Si – W (Silicon – Tungsten)

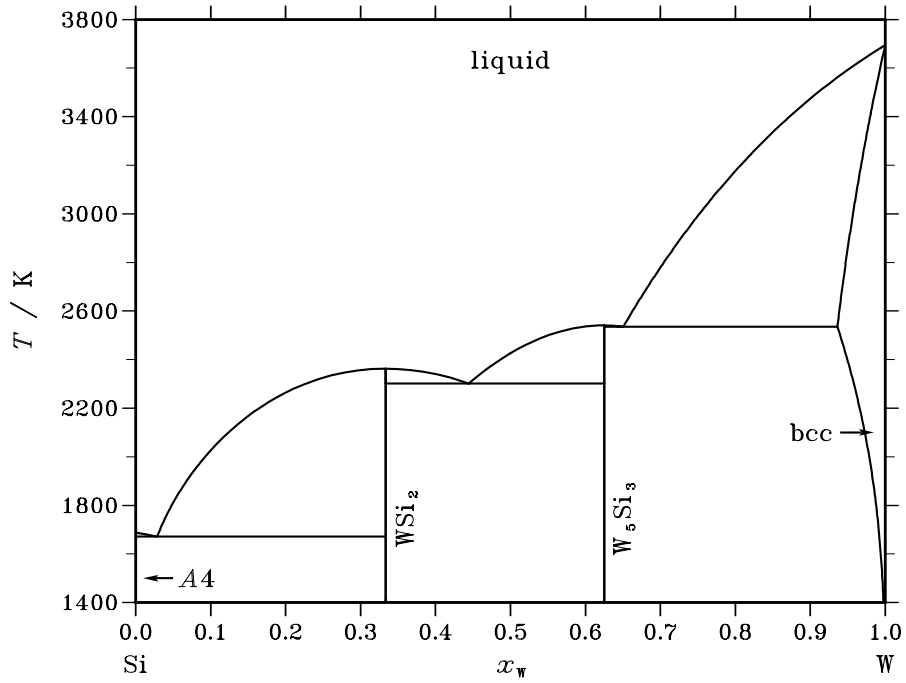

Fig. 1. Calculated phase diagram for the system Si-W.

The phase diagram of Si-W has been reported by Nagender Naidu *et al.* [89Nag]. A critical thermodynamic assessment has been given by [89Vah] and it was updated later by [03Che]. The system presents a complete mutual solubility in the liquid state, a negligible solubility of W in crystalline Si, and a limited solubility of Si in bcc-W. There are two compounds in the system, WSi_2 and W_5Si_3, with a narrow homogeneity range. The solution phases were modelled with a simple substitutional model, by using either a second-order Redlich-Kister polynomial (liquid) or a constant term (bcc). The compounds were considered as stoichiometric. 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 W-concentrations less than 16 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	$(Si,W)_1$
$A4$	$A4$	C(diamond)	$cF8$	$Fd\overline{3}m$	DIAMOND_A4	Si_1
WSi_2	$C11_b$	$MoSi_2$	$tI6$	$I4/mmm$	WSI2	W_1Si_2
W_5Si_3	$D8_m$	W_5Si_3	$tI32$	$I4/mcm$	W5SI3	W_5Si_3
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Si,W)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{W}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons$ W_5Si_3	congruent	2540.8	0.625	0.625		−39599
liquid $\rightleftharpoons$ W_5Si_3 + bcc	eutectic	2535.9	0.650	0.625	0.936	−38948
liquid $\rightleftharpoons$ WSi_2	congruent	2363.0	0.333	0.333		−54676
liquid $\rightleftharpoons$ WSi_2 + W_5Si_3	eutectic	2301.5	0.444	0.333	0.625	−46751
liquid $\rightleftharpoons$ $A4$ + WSi_2	eutectic	1671.1	0.028	0.000	0.333	−49630

Table IIIa. Integral quantities for the liquid phase at 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	−12900	−10978	0.915	−7224	−1.788	0.000
0.200	−21579	−19516	0.982	−12842	−3.178	0.000
0.300	−27521	−25615	0.908	−16855	−4.171	0.000
0.400	−31014	−29274	0.829	−19263	−4.767	0.000
0.500	−32168	−30494	0.797	−20065	−4.966	0.000
0.600	−31014	−29274	0.829	−19263	−4.767	0.000
0.700	−27521	−25615	0.908	−16855	−4.171	0.000
0.800	−21579	−19516	0.982	−12842	−3.178	0.000
0.900	−12900	−10978	0.915	−7223	−1.788	0.000
1.000	0	0	0.000	0	0.000	0.000

