Ge – Si (Germanium – Silicon)

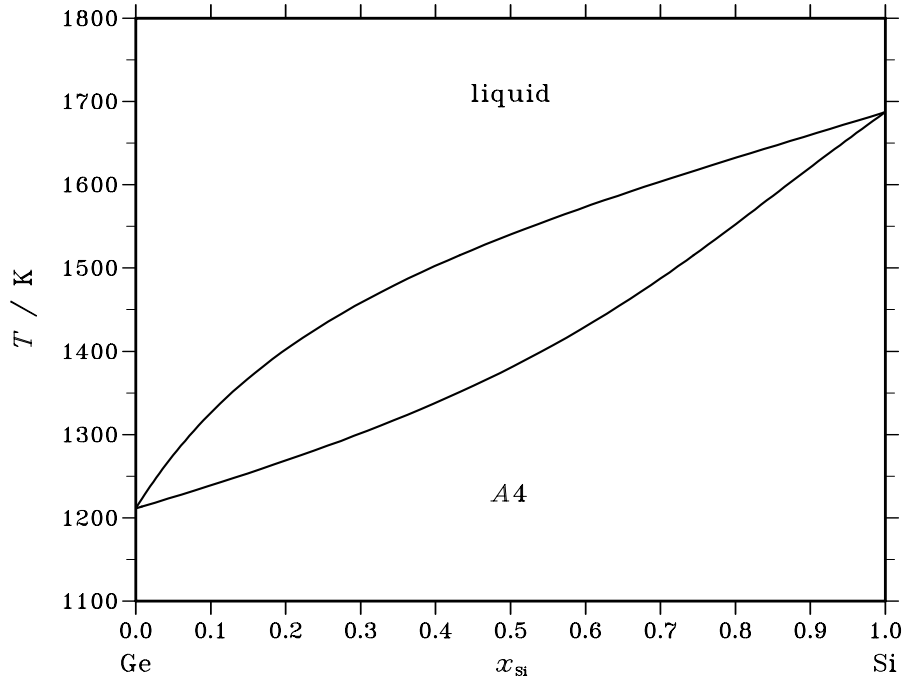

Fig. 1. Calculated phase diagram for the system Ge-Si.

The phase diagram for the Ge-Si system is very simple showing complete solubility in both the liquid phase and the crystalline diamond structure. Data for the system have been reviewed by Olesinski and Abbaschian [84Ole]. The solidus and liquidus phase boundaries have been determined experimentally by Stöhr and Klemm [39Sto] and Hassion *et al.* [55Has]. There have been few measurements of the thermodynamic properties of the system. Bergman *et al.* [93Ber] have measured the partial enthalpy of Si in liquid alloys at 1327 K by drop calorimetry for mole fractions of Si up to 0.03 and the vapour pressures of both components in the liquid at 1723 K by Knudsen cell mass spectrometry. Their measurements indicate that the liquid phase thermodynamic properties can be represented by a regular solution model and data were developed by Dinsdale [98Din] to be consistent with the partial enthalpy and vapour pressure measurements. A regular solution parameter for the crystalline phase derived by Olesinski and Abbaschian [84Ole] from the phase boundary information was also adopted. The assessed data are in good agreement with the experimental data for the system.

Table I. Phases, structures and models.

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

Table IIa. Integral quantities for the liquid phase at 1723 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	−4117	595	2.735	540	0.032	0.000
0.200	−6209	1058	4.217	960	0.057	0.000
0.300	−7491	1388	5.153	1260	0.074	0.000
0.400	−8201	1586	5.681	1440	0.085	0.000
0.500	−8430	1653	5.852	1500	0.089	0.000
0.600	−8201	1586	5.681	1440	0.085	0.000
0.700	−7491	1388	5.153	1260	0.074	0.000
0.800	−6209	1058	4.217	960	0.057	0.000
0.900	−4117	595	2.735	540	0.032	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIb. Partial quantities for Ge in the liquid phase at 1723 K.

