Mn – Ti (Manganese – Titanium)

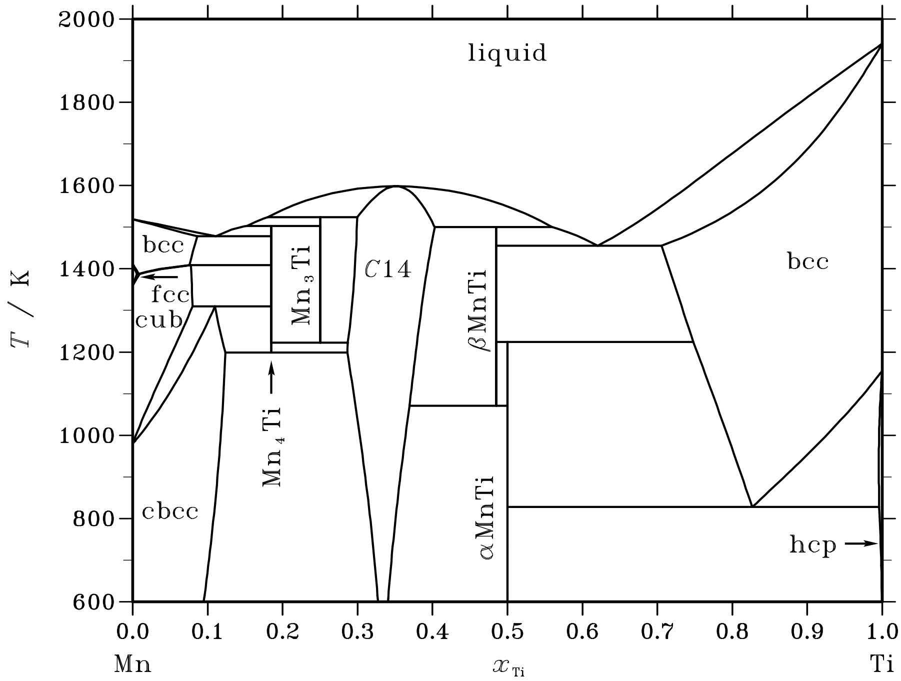

Fig. 1. Calculated phase diagram for the system Mn-Ti.

The Mn-Ti system is characterised by complete mixing of the elements in the liquid phase, substantial solubility of Mn in bcc-Ti, low solubility of Mn in hcp-Ti, limited solubility of Ti in the Mn based solid solution phases and the formation of a number of intermetallic phases of which Mn_2Ti ($C14$) exists over a wide homogeneity range. Although the broad features of the phase diagram are clear, the details are still in doubt with a fair degree of discrepancy between different experimental studies. There appear to be no measurements of the thermodynamic properties in the system. The available experimental data for the system have been thoroughly reviewed by Murray [87Mur]. The dataset adopted by SGTE for this system is taken from the critical assessment of Saunders [93Sau, 98Ans] which is good agreement with the bulk of the experimental studies for the system.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Mn,Ti)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Mn,Ti)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Mn,Ti)_1$
cbcc	$A12$	αMn	$cI58$	$I\overline{4}3m$	CBCC_A12	$(Mn,Ti)_1$
cub	$A13$	βMn	$cP20$	$P4_132$	CUB_A13	$(Mn,Ti)_1$
Mn_4Ti	$\cdots$	δ(Mo,Ni)	$hR53$	$R\overline{3}m$	MN4TI	$Mn_{163}Ti_{37}$
Mn_3Ti	$\cdots$	$\cdots$	$o*$*	$\cdots$	MN3TI	Mn_3Ti_1
$C14$	$C14$	$MgZn_2$	$hP12$	$P6_3/mmc$	C14_LAVES	$(Mn,Ti)_2(Mn,Ti)_1$
βMnTi	$\cdots$	$\cdots$	$\cdots$	$\cdots$	TIMN_BETA	$Mn_{103}Ti_{97}$
αMnTi	$\cdots$	$\cdots$	$t*58$	$\cdots$	TIMN_ALPHA	Mn_1Ti_1
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Mn,Ti)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ti}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid ⇌ $C14$	congruent	1598.0	0.351	0.351		−15248
liquid + $C14$ ⇌ Mn_3Ti	peritectic	1523.5	0.180	0.300	0.250	−6137
liquid + Mn_3Ti ⇌ Mn_4Ti	peritectic	1502.9	0.153	0.250	0.185	−9662
$C14$ + liquid ⇌ βMnTi	peritectic	1500.2	0.403	0.560	0.485	−6183
liquid ⇌ bcc + Mn_4Ti	eutectic	1478.0	0.111	0.086	0.185	−12520
liquid ⇌ βMnTi + bcc	eutectic	1455.5	0.620	0.485	0.706	−9432
bcc + Mn_4Ti ⇌ cub	peritectoid	1408.6	0.076	0.185	0.078	−4038
bcc ⇌ fcc + cub	eutectoid	1387.6	0.008	0.005	0.009	−3387
cub + Mn_4Ti ⇌ cbcc	peritectoid	1309.3	0.080	0.185	0.110	−1642
βMnTi + bcc ⇌ αMnTi	peritectoid	1224.0	0.485	0.748	0.500	−510
Mn_3Ti ⇌ Mn_4Ti + $C14$	eutectoid	1222.3	0.250	0.185	0.287	−445
Mn_4Ti ⇌ cbcc + $C14$	eutectoid	1198.5	0.185	0.124	0.286	−1862
βMnTi ⇌ $C14$ + αMnTi	eutectoid	1071.3	0.485	0.369	0.500	−401
bcc ⇌ αMnTi + hcp	eutectoid	827.6	0.827	0.500	0.996	−4142