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

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

x_{Si}	ΔG_{Si} [J/mol]	ΔH_{Si} [J/mol]	ΔS_{Si} [J/(mol·K)]	$G_{\mathrm{Si}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Si}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Si}	γ_{Si}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2642	−1220	0.677	−803	−0.199	0.860	0.955
0.800	−7107	−4879	1.061	−3210	−0.795	0.666	0.832
0.700	−13451	−10978	1.178	−7224	−1.788	0.463	0.661
0.600	−21761	−19516	1.069	−12842	−3.178	0.288	0.479
0.500	−32168	−30494	0.797	−20065	−4.966	0.158	0.317
0.400	−44893	−43911	0.468	−28894	−7.151	0.076	0.191
0.300	−60350	−59767	0.277	−39328	−9.733	0.032	0.105
0.200	−79469	−78064	0.669	−51367	−12.713	0.011	0.053
0.100	−105216	−98799	3.056	−65012	−16.089	0.002	0.024
0.000	$-\infty$	−121974	∞	−80261	−19.863	0.000	0.010

Reference state: Si(liquid)

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

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
0.000	$-\infty$	−121974	∞	−80261	−19.863	0.000	0.010
0.100	−105216	−98799	3.056	−65012	−16.089	0.002	0.024
0.200	−79469	−78064	0.669	−51367	−12.713	0.011	0.053
0.300	−60350	−59767	0.277	−39328	−9.733	0.032	0.105
0.400	−44893	−43911	0.468	−28894	−7.151	0.076	0.191
0.500	−32168	−30494	0.797	−20065	−4.966	0.158	0.317
0.600	−21761	−19516	1.069	−12842	−3.178	0.288	0.479
0.700	−13451	−10978	1.178	−7223	−1.788	0.463	0.661
0.800	−7107	−4879	1.061	−3210	−0.795	0.666	0.832
0.900	−2642	−1220	0.677	−803	−0.199	0.860	0.955
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: W(liquid)

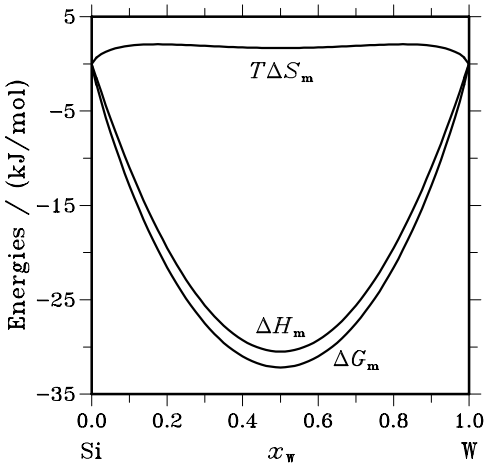

Fig. 2. Integral quantities of the liquid phase at T= K.

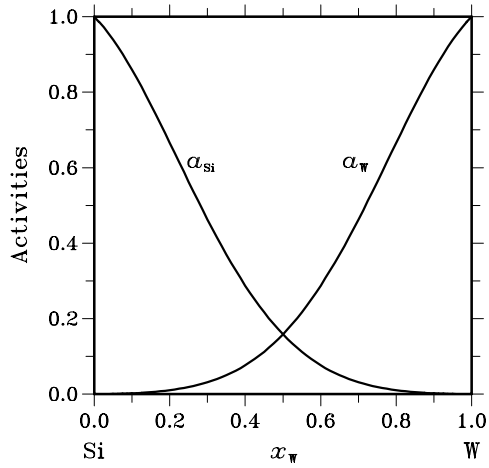

Fig. 3. Activities in the liquid phase at T= K.

Table IVa. Integral quantities for the stable phases at 2600 K.

Phase	x_W	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)]
liquid	0.000	0	0	0.000	0	0.000	0.000
	0.100	−11810	−5760	2.327	−4782	−0.376	0.004
	0.200	−18976	−9081	3.806	−8158	−0.355	0.007
	0.300	−23333	−9962	5.142	−10127	0.063	0.011
	0.400	−25239	−8404	6.475	−10690	0.879	0.014
	0.500	−24830	−4407	7.855	−9846	2.092	0.018
	0.600	−22145	2030	9.298	−7596	3.702	0.021
	0.663	−19276	7327	10.232	−5460	4.918	0.023
bcc	0.939	−4659	−800	1.484	326	−0.433	0.002
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Si(liquid), W(bcc)

Table IVb. Partial quantities for Si in the stable phases at 2600 K.

