Si – Te (Silicon – Tellurium)

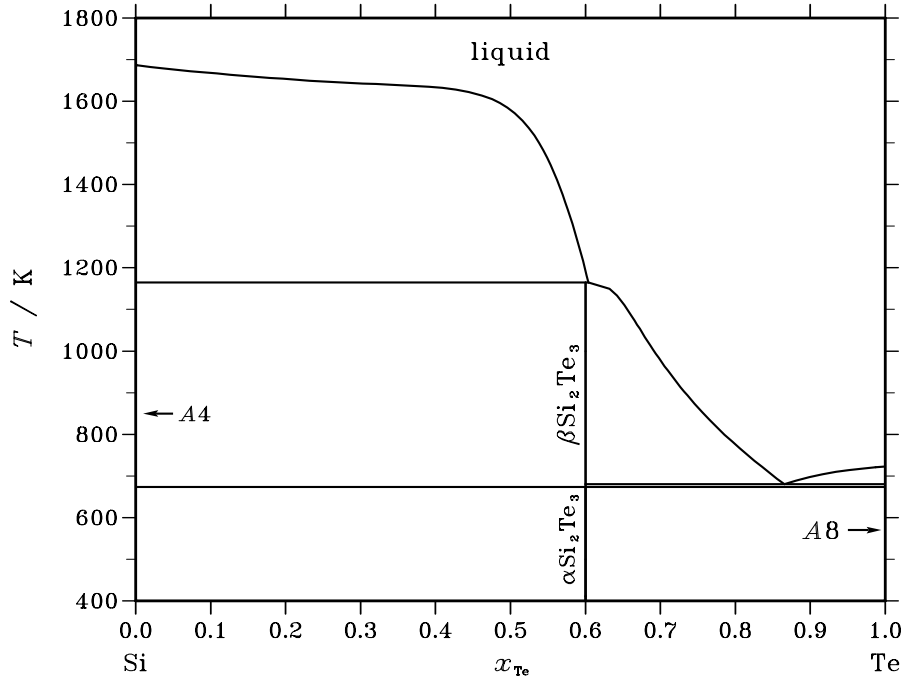

Fig. 1. Calculated phase diagram for the system Si-Te.

The Si-Te system has been assessed by [99Feu]. There is one intermediate compound, Si_2Te_3, which undergoes a polymorphic transition at 674 K. No solubility range has been observed for the two forms of this compound, as well as for Si and Te. Si_2Te_3 decomposes peritectically at 1165 K and a eutectic reaction occurs at 680 K.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Si,Te)_1$
$A4$	$A4$	C(diamond)	$cF8$	$Fd\overline{3}m$	DIAMOND_A4	Si_1
αSi_2Te_3	⋯	αSi_2Te_3	$hP40$	$P\overline{3}1c$	SI2TE3_LT	Si_2Te_3
βSi_2Te_3	⋯	⋯	⋯	⋯	SI2TE3_HT	Si_2Te_3
$A8$	$A8$	γSe	$hP3$	$P3_121$	TRIGONAL_A8	Te_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Te}			$\Delta_r H$ / (J/mol)
$A4$ + liquid $\rightleftharpoons$ βSi_2Te_3	peritectic	1165.1	0.000	0.604	0.600	−24537
liquid $\rightleftharpoons$ βSi_2Te_3 + $A8$	eutectic	680.2	0.865	0.600	1.000	−15633
$\beta Si_2Te_3 \rightleftharpoons \alpha Si_2Te_3$	polymorphic	674.0	0.600	0.600		−157