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)]	$G^{\mathrm{E}}_{\mathrm{m}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{m}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−4495	−2959	0.768	911	−1.935	0.000
0.200	−6747	−5306	0.721	1574	−3.440	0.000
0.300	−8150	−7022	0.564	2008	−4.515	0.000
0.400	−8964	−8093	0.436	2227	−5.160	0.000
0.500	−9276	−8500	0.388	2250	−5.375	0.000
0.600	−9099	−8227	0.436	2093	−5.160	0.000
0.700	−8386	−7258	0.564	1772	−4.515	0.000
0.800	−7016	−5574	0.721	1306	−3.440	0.000
0.900	−4697	−3161	0.768	709	−1.935	0.000
1.000	0	0	0.000	0	0.000	0.000

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

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

x_{Mn}	ΔG_{Mn} [J/mol]	ΔH_{Mn} [J/mol]	ΔS_{Mn} [J/(mol·K)]	G^E_{Mn} [J/mol]	S^E_{Mn} [J/(mol·K)]	a_{Mn}	γ_{Mn}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1626	−304	0.661	126	−0.215	0.907	1.008
0.800	−3227	−1237	0.995	483	−0.860	0.824	1.029
0.700	−4894	−2833	1.031	1037	−1.935	0.745	1.064
0.600	−6741	−5126	0.807	1754	−3.440	0.667	1.111
0.500	−8926	−8150	0.388	2600	−5.375	0.585	1.169
0.400	−11695	−11938	−0.121	3542	−7.740	0.495	1.237
0.300	−15474	−16523	−0.525	4547	−10.535	0.394	1.314
0.200	−21183	−21939	−0.378	5581	−13.760	0.280	1.399
0.100	−31680	−28220	1.730	6610	−17.415	0.149	1.488
0.000	$-\infty$	−35400	∞	7600	−21.500	0.000	1.579

Reference state: Mn(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^E_{Ti} [J/mol]	S^E_{Ti} [J/(mol·K)]	a_{Ti}	γ_{Ti}
0.000	$-\infty$	−32600	∞	10400	−21.500	0.000	1.869
0.100	−30319	−26860	1.730	7970	−17.415	0.161	1.615
0.200	−20824	−21581	−0.378	5939	−13.760	0.286	1.429
0.300	−15748	−16797	−0.525	4273	−10.535	0.388	1.293
0.400	−12299	−12542	−0.121	2938	−7.740	0.477	1.193
0.500	−9626	−8850	0.388	1900	−5.375	0.561	1.121
0.600	−7368	−5754	0.807	1126	−3.440	0.642	1.070
0.700	−5348	−3287	1.031	583	−1.935	0.725	1.036
0.800	−3474	−1483	0.995	237	−0.860	0.811	1.014
0.900	−1698	−376	0.661	54	−0.215	0.903	1.003
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(liquid)