Phase	x_{Si}	ΔG_{Si} [J/mol]	ΔH_{Si} [J/mol]	ΔS_{Si} [J/(mol·K)]	G^E_{Si} [J/mol]	S^E_{Si} [J/(mol·K)]	a_{Si}	γ_{Si}
liquid	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−2981	−1220	0.677	−703	−0.199	0.871	0.968
	0.800	−7637	−4879	1.061	−2813	−0.795	0.702	0.878
	0.700	−14040	−10978	1.178	−6330	−1.788	0.522	0.746
	0.600	−22296	−19516	1.069	−11253	−3.178	0.357	0.594
	0.500	−32567	−30494	0.797	−17582	−4.966	0.222	0.443
	0.400	−45127	−43911	0.468	−25319	−7.151	0.124	0.310
	0.337	−54409	−53597	0.312	−30903	−8.728	0.081	0.239
bcc	0.061	−54409	−12421	16.149	5940	−7.062	0.081	1.316
	0.000	−∞	−13714	∞	4647	−7.062	0.000	1.240

Reference state: Si(liquid)

Table IVc. Partial quantities for W in the stable phases at 2600 K.

Phase	x_W	ΔG_W [J/mol]	ΔH_W [J/mol]	ΔS_W [J/(mol·K)]	G^E_W [J/mol]	S^E_W [J/(mol·K)]	a_W	γ_W
liquid	0.000	−∞	−69801	∞	−54857	−5.748	0.000	0.079
	0.100	−91271	−46625	17.171	−41494	−1.973	0.015	0.147
	0.200	−64331	−25890	14.785	−29538	1.403	0.051	0.255
	0.300	−45016	−7594	14.393	−18989	4.383	0.125	0.415
	0.400	−29654	8263	14.584	−9846	6.965	0.254	0.634
	0.500	−17094	21680	14.913	−2110	9.150	0.454	0.907
	0.600	−6823	32658	15.185	4220	10.938	0.729	1.216
	0.663	−1409	38311	15.277	7479	11.858	0.937	1.413
bcc	0.939	−1409	−41	0.526	−41	0.000	0.937	0.998
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: W(bcc)

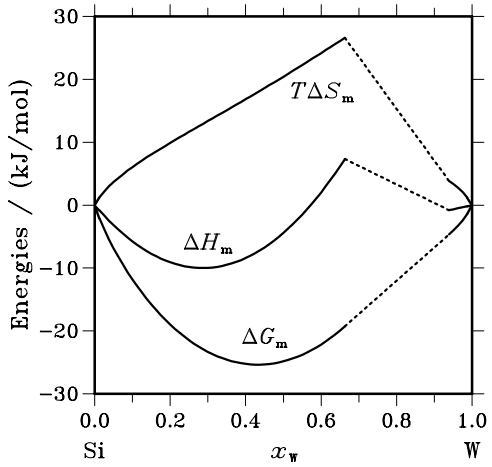

Fig. 4. Integral quantities of the stable phases at T=2600 K.

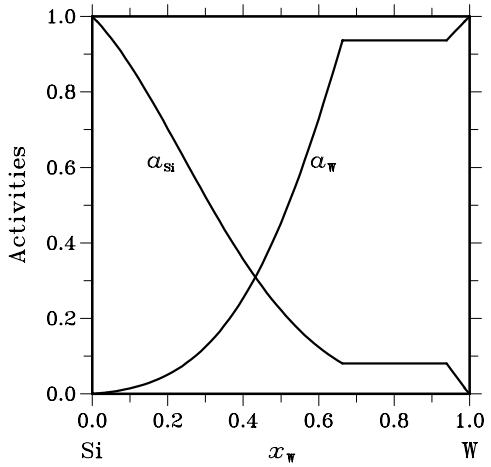

Fig. 5. Activities in the stable phases at T=2600 K.

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

Compound	x_{W}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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))
W_1Si_2	0.333	−31921	−31393	1.771	1.488
W_5Si_3	0.625	−19358	−17975	4.639	−0.151

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