Mg – Si (Magnesium – Silicon)

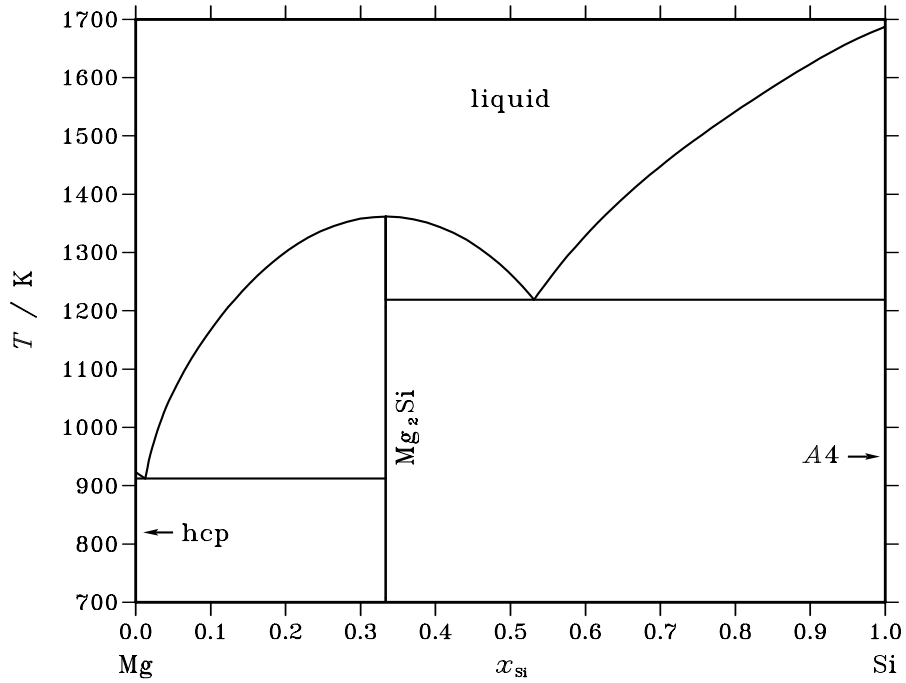

Fig. 1. Calculated phase diagram for the system Mg-Si.

The thermodynamic and phase equilibrium data in the system Mg-Si have been critically assessed by [88Nay]. Also, the thermodynamic model parameters of the four phases in this system (liquid, hcp, $A4$, and Mg_2Si) have been assessed in several works [81Dor, 86Lud, 97Feu, 00Yan]. In all cases liquid and hcp have been modelled as solution phases, Mg_2Si has been treated as a stoichiometric compound and $A4$ is given as pure Si. The most recent thermodynamic assessment of the Mg-Si system [00Yan] has been selected. This assessment has been chosen because of the very good fit to experimental data and because of the lowest total number of parameters (10 compared to 13-17 in other assessments) introduced in the models. The description should not be used at temperatures above 2800 K, where an inverse miscibility gap in the liquid phase starts to develop.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Mg,Si)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Mg,Si)_1$
Mg_2Si	$C1$	CaF_2	$cF12$	$Fm\bar{3}m$	MG2SI	Mg_2Si_1
$A4$	$A4$	C(diamond)	$cF8$	$Fd\bar{3}m$	DIAMOND_A4	Si_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Si}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ Mg_2Si	congruent	1361.5	0.333	0.333		−26535
liquid $\rightleftharpoons$ Mg_2Si + $A4$	eutectic	1219.2	0.531	0.333	1.000	−28179
liquid $\rightleftharpoons$ hcp + Mg_2Si	eutectic	912.6	0.013	0.000	0.333	−9044

Table IIIa. Integral quantities for the liquid phase at 2200 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	−6680	−6228	0.335	−3031	−2.368	0.000
0.200	−11245	−12101	−0.634	−5628	−4.795	0.000
0.300	−14456	−16489	−1.506	−7599	−6.585	0.000
0.400	−16364	−18683	−1.718	−8810	−7.314	0.000
0.500	−16965	−18406	−1.067	−9185	−6.830	0.000
0.600	−16263	−15803	0.340	−8708	−5.256	0.000
0.700	−14278	−11449	2.096	−7421	−2.983	0.000
0.800	−11042	−6341	3.482	−5425	−0.679	0.000
0.900	−6527	−1908	3.422	−2878	0.719	0.000
1.000	0	0	0.000	0	0.000	0.000