x_{Ge}	ΔG_{Ge} [J/mol]	ΔH_{Ge} [J/mol]	ΔS_{Ge} [J/(mol·K)]	$G_{\mathrm{Ge}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Ge}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Ge}	γ_{Ge}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1449	66	0.880	60	0.004	0.904	1.004
0.800	−2957	264	1.869	240	0.014	0.814	1.017
0.700	−4570	595	2.997	540	0.032	0.727	1.038
0.600	−6358	1058	4.304	960	0.057	0.642	1.069
0.500	−8430	1653	5.852	1500	0.089	0.555	1.110
0.400	−10967	2380	7.746	2160	0.127	0.465	1.163
0.300	−14308	3239	10.184	2940	0.173	0.368	1.228
0.200	−19217	4230	13.608	3840	0.227	0.261	1.307
0.100	−28127	5354	19.432	4860	0.287	0.140	1.404
0.000	−∞	6610	∞	6000	0.354	0.000	1.520

Reference state: Ge(liquid)

Table IIc. Partial quantities for Si in the liquid phase at 1723 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	−∞	6610	∞	6000	0.354	0.000	1.520
0.100	−28127	5354	19.432	4860	0.287	0.140	1.404
0.200	−19217	4230	13.608	3840	0.227	0.261	1.307
0.300	−14308	3239	10.184	2940	0.173	0.368	1.228
0.400	−10967	2380	7.746	2160	0.127	0.465	1.163
0.500	−8430	1653	5.852	1500	0.089	0.555	1.110
0.600	−6358	1058	4.304	960	0.057	0.642	1.069
0.700	−4570	595	2.997	540	0.032	0.727	1.038
0.800	−2957	264	1.869	240	0.014	0.814	1.017
0.900	−1449	66	0.880	60	0.004	0.904	1.004
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Si(liquid)

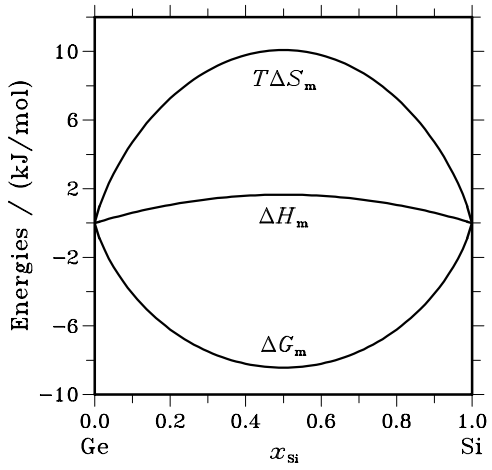

Fig. 2. Integral quantities of the liquid phase at T=1723 K.

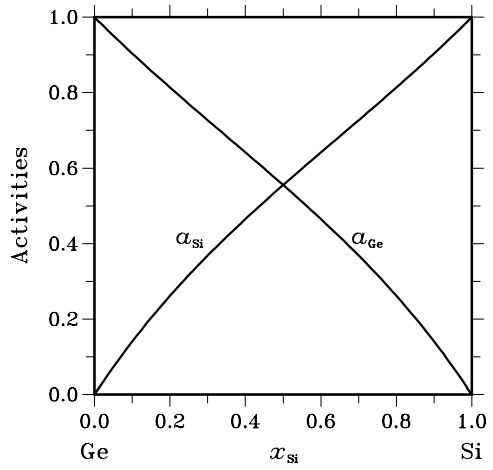

Fig. 3. Activities in the liquid phase at T=1723 K.

Table IIIa. Integral quantities for the stable phases at 1100 K.

Phase	x_{Si}	ΔG_{m} [J/mol]	ΔH_{m} [J/mol]	ΔS_{m} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{m}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{m}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
$A4$	0.000	0	0	0.000	0	0.000	0.000
	0.100	−2658	315	2.703	315	0.000	0.000
	0.200	−4017	560	4.161	560	0.000	0.000
	0.300	−4852	735	5.079	735	0.000	0.000
	0.400	−5315	840	5.596	840	0.000	0.000
	0.500	−5465	875	5.763	875	0.000	0.000
	0.600	−5315	840	5.596	840	0.000	0.000
	0.700	−4852	735	5.079	735	0.000	0.000
	0.800	−4017	560	4.161	560	0.000	0.000
	0.900	−2658	315	2.703	315	0.000	0.000
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Ge($A4$), Si($A4$)

Table IIIb. Partial quantities for Ge in the stable phases at 1100 K.

