Sn – Ti (Tin – Titanium)

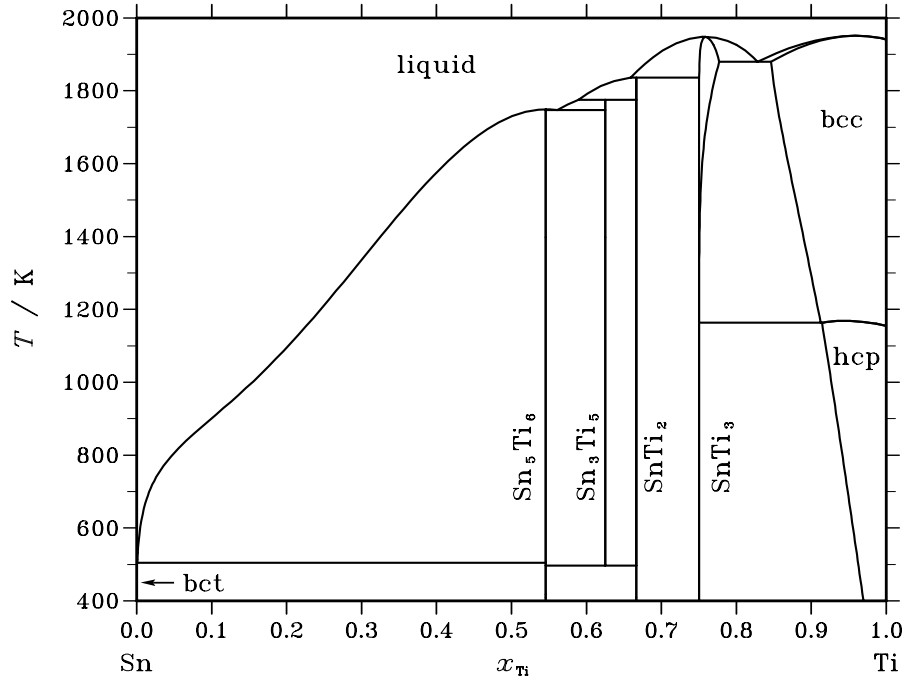

Fig. 1. Calculated phase diagram for the system Sn-Ti.

An understanding of phase equilibria and thermodynamic properties in the Sn-Ti system is important in order to make predictions of the phase diagram and behaviour of alloys in the Ti-Al-Sn system which is of potential interest to the aerospace industry. There have been relatively few studies of these properties in the Sn-Ti system. The information has been comprehensively reviewed by Murray [87Mur]. The critically assessed data adopted by SGTE have been taken from the work of Hayes [98Ans] and is in good agreement with the experimental information. The phase diagram of the system has been studied in many investigations [54Fin, 55McQ, 56McQ, 57Pie, 60Kor, 60Gla, 62Ere]. Thermodynamic properties have been determined calorimetrically by [81Esi, 86Nik]. Activities of one or both components have been determined by [73Geg, 80And, 82Alg].

The phase diagram for the system is characterised by complete mixing in the liquid phase, appreciable solubility of Sn in both hcp-Ti and bcc-Ti, negligible solubility of Ti in bct-Sn and the formation of a series of four Ti rich intermetallic compounds, two of which $SnTi_3$ and Sn_5Ti_6 melt congruently. The $SnTi_3$ phase has been modelled with two sublattices to allow for its existence over a range of homogeneity.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Sn,Ti)_1$
bct	$A5$	βSn	$tI4$	$I4_1/amd$	BCT_A5	$(Sn,Ti)_1$
βSn_5Ti_6	$\cdots$	βTi_6Sn_5	$hP22$	$P6_3/mmc$ or $P\overline{3}1c$	SN5TI6	Sn_5Ti_6
αSn_5Ti_6	$\cdots$	Ni_6Sn_5	$oI44$	$Immm$	SN5TI6	Sn_5Ti_6
Sn_3Ti_5	$D8_8$	Mn_5Si_3	$hP16$	$P6_3/mcm$	D88_SN3TI5	Sn_3Ti_5
$SnTi_2$	$D8_2$	Cu_5Zn_8	$cI52$	$I\overline{4}3m$	D82_SNTI2	Sn_1Ti_2
$SnTi_3$	$D0_{19}$	Ni_3Sn	$hP8$	$P6_3/mmc$	D019_SNTI3	$(Sn,Ti)_1(Sn,Ti)_3$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Sn,Ti)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Sn,Ti)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ti}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ bcc	congruent	1951.3	0.959	0.959		−14749
liquid $\rightleftharpoons$ $SnTi_3$	congruent	1948.1	0.759	0.759		−24635
liquid $\rightleftharpoons$ $SnTi_3$ + bcc	eutectic	1879.8	0.828	0.777	0.846	−16246
liquid + $SnTi_3$ $\rightleftharpoons$ $SnTi_2$	peritectic	1835.9	0.659	0.750	0.667	−25313
liquid + $SnTi_2$ $\rightleftharpoons$ Sn_3Ti_5	peritectic	1774.7	0.589	0.667	0.625	−13442
liquid $\rightleftharpoons$ Sn_5Ti_6	congruent	1749.3	0.545	0.545		−24434
liquid $\rightleftharpoons$ Sn_5Ti_6 + Sn_3Ti_5	eutectic	1746.9	0.561	0.545	0.625	−24632
bcc $\rightleftharpoons$ hcp	congruent	1168.7	0.945	0.945		−3487
bcc $\rightleftharpoons$ $SnTi_3$ + hcp	eutectoid	1163.3	0.913	0.750	0.914	−3217
liquid $\rightleftharpoons$ bct + Sn_5Ti_6	eutectic	504.8	0.001	0.000	0.545	−7056
Sn_3Ti_5 $\rightleftharpoons$ Sn_5Ti_6 + $SnTi_2$	eutectoid	496.5	0.625	0.545	0.667	−84