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

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

x_{Mg}	ΔG_{Mg} [J/mol]	ΔH_{Mg} [J/mol]	ΔS_{Mg} [J/(mol·K)]	$G_{\mathrm{Mg}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Mg}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Mg}	γ_{Mg}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1362	47	1.044	−180	0.168	0.886	0.984
0.800	−3510	−1534	1.464	−1005	−0.392	0.731	0.914
0.700	−6778	−6369	0.303	−2774	−2.663	0.547	0.781
0.600	−11341	−14804	−2.565	−5607	−6.813	0.364	0.607
0.500	−17230	−25906	−6.427	−9450	−12.190	0.215	0.431
0.400	−24356	−37462	−9.708	−14071	−17.326	0.114	0.285
0.300	−32579	−45980	−9.927	−19065	−19.937	0.055	0.183
0.200	−41913	−46690	−3.539	−23848	−16.921	0.024	0.119
0.100	−53507	−33542	14.788	−27661	−4.356	0.009	0.085
0.000	$-\infty$	794	∞	−29570	22.492	0.000	0.072

Reference state: Mg(liquid)

Table IIIc. 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)]	$G_{\mathrm{Si}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Si}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Si}	γ_{Si}
0.000	$-\infty$	−59206	∞	−31688	−20.384	0.000	0.059
0.100	−54536	−62702	−6.049	−28690	−25.194	0.008	0.078
0.200	−42184	−54370	−9.027	−24119	−22.409	0.023	0.117
0.300	−32371	−40100	−5.725	−18857	−15.736	0.056	0.186
0.400	−23899	−24502	−0.447	−13614	−8.065	0.119	0.297
0.500	−16701	−10906	4.292	−8920	−1.471	0.226	0.452
0.600	−10867	−1364	7.039	−5133	2.792	0.380	0.633
0.700	−6435	3351	7.248	−2431	4.283	0.564	0.805
0.800	−3324	3746	5.237	−819	3.382	0.744	0.930
0.900	−1307	1607	2.159	−125	1.283	0.890	0.989
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Si(liquid)

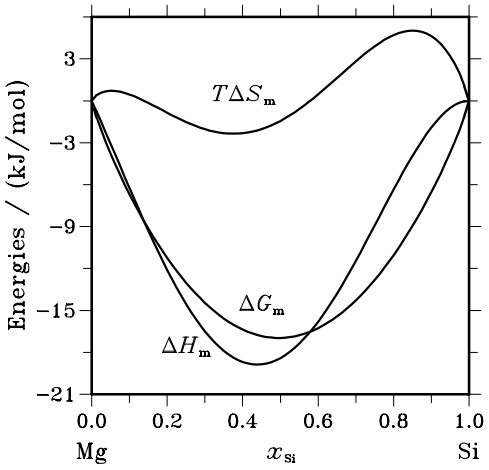

Fig. 2. Integral quantities of the liquid phase at T=2200 K.

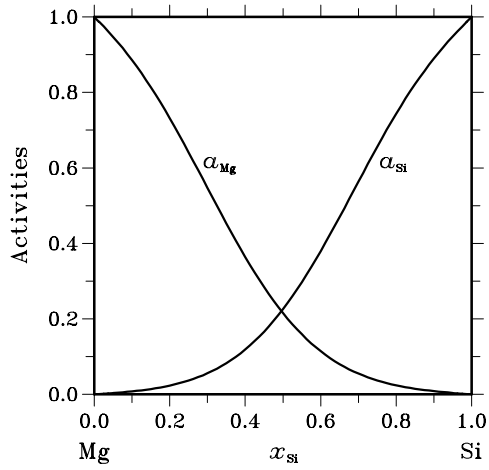

Fig. 3. Activities in the liquid phase at T=2200 K.

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

Compound	x_{Si}	$\Delta_f G^\circ$ / (J/mol)	$\Delta_f H^\circ$ / (J/mol)	$\Delta_f S^\circ$ / (J/(mol·K))	$\Delta_f C_P^\circ$ / (J/(mol·K))
Mg_2Si_1	0.333	−19910	−21370	−4.895	0.000

References

[81Dor] P. Dörner, H. Krieg, H.L. Lukas, R. Müller, G. Petzow: Calphad **5** (1981) 41–55.
[86Lud] D. Lüdecke: Z. Metallkd. **77** (1986) 278–283.
[88Nay] A.A. Nayeb-Hashemi, J.B. Clark in: "Phase Diagrams of Binary Magnesium Alloys", ASM Int., Metals Park, OH, 1988, pp. 280–288.
[97Feu] H. Feufel, T. Gödecke, H.L. Lukas, F. Sommer: J. Alloys Comp. **247** (1997) 31–42.
[00Yan] X.-Y. Yan, F. Zhang, Y.A. Chang: J. Phase Equilbria **21** (2000) 379–384.