Mn – Si (Manganese – Silicon)

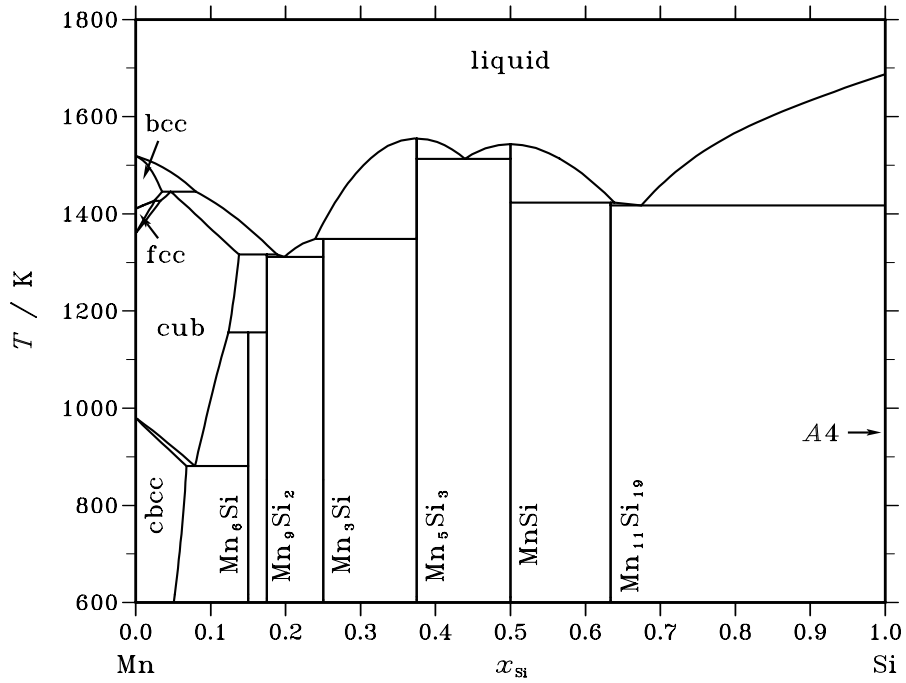

Fig. 1. Calculated phase diagram for the system Mn-Si.

The phase diagram for the Mn-Si system is characterised by continuous mixing between the two components in the liquid phase, the formation of a large number of intermetallic compound phases, substantial solubility of silicon in the cbcc-Mn and cub-Mn phases with rather lower solubility in the higher temperature fcc and bcc phases. The solubility of Mn in crystalline silicon is very low. The experimental data for the system are fairly extensive. Measurements have been made of the enthalpies and partial Gibbs energies in the liquid phase and the heat capacities, enthalpies of formation and vapour pressures of the compound phases. The dataset adopted by SGTE is from the critical assessment of Tibbals [91Tib, 98Ans] and is in good agreement with the experimental data. Other critical assessments for the system have been carried out by Gisby and Dinsdale [88Gis], Chevalier *et al.* [95Che], Chakraborti and Lukas [89Cha] and Kaufman [79Kau].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Mn,Si)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Mn,Si)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Mn,Si)_1$
cbcc	$A12$	αMn	$cI58$	$I\overline{4}3m$	CBCC_A12	$(Mn,Si)_1$
cub	$A13$	βMn	$cP20$	$P4_132$	CUB_A13	$(Mn,Si)_1$
Mn_6Si	⋯	⋯	$hR53$	$R\overline{3}$	MN6SI	$Mn_{17}Si_3$
Mn_9Si_2	⋯	⋯	$oI186$	$Immm$	MN9SI2	$Mn_{33}Si_7$
αMn_3Si	⋯	⋯	⋯	⋯	M3SI	Mn_3Si_1
βMn_3Si	$D0_3$	$AlFe_3$	$cF16$	$Fm\overline{3}m$	M3SI	Mn_3Si_1
Mn_5Si_3	$D8_8$	Mn_5Si_3	$hP16$	$P6_3/mcm$	D88_M5SI3	Mn_5Si_3
MnSi	$B20$	FeSi	$cP8$	$P2_13$	B20_M1SI1	Mn_1Si_1
$Mn_{11}Si_{19}$	⋯	⋯	$tP120$	$P\overline{4}n2$	MN11SI19	$Mn_{11}Si_{19}$
$A4$	$A4$	C(diamond)	$cF8$	$Fd\overline{3}m$	DIAMOND_A4	Si_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Si}			$\Delta_r H$ / (J/mol)
liquid ⇌ Mn_5Si_3	congruent	1555.5	0.375	0.375		−24428
liquid ⇌ MnSi	congruent	1543.6	0.500	0.500		−28076
liquid ⇌ Mn_5Si_3 + MnSi	eutectic	1513.4	0.439	0.375	0.500	−25341
bcc + liquid ⇌ cub	peritectic	1445.3	0.035	0.080	0.047	−7910
bcc + cub ⇌ fcc	peritectoid	1426.6	0.024	0.033	0.025	−1386
MnSi + liquid ⇌ $Mn_{11}Si_{19}$	peritectic	1423.4	0.500	0.639	0.633	−33818
liquid ⇌ $Mn_{11}Si_{19}$ + $A4$	eutectic	1417.1	0.674	0.633	1.000	−35863
liquid + Mn_5Si_3 ⇌ Mn_3Si	peritectic	1348.0	0.239	0.375	0.250	−13458
cub + liquid ⇌ Mn_9Si_2	peritectic	1316.3	0.138	0.189	0.175	−10436
liquid ⇌ Mn_9Si_2 + Mn_3Si	eutectic	1311.0	0.198	0.175	0.250	−14258
cub + Mn_9Si_2 ⇌ Mn_6Si	peritectoid	1155.8	0.124	0.175	0.150	−702
cub ⇌ cbcc + Mn_6Si	eutectoid	881.0	0.079	0.068	0.150	−2122

