Si – Y (Silicon – Yttrium)

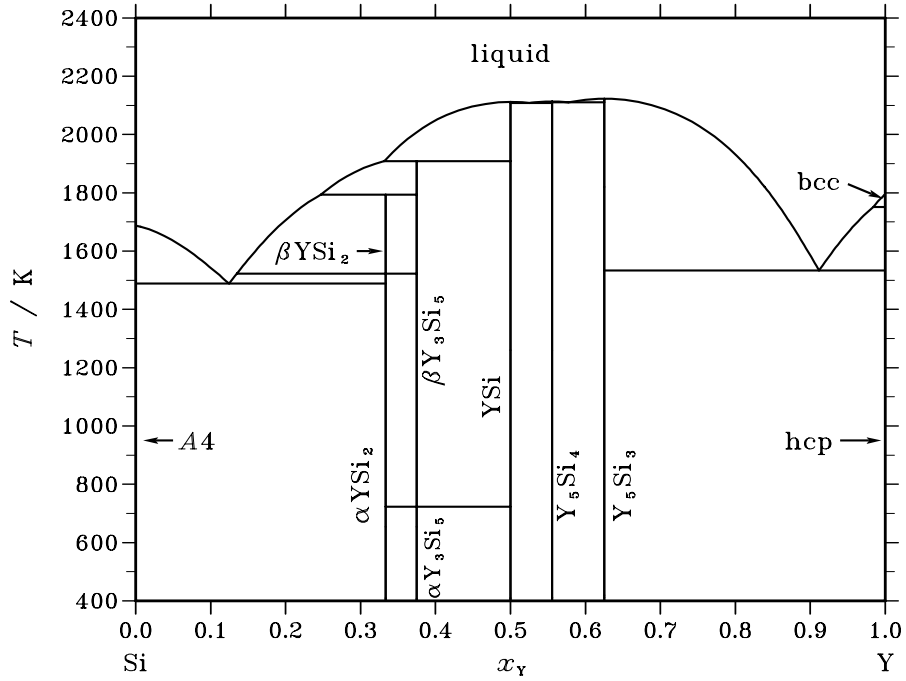

Fig. 1. Calculated phase diagram for the system Si-Y.

Silicides of Y and rare earth metals received considerable attention since it was found that a significant number of these alloys may be utilised in electronic and nuclear technology. Several of these alloys have rather exceptional qualities with respect to absorption of hydrogen gas and superconductivity. Many of these alloys have potential applications in high temperature industrial processes.

The phase diagram of the Si-Y system has been first given by [61Lun] and in this form is quoted by [90Mas]. In this system, five intermetallic phases Y_5Si_3, Y_5Si_4, YSi, Y_3Si_5, and YSi_2 with no homogeneity ranges have been considered. The Si-Y system has been thermodynamically assessed by [89Ran] and [91Luk] and the latter has been selected here. The phase diagram computed using this dataset agrees with [90Mas].

Structures and phase equilibria in the Si-Y system have also been investigated and critically reviewed by [90But]. In this work, thermal analysis, metallography, and microhardness measurements have been used to examine the system. The Y_5Si_3 phase has been confirmed as the most stable silicide. It was suggested that metal vacancies can be present in the structure of this phase leading to silicon-rich Y_5Si_{3+x}, which structurally evolves into Y_5Si_4. A very flat liquidus around Y_5Si_4 and YSi has been considered to modify previous phase diagrams postulating peritectic (instead of eutectic) formation of the Y_5Si_4 and YSi phases. This phase diagram has been also accepted by Okamoto [91Oka].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Si,Y)_1$
$A4$	$A4$	C(diamond)	$cF8$	$Fd\overline{3}m$	DIAMOND_A4	Si_1
αYSi_2	$C32$	AlB_2	$hP3$	$P6/mmm$	SI2Y_R	Si_2Y_1
βYSi_2	C_c	$ThSi_2$	$tI12$	$I4_1/amd$	SI2Y_H	Si_2Y_1
αY_3Si_5	C_c	$ThSi_2$	$tI12$	$I4_1/amd$	SI5Y3_R	Si_5Y_3
βY_3Si_5	⋯	⋯	⋯	⋯	SI5Y3_H	Si_5Y_3
YSi	$B33$	CrB	$oC8$	$Cmcm$	SIY	Si_1Y_1
Y_5Si_4	⋯	⋯	$oP36$	$Pnma$	SI4Y5	Si_4Y_5
Y_5Si_3	$D8_8$	Mn_5Si_3	$hP16$	$P6_3/mcm$	SI3Y5	Si_3Y_5
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Si,Y)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Si,Y)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_Y			$\Delta_r H$ / (J/mol)
liquid ⇌ Y_5Si_3	congruent	2123.0	0.625	0.625		−51850
liquid ⇌ Y_5Si_4	congruent	2113.0	0.556	0.556		−56570
liquid ⇌ YSi	congruent	2111.3	0.500	0.500		−61113
liquid ⇌ Y_5Si_4 + Y_5Si_3	eutectic	2110.5	0.578	0.556	0.625	−54790
liquid ⇌ YSi + Y_5Si_4	eutectic	2108.0	0.525	0.500	0.556	−58842
liquid + YSi ⇌ βY_3Si_5	peritectic	1908.0	0.331	0.500	0.375	−48231
liquid + βY_3Si_5 ⇌ βYSi_2	peritectic	1793.0	0.247	0.375	0.333	−21349
bcc ⇌ liquid + hcp	degenerate	1751.1	1.000	0.984	1.000	−4886
liquid ⇌ Y_5Si_3 + hcp	eutectic	1533.0	0.912	0.625	1.000	−20248
βYSi_2 ⇌ αYSi_2	polymorphic	1523.0	0.333	0.333		−1523
liquid ⇌ $A4$ + αYSi_2	eutectic	1488.4	0.124	0.000	0.333	−54095
βY_3Si_5 ⇌ αY_3Si_5	polymorphic	723.0	0.375	0.375		−723