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

x_{Te}	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	−6676	−2505	2.454	−2081	−0.249	0.388
0.200	−12574	−5480	4.173	−5501	0.012	0.460
0.300	−18249	−8777	5.572	−9615	0.493	0.475
0.400	−23806	−12507	6.647	−14294	1.051	0.463
0.500	−29153	−16748	7.297	−19355	1.534	0.430
0.600	−33149	−20747	7.295	−23636	1.699	0.352
0.700	−31432	−20417	6.479	−22797	1.400	0.189
0.800	−23383	−14749	5.079	−16310	0.918	0.070
0.900	−12702	−7650	2.972	−8107	0.269	0.042
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. 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)]	$G_{\mathrm{Si}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Si}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Si}	γ_{Si}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−592	328	0.542	897	−0.334	0.959	1.066
0.800	−1056	765	1.071	2099	−0.785	0.928	1.160
0.700	−1425	1694	1.835	3617	−1.131	0.904	1.292
0.600	−1808	3459	3.098	5413	−1.149	0.880	1.467
0.500	−3871	5310	5.401	5927	−0.363	0.760	1.521
0.400	−20044	−2386	10.387	−7093	2.768	0.242	0.605
0.300	−72123	−49591	13.254	−55105	3.243	0.006	0.020
0.200	−100702	−67799	19.355	−77953	5.973	0.001	0.004
0.100	−116928	−74676	24.854	−84381	5.709	0.000	0.003
0.000	$-\infty$	−32411	∞	−4276	−16.550	0.000	0.739

Reference state: Si(liquid)

Table IIIc. Partial quantities for Te in the liquid phase at 1700 K.

x_{Te}	ΔG_{Te} [J/mol]	ΔH_{Te} [J/mol]	ΔS_{Te} [J/(mol·K)]	$G_{\mathrm{Te}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Te}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Te}	γ_{Te}
0.000	$-\infty$	0	∞	0	0.000	0.000	1.000
0.100	−61426	−28002	19.661	−28880	0.516	0.013	0.130
0.200	−58648	−30459	16.582	−35899	3.200	0.016	0.079
0.300	−57507	−33208	14.293	−40489	4.283	0.017	0.057
0.400	−56804	−36455	11.970	−43853	4.352	0.018	0.045
0.500	−54435	−38807	9.193	−44637	3.430	0.021	0.043
0.600	−41885	−32988	5.233	−34665	0.986	0.052	0.086
0.700	−13993	−7914	3.576	−8951	0.610	0.372	0.531
0.800	−4053	−1486	1.510	−899	−0.345	0.751	0.938
0.900	−1121	−202	0.540	368	−0.336	0.924	1.026
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Te(liquid)

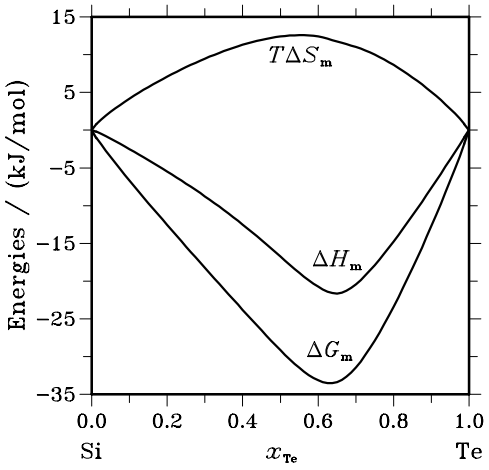

Fig. 2. Integral quantities of the liquid phase at T=1700 K.

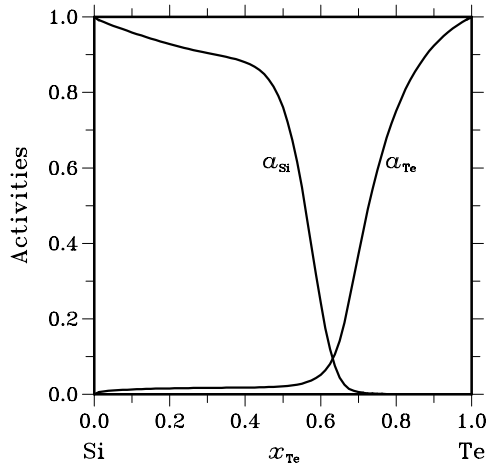

Fig. 3. Activities in the liquid phase at T=1700 K.

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

Compound	x_{Te}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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))
βSi_2Te_3	0.600	−18094	−14043	13.587	0.000
αSi_2Te_3	0.600	−18182	−14200	13.355	0.000

References

[99Feu] Y. Feutelais, A. Schlieper, S.G. Fries: Calphad **23** (1999) 365–378.