Fe – Si (Iron – Silicon)

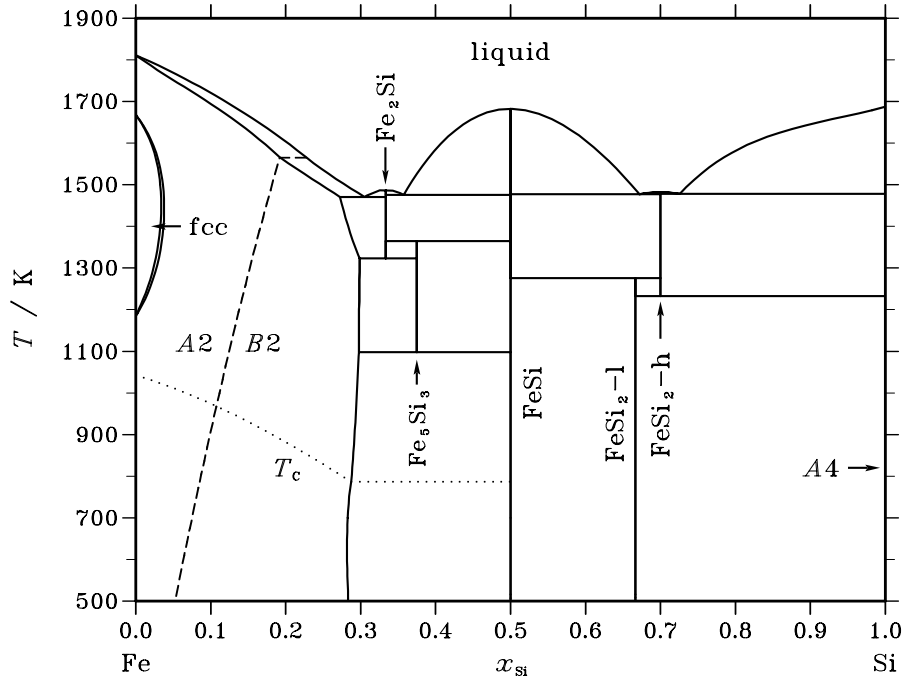

Fig. 1. Calculated phase diagram for the system Fe-Si.

There is complete solubility in the liquid and a considerable solubility of Si in bcc-Fe. This is partially due to the fact that Si stabilises an ordering transformation in the bcc phase. The $B2$ ordered phase is included in the modelling but the low temperature ordering to $D0_3$ has not been considered in the present assessment [91Lac]. The fcc phase is confined into a narrow "gamma-loop" and there are 5 compounds, all modelled as stoichiometric phases.
Si is an important alloying element for steel processing. But it is also used in hard magnets and as cheap bcc stabiliser. It also forms a strong oxide that can protect the surface. It is interesting to use it in higher amounts in stainless steels. But the relations between Si and other alloying elements are very complicated and much information from higher order systems are still missing.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Fe,Si)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Fe,Si)_1$
$A2$	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Fe,Si)_1$
$B2$	$B2$	CsCl	$cP2$	$Pm3m$	B2_BCC	$(Fe,Si)_1(Fe,Si)_1$
Fe_2Si	···	···	$hP6$	$P\overline{3}m1$	FE2SI	Fe_2Si_1
Fe_5Si_3	$D8_8$	Mn_5Si_3	$hP16$	$P6_3/mcm$	D88_M5SI3	Fe_5Si_3
FeSi	$B20$	FeSi	$cP8$	$P2_13$	B20_M1SI1	Fe_1Si_1
$FeSi_2$-l	···	···	$tP3$	$P4/mmm$	FESI2_L	Fe_1Si_2
$FeSi_2$-h	···	···	$oC48$	$Cmca$	FESI2_H	Fe_3Si_7
$A4$	$A4$	C(diamond)	$cF8$	$Fd\overline{3}m$	DIAMOND_FCC_A4	Si_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Si}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons$ FeSi	congruent	1682.3	0.500	0.500		−26822
liquid $\rightleftharpoons$ Fe_2Si	congruent	1487.9	0.333	0.333		−11921
liquid $\rightleftharpoons$ $FeSi_2$-h	congruent	1481.9	0.700	0.700		−23420
liquid $\rightleftharpoons$ $FeSi_2$-h + $A4$	eutectic	1478.3	0.726	0.700	1.000	−24337
liquid $\rightleftharpoons$ FeSi + $FeSi_2$-h	eutectic	1477.2	0.672	0.500	0.700	−23167
liquid $\rightleftharpoons$ Fe_2Si + FeSi	eutectic	1475.7	0.357	0.333	0.500	−13504
liquid $\rightleftharpoons$ $B2$ + Fe_2Si	eutectic	1470.6	0.305	0.272	0.333	−13341
Fe_2Si + FeSi $\rightleftharpoons$ Fe_5Si_3	peritectoid	1364.5	0.333	0.500	0.375	−3234
Fe_2Si $\rightleftharpoons$ $B2$ + Fe_5Si_3	eutectoid	1322.9	0.333	0.299	0.375	−4796
FeSi + $FeSi_2$-h $\rightleftharpoons$ $FeSi_2$-l	peritectoid	1275.7	0.500	0.700	0.667	−4945
$FeSi_2$-h $\rightleftharpoons$ $FeSi_2$-l + $A4$	eutectoid	1232.9	0.700	0.667	1.000	−4996
Fe_5Si_3 $\rightleftharpoons$ $B2$ + FeSi	eutectoid	1098.1	0.375	0.298	0.500	−898

