Ga – Si (Gallium – Silicon)

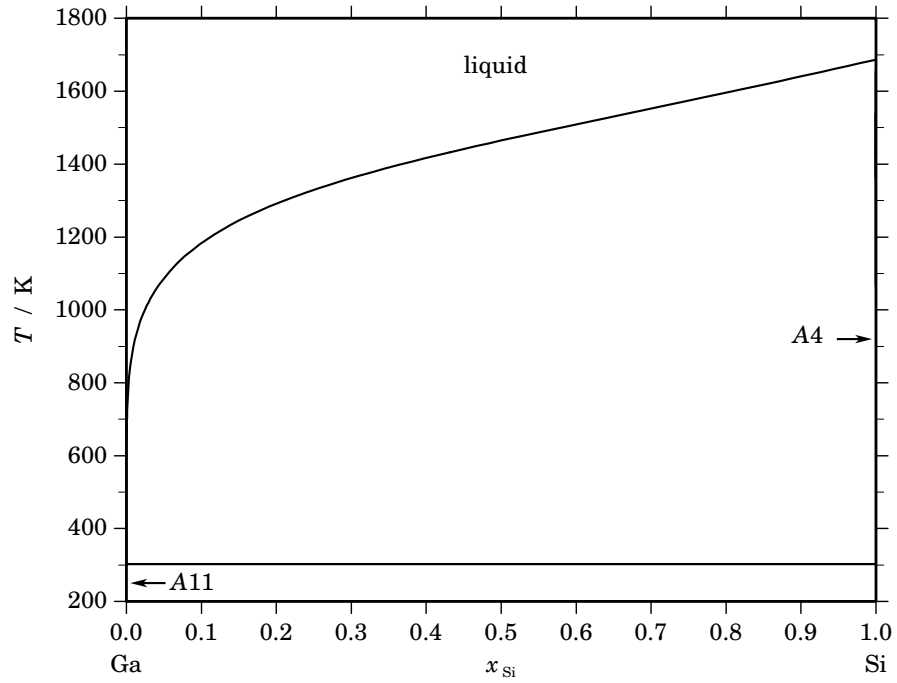

Fig. 1. Calculated phase diagram for the system Ga-Si.

The system Ga-Si is of interest for the semiconductor industry. Ga can be used as a p-type dopant in Si and furthermore, thin films of silicon can be grown from its solution in Ga melts by liquid phase epitaxy. A thorough review on the gallium-silicon system has been given by Olesinski *et al.* [1985Ole]. Since then, it seems that only one major thermodynamic investigation has been published for this system [2004Sud]. The selected dataset has been optimised by [2005Fra]. The phase diagram of Ga-Si is simple eutectic and almost degenerate on the Ga-side. For the optimisation of the liquidus curve, data from 3 experimental investigations have been selected which are in good mutual agreement [1948Kle, 1953Kec, 1977Gir]. For the solid solubility of gallium in crystalline silicon the data of [1960Tru, 1977Gir] have been chosen. In a recent investigation mixing enthalpies for the melt have been reported [2004Sud] across the whole composition range. These data compare well with the partial enthalpy of Si in Ga-rich melts which have been given in [1983Tma].

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Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Ga,Si)_1$
$A11$	$A11$	αGa	$oC8$	$Cmca$	ORTHORHOMBIC_CMCA	Ga_1
$A4$	$A4$	C(diamond)	$cF8$	$Fd\overline{3}m$	DIAMOND_A4	$(Ga,Si)_1$

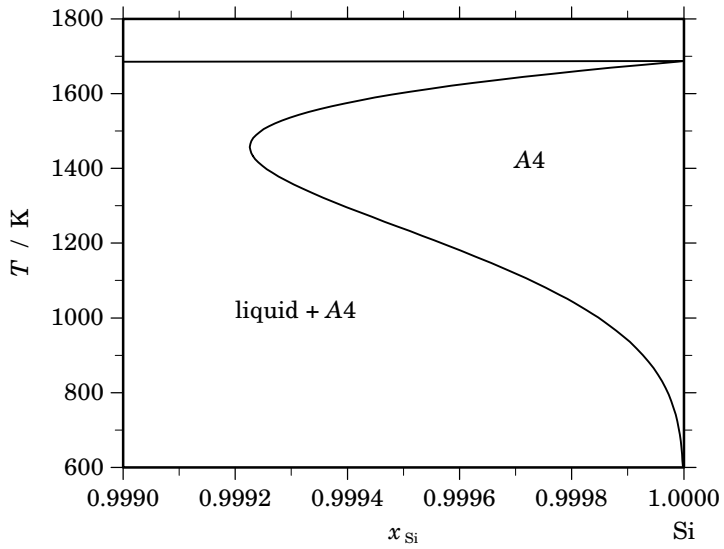

Fig. 2. Partial phase diagram for the system Ga-Si.