Table IIIa. Integral quantities for the liquid phase at 2200 K.

x_Y	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)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−26046	−14375	5.305	−20100	2.602	0.000
0.200	−41319	−28787	5.696	−32165	1.536	0.000
0.300	−49414	−40984	3.832	−38240	−1.247	0.000
0.400	−52274	−49312	1.346	−39963	−4.249	0.000
0.500	−51250	−52706	−0.662	−38571	−6.425	0.000
0.600	−47210	−50698	−1.585	−34899	−7.181	0.000
0.700	−40553	−43410	−1.299	−29379	−6.378	0.000
0.800	−31192	−31559	−0.167	−22039	−4.327	0.000
0.900	−18451	−16454	0.907	−12504	−1.795	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Si in the liquid phase at 2200 K.

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}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−6318	442	3.073	−4391	2.197	0.708	0.787
0.800	−18721	−1527	7.815	−14639	5.960	0.359	0.449
0.700	−33787	−9517	11.032	−27263	8.066	0.158	0.225
0.600	−49335	−25357	10.899	−39991	6.652	0.067	0.112
0.500	−64436	−49097	6.973	−51757	1.209	0.030	0.059
0.400	−79468	−79007	0.209	−62707	−7.409	0.013	0.032
0.300	−96214	−111578	−6.984	−74191	−16.994	0.005	0.017
0.200	−118209	−141521	−10.596	−88769	−23.978	0.002	0.008
0.100	−152329	−161767	−4.290	−110211	−23.435	0.000	0.002
0.000	−∞	−163468	∞	−143491	−9.081	0.000	0.000

Reference state: Si(liquid)

Table IIIc. Partial quantities for Y in the liquid phase at 2200 K.

x_Y	ΔG_Y [J/mol]	ΔH_Y [J/mol]	ΔS_Y [J/(mol·K)]	G^E_Y [J/mol]	S^E_Y [J/(mol·K)]	a_Y	γ_Y
0.000	−∞	−134592	∞	−248979	51.994	0.000	0.000
0.100	−203597	−147734	25.392	−161478	6.247	0.000	0.000
0.200	−131712	−137825	−2.779	−102272	−16.160	0.001	0.004
0.300	−85876	−114408	−12.969	−63853	−22.979	0.009	0.030
0.400	−56682	−85244	−12.983	−39921	−20.601	0.045	0.113
0.500	−38064	−56315	−8.296	−25385	−14.059	0.125	0.250
0.600	−25705	−31825	−2.782	−16361	−7.029	0.245	0.409
0.700	−16698	−14194	1.138	−10174	−1.828	0.401	0.573
0.800	−9437	−4068	2.441	−5356	0.585	0.597	0.746
0.900	−3575	−308	1.485	−1648	0.609	0.822	0.914
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Y(liquid)

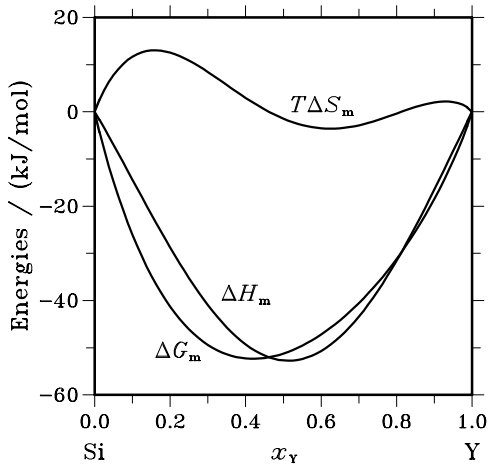

Fig. 2. Integral quantities of the liquid phase at T=2200 K.

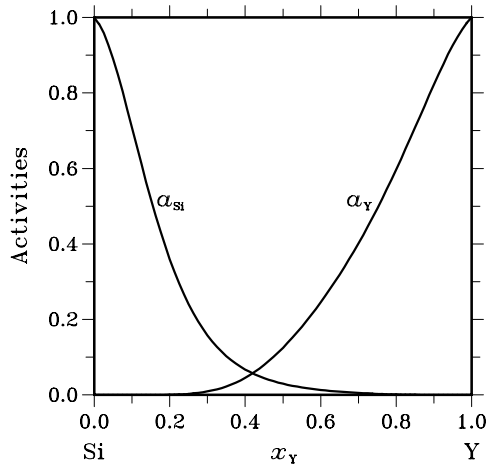

Fig. 3. Activities in the liquid phase at T=2200 K.

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

Compound	x_{Y}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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))
$\alpha\mathrm{Y_1Si_2}$	0.333	−67124	−69848	−9.136	0.000
$\beta\mathrm{Y_1Si_2}$	0.333	−65900	−68325	−8.136	0.000
$\alpha\mathrm{Y_3Si_5}$	0.375	−70713	−73591	−9.654	0.000
$\beta\mathrm{Y_3Si_5}$	0.375	−70288	−72868	−8.654	0.000
$\mathrm{Y_1Si_1}$	0.500	−77338	−80332	−10.042	0.000
$\mathrm{Y_5Si_4}$	0.556	−74290	−77166	−9.646	0.000
$\mathrm{Y_5Si_3}$	0.625	−69124	−71800	−8.975	0.000

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