delta_{\mathrm{f}}C^{\circ}_{P}$ / (J/(mol·K))
Ta_1Si_2	0.333	−39713	−39390	1.083	−1.095
Ta_5Si_3	0.625	−42024	−41800	0.752	−0.226
Ta_2Si_1	0.667	−41627	−41783	−0.522	−0.237
Ta_3Si_1	0.750	−37917	−38665	−2.507	−0.263

References

[88Sud] V.S. Sudavtsova: Urk. Khim. Zh. **54** (1988) 996–997.
[89Vah] C. Vahlas, P.-Y. Chevalier, E. Blanquet: Calphad **13** (1989) 273–292.
[03Che] P.-Y. Chevalier, E. Fischer: unpublished work, 2003.