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Si}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons$ $A11$ + $A4$	eutectic	302.9	0.000	0.000	1.000	−5590

Table IIIa. Integral quantities for the liquid phase at 1750 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	−4282	1656	3.393	448	0.690	0.000
0.200	−6485	2944	5.388	796	1.227	0.000
0.300	−7843	3864	6.690	1045	1.611	0.000
0.400	−8598	4416	7.437	1195	1.841	0.000
0.500	−8841	4600	7.681	1244	1.918	0.000
0.600	−8598	4416	7.437	1195	1.841	0.000
0.700	−7843	3864	6.690	1045	1.611	0.000
0.800	−6485	2944	5.388	796	1.227	0.000
0.900	−4282	1656	3.393	448	0.690	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Ga in the liquid phase at 1750 K.

x_{Ga}	ΔG_{Ga} [J/mol]	ΔH_{Ga} [J/mol]	ΔS_{Ga} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ga}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ga}}$ [J/(mol·K)]	a_{Ga}	γ_{Ga}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1483	184	0.953	50	0.077	0.903	1.003
0.800	−3048	736	2.162	199	0.307	0.811	1.014
0.700	−4742	1656	3.656	448	0.690	0.722	1.031
0.600	−6636	2944	5.474	796	1.227	0.634	1.056
0.500	−8841	4600	7.681	1244	1.918	0.545	1.089
0.400	−11541	6624	10.380	1792	2.761	0.452	1.131
0.300	−15079	9016	13.769	2439	3.758	0.355	1.182
0.200	−20232	11776	18.291	3186	4.909	0.249	1.245
0.100	−29472	14904	25.358	4032	6.213	0.132	1.319
0.000	−∞	18400	∞	4978	7.670	0.000	1.408

Reference state: Ga(liquid)

Table IIIc. Partial quantities for Si in the liquid phase at 1750 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	−∞	18400	∞	4978	7.670	0.000	1.408
0.100	−29472	14904	25.358	4032	6.213	0.132	1.319
0.200	−20232	11776	18.291	3186	4.909	0.249	1.245
0.300	−15079	9016	13.769	2439	3.758	0.355	1.182
0.400	−11541	6624	10.380	1792	2.761	0.452	1.131
0.500	−8841	4600	7.681	1244	1.918	0.545	1.089
0.600	−6636	2944	5.474	796	1.227	0.634	1.056
0.700	−4742	1656	3.656	448	0.690	0.722	1.031
0.800	−3048	736	2.162	199	0.307	0.811	1.014
0.900	−1483	184	0.953	50	0.077	0.903	1.003
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Si(liquid)

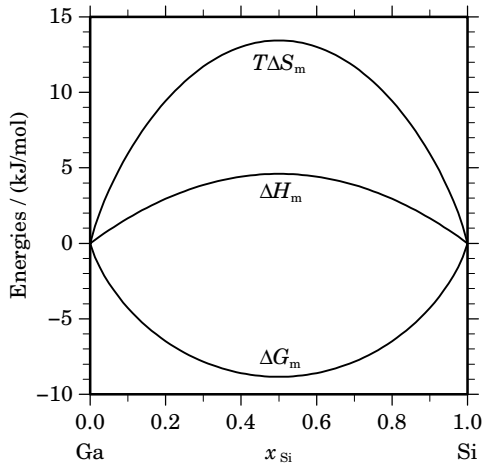

Fig. 3. Integral quantities of the liquid phase at T=1750 K.

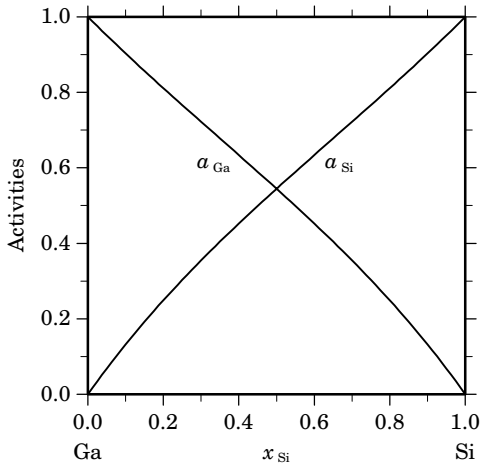

Fig. 4. Activities in the liquid phase at T=1750 K.