Table IIIa. Integral quantities for the liquid phase at 1873 K.

x_{Si}	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	−13944	−15436	−0.797	−8882	−3.500	0.000
0.200	−23761	−27059	−1.761	−15968	−5.921	0.000
0.300	−30033	−35033	−2.670	−20520	−7.749	0.000
0.400	−32776	−39627	−3.657	−22295	−9.253	0.000
0.500	−32248	−41109	−4.731	−21453	−10.494	0.000
0.600	−28943	−39664	−5.724	−18462	−11.319	0.000
0.700	−23521	−35294	−6.286	−14008	−11.365	0.000
0.800	−16691	−27729	−5.893	−8898	−10.054	0.000
0.900	−9033	−16330	−3.896	−3970	−6.599	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Fe in the liquid phase at 1873 K.

x_{Fe}	ΔG_{Fe} [J/mol]	ΔH_{Fe} [J/mol]	ΔS_{Fe} [J/(mol·K)]	$G_{\mathrm{Fe}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Fe}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Fe}	γ_{Fe}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2370	−1922	0.239	−729	−0.637	0.859	0.954
0.800	−7648	−7540	0.057	−4173	−1.798	0.612	0.765
0.700	−16572	−16325	0.132	−11018	−2.834	0.345	0.493
0.600	−28606	−27640	0.516	−20651	−3.731	0.159	0.266
0.500	−42326	−41109	0.650	−31531	−5.114	0.066	0.132
0.400	−55832	−56992	−0.620	−41562	−8.238	0.028	0.069
0.300	−67214	−76558	−4.988	−48465	−14.999	0.013	0.045
0.200	−75213	−102453	−14.544	−50149	−27.925	0.008	0.040
0.100	−80943	−139076	−31.037	−45085	−50.182	0.006	0.055
0.000	$-\infty$	−192952	∞	−32679	−85.570	0.000	0.123

Reference state: Fe(liquid)

Table IIIc. Partial quantities for Si in the liquid phase at 1873 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}
0.000	$-\infty$	−173560	∞	−93913	−42.524	0.000	0.002
0.100	−118117	−137065	−10.117	−82258	−29.262	0.001	0.005
0.200	−88213	−105133	−9.034	−63149	−22.415	0.003	0.017
0.300	−61442	−78686	−9.207	−42692	−19.217	0.019	0.064
0.400	−39031	−57607	−9.918	−24762	−17.536	0.082	0.204
0.500	−22169	−41109	−10.112	−11375	−15.875	0.241	0.482
0.600	−11018	−28111	−9.126	−3062	−13.374	0.493	0.821
0.700	−4795	−17610	−6.842	759	−9.807	0.735	1.050
0.800	−2061	−9048	−3.731	1415	−5.586	0.876	1.095
0.900	−1043	−2692	−0.880	598	−1.756	0.935	1.039
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Si(liquid)

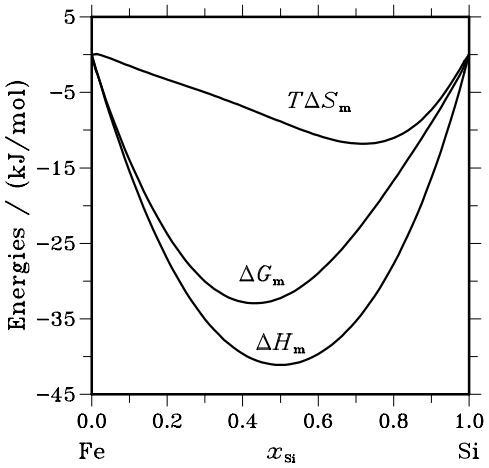

Fig. 2. Integral quantities of the liquid phase at T=1873 K.

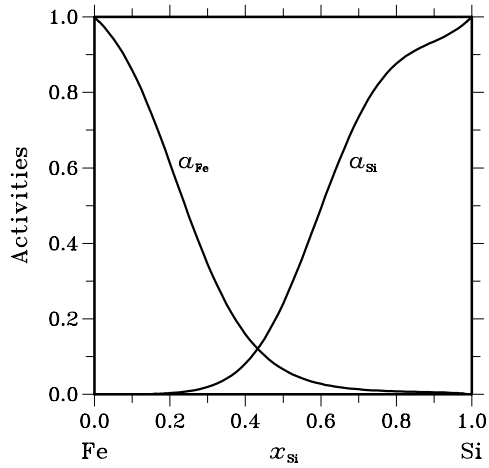

Fig. 3. Activities in the liquid phase at T=1873 K.

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

Compound	x_{Si}	$\Delta_f G^\circ$ / (J/mol)	$\Delta_f H^\circ$ / (J/mol)	$\Delta_f S^\circ$ / (J/(mol·K))	$\Delta_f C^\circ_P$ / (J/(mol·K))
Fe_2Si_1	0.333	−20613	−17652	9.929	−0.278
Fe_5Si_3	0.375	−26130	−24425	5.720	−0.261
Fe_1Si_1	0.500	−32573	−31806	2.572	−0.209
$FeSi_2$-l	0.667	−24248	−24333	−0.285	−0.139
$FeSi_2$-h	0.700	−18036	−16904	3.795	−0.125

References

[91Lac] J. Lacaze, B. Sundman: Metall. Trans. A **22A** (1991) 2211–2223.