Table IIIa. Integral quantities for the liquid phase at 2000 K.

x_{Ti}	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	−12205	−4922	3.641	−6799	0.939	0.000
0.200	−21439	−10171	5.634	−13118	1.474	0.000
0.300	−28728	−15214	6.757	−18570	1.678	0.000
0.400	−33960	−19519	7.221	−22768	1.625	0.000
0.500	−36853	−22552	7.151	−25327	1.388	0.000
0.600	−37051	−23781	6.635	−25860	1.040	0.000
0.700	−34138	−22673	5.733	−23980	0.654	0.000
0.800	−27622	−18695	4.463	−19301	0.303	0.000
0.900	−16842	−11315	2.763	−11436	0.061	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Sn(liquid), Ti(liquid)

Table IIIb. Partial quantities for Sn in the liquid phase at 2000 K.

x_{Sn}	ΔG_{Sn} [J/mol]	ΔH_{Sn} [J/mol]	ΔS_{Sn} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Sn}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Sn}}$ [J/(mol·K)]	a_{Sn}	γ_{Sn}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1928	252	1.090	−176	0.214	0.891	0.989
0.800	−4929	299	2.614	−1219	0.759	0.743	0.929
0.700	−9832	−926	4.453	−3901	1.487	0.554	0.791
0.600	−17491	−4488	6.501	−8996	2.254	0.349	0.582
0.500	−28803	−11453	8.675	−17277	2.912	0.177	0.354
0.400	−44753	−22885	10.934	−29516	3.315	0.068	0.169
0.300	−66506	−39850	13.328	−46485	3.317	0.018	0.061
0.200	−95722	−63415	16.154	−68959	2.772	0.003	0.016
0.100	−135999	−94643	20.678	−97709	1.533	0.000	0.003
0.000	−∞	−134602	∞	−133509	−0.547	0.000	0.000

Reference state: Sn(liquid)

Table IIIc. Partial quantities for Ti in the liquid phase at 2000 K.

x_{Ti}	ΔG_{Ti} [J/mol]	ΔH_{Ti} [J/mol]	ΔS_{Ti} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ti}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ti}}$ [J/(mol·K)]	a_{Ti}	γ_{Ti}
0.000	−∞	−45811	∞	−69107	11.648	0.000	0.016
0.100	−104700	−51491	26.604	−66410	7.460	0.002	0.018
0.200	−87479	−52049	17.715	−60715	4.333	0.005	0.026
0.300	−72817	−48552	12.133	−52797	2.122	0.013	0.042
0.400	−58663	−42064	8.300	−43426	0.681	0.029	0.073
0.500	−44904	−33650	5.627	−33377	−0.137	0.067	0.134
0.600	−31917	−24378	3.770	−23422	−0.478	0.147	0.245
0.700	−20265	−15311	2.477	−14334	−0.488	0.296	0.422
0.800	−10597	−7515	1.541	−6886	−0.315	0.529	0.661
0.900	−3602	−2056	0.773	−1850	−0.103	0.805	0.895
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(liquid)

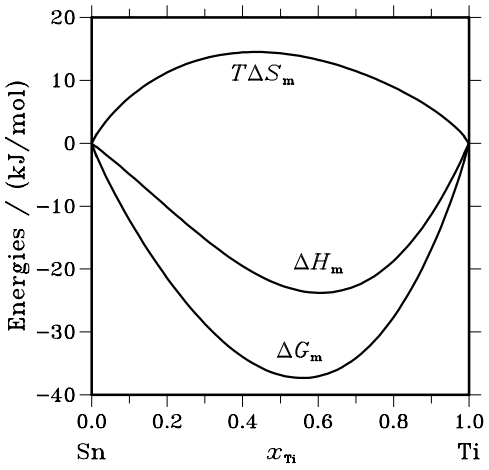

Fig. 2. Integral quantities of the liquid phase at T=2000 K.

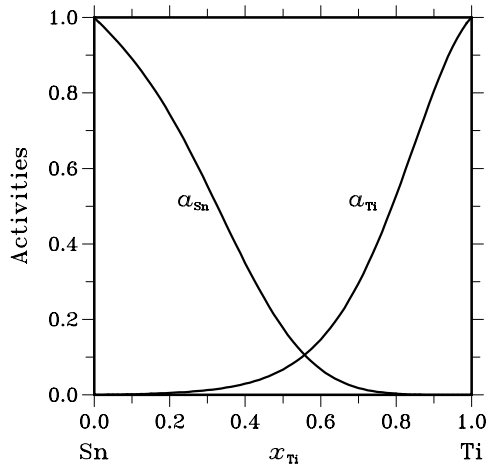

Fig. 3. Activities in the liquid phase at T=2000 K.

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

Compound	x_{Ti}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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))
Sn_5Ti_6	0.545	−38877	−37921	3.208	−0.020
Sn_3Ti_5	0.625	−39926	−39466	1.543	−0.016
$SnTi_2$	0.667	−40526	−40403	0.412	−0.014
$SnTi_3$	0.750	−37392	−37446	−0.179	−0.011

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