Phase	x_{Ge}	ΔG_{Ge} [J/mol]	ΔH_{Ge} [J/mol]	ΔS_{Ge} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ge}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ge}}$ [J/(mol·K)]	a_{Ge}	γ_{Ge}
$A4$	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−929	35	0.876	35	0.000	0.903	1.004
	0.800	−1901	140	1.855	140	0.000	0.812	1.015
	0.700	−2947	315	2.966	315	0.000	0.725	1.035
	0.600	−4112	560	4.247	560	0.000	0.638	1.063
	0.500	−5465	875	5.763	875	0.000	0.550	1.100
	0.400	−7120	1260	7.619	1260	0.000	0.459	1.148
	0.300	−9296	1715	10.010	1715	0.000	0.362	1.206
	0.200	−12480	2240	13.382	2240	0.000	0.256	1.278
	0.100	−18224	2835	19.145	2835	0.000	0.136	1.363
	0.000	$-\infty$	3500	∞	3500	0.000	0.000	1.466

Reference state: Ge($A4$)

Table IIIc. Partial quantities for Si in the stable phases at 1100 K.

Phase	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}
$A4$	0.000	$-\infty$	3500	∞	3500	0.000	0.000	1.466
	0.100	−18224	2835	19.145	2835	0.000	0.136	1.363
	0.200	−12480	2240	13.382	2240	0.000	0.256	1.278
	0.300	−9296	1715	10.010	1715	0.000	0.362	1.206
	0.400	−7120	1260	7.619	1260	0.000	0.459	1.148
	0.500	−5465	875	5.763	875	0.000	0.550	1.100
	0.600	−4112	560	4.247	560	0.000	0.638	1.063
	0.700	−2947	315	2.966	315	0.000	0.725	1.035
	0.800	−1901	140	1.855	140	0.000	0.812	1.015
	0.900	−929	35	0.876	35	0.000	0.903	1.004
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Si($A4$)

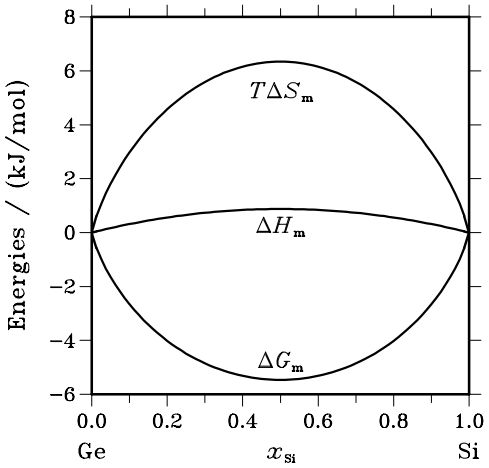

Fig. 4. Integral quantities of the stable phases at T=1100 K.

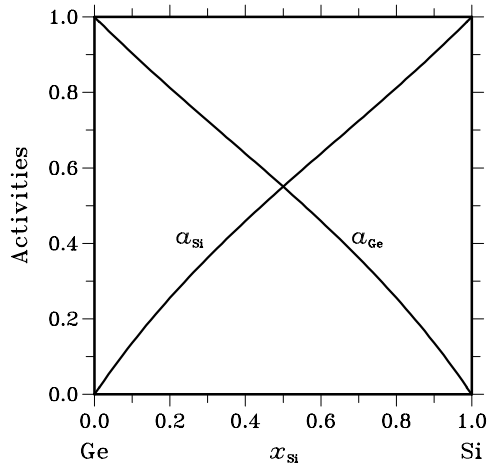

Fig. 5. Activities in the stable phases at T=1100 K.

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