Table IIIa. Integral quantities for the liquid phase at 1700 K.

x_{Si}	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	−13073	−11658	0.832	−8478	−1.871	0.000
0.200	−22678	−22469	0.123	−15605	−4.038	0.000
0.300	−29061	−30506	−0.850	−20426	−5.929	0.000
0.400	−32117	−34752	−1.550	−22604	−7.146	0.000
0.500	−32061	−34954	−1.702	−22263	−7.465	0.000
0.600	−29350	−31462	−1.243	−19837	−6.838	0.000
0.700	−24545	−25074	−0.311	−15910	−5.391	0.000
0.800	−18138	−16883	0.738	−11065	−3.422	0.000
0.900	−10320	−8120	1.294	−5725	−1.409	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Mn in the liquid phase at 1700 K.

x_{Mn}	ΔG_{Mn} [J/mol]	ΔH_{Mn} [J/mol]	ΔS_{Mn} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Mn}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Mn}}$ [J/(mol·K)]	a_{Mn}	γ_{Mn}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1946	−18	1.134	−457	0.258	0.871	0.968
0.800	−6606	−3142	2.038	−3452	0.182	0.627	0.783
0.700	−14932	−11780	1.854	−9891	−1.111	0.348	0.497
0.600	−26357	−25907	0.265	−19137	−3.982	0.155	0.258
0.500	−39428	−43684	−2.503	−29631	−8.267	0.061	0.123
0.400	−52462	−62080	−5.657	−39511	−13.276	0.024	0.061
0.300	−64254	−77493	−7.788	−47236	−17.798	0.011	0.035
0.200	−74954	−86372	−6.716	−52205	−20.098	0.005	0.025
0.100	−87923	−85833	1.230	−55377	−17.915	0.002	0.020
0.000	−∞	−74286	∞	−59892	−8.467	0.000	0.014

Reference state: Mn(liquid)

Table IIIc. Partial quantities for Si in the liquid phase at 1700 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}
0.000	−∞	−111784	∞	−86494	−14.877	0.000	0.002
0.100	−113214	−116420	−1.886	−80668	−21.031	0.000	0.003
0.200	−86968	−99781	−7.537	−64219	−20.919	0.002	0.011
0.300	−62027	−74199	−7.160	−45010	−17.170	0.012	0.041
0.400	−40756	−48020	−4.273	−27805	−11.891	0.056	0.140
0.500	−24693	−26225	−0.901	−14896	−6.664	0.174	0.349
0.600	−13942	−11050	1.701	−6721	−2.547	0.373	0.622
0.700	−7526	−2609	2.893	−2485	−0.073	0.587	0.839
0.800	−3934	489	2.602	−780	0.746	0.757	0.946
0.900	−1697	515	1.301	−208	0.425	0.887	0.985
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Si(liquid)

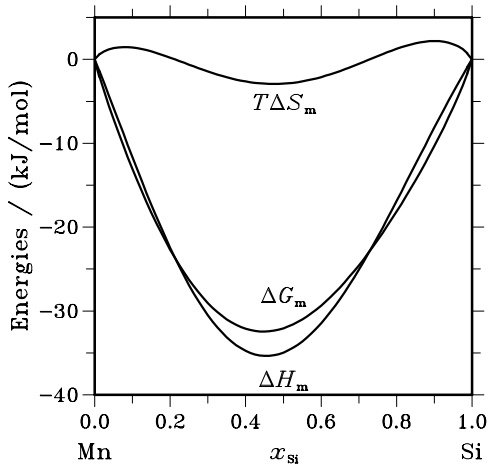

Fig. 2. Integral quantities of the liquid phase at T=1700 K.

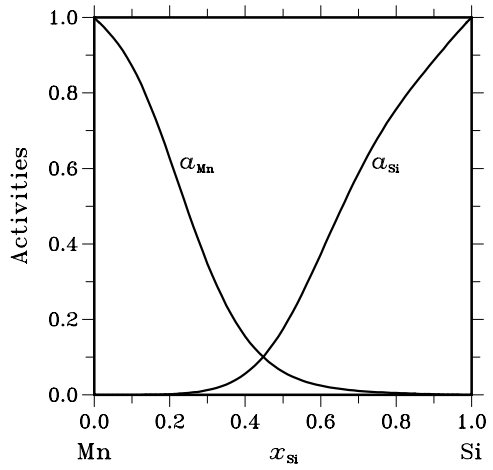

Fig. 3. Activities in the liquid phase at T=1700 K.

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

Compound	x_{Si}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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))
Mn_6Si	0.150	−12416	−12179	0.793	1.577
Mn_9Si_2	0.175	−14138	−13917	0.741	2.156
Mn_3Si_1	0.250	−18826	−18280	1.830	0.053
Mn_5Si_3	0.375	−26069	−24827	4.166	4.033
Mn_1Si_1	0.500	−28870	−28006	2.896	−4.727
$Mn_{11}Si_{19}$	0.633	−21641	−20411	4.124	5.155

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