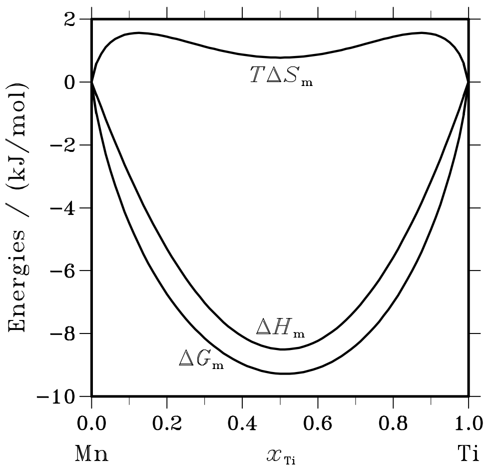

Fig. 2. Integral quantities of the liquid phase at T=2000 K.

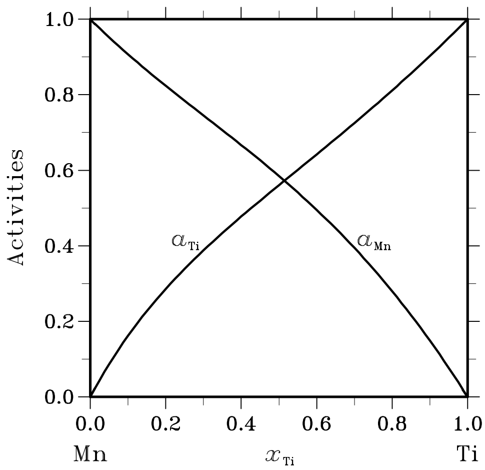

Fig. 3. Activities in the liquid phase at T=2000 K.

Table IVa. Integral quantities for the stable phases at 1450 K.

Phase	x_{Ti}	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)]
bcc	0.000	0	0	0.000	0	0.000	0.000
	0.082	−3039	−1802	0.854	373	−1.500	−0.008
Mn_4Ti	0.185	−5605	−7317	−1.181			0.660
Mn_3Ti	0.250	−6912	−9321	−1.662			1.086
$C14$	0.298	−7769	−10985	−2.218	−427	−7.282	4.523
	0.300	−7807	−11043	−2.231	−443	−7.310	4.604
	0.398	−8330	−10368	−1.406	−228	−6.993	4.361
βMnTi	0.485	−7878	−9543	−1.148			2.627
bcc	0.707	−6008	−4722	0.887	1289	−4.145	−0.008
	0.800	−5008	−3614	0.962	1024	−3.199	−0.005
	0.900	−3325	−2015	0.903	594	−1.799	−0.003
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Mn(bcc), Ti(bcc)

Table IVb. Partial quantities for Mn in the stable phases at 1450 K.

Phase	x_{Mn}	ΔG_{Mn} [J/mol]	ΔH_{Mn} [J/mol]	ΔS_{Mn} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Mn}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Mn}}$ [J/(mol·K)]	a_{Mn}	γ_{Mn}
bcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.918	−1007	−172	0.576	21	−0.133	0.920	1.002
Mn_4Ti	0.815	−1007	2567	2.465			0.920	
	0.815	−1883	−1611	0.188			0.855	
Mn_3Ti	0.750	−1883	−1611	0.188			0.855	
	0.750	−2436	−632	1.244			0.817	
$C14$	0.702	−2436	−2898	−0.319	1828	−3.259	0.817	1.164
	0.700	−2558	−3103	−0.376	1742	−3.341	0.809	1.155
	0.602	−10387	−22151	−8.113	−4276	−12.327	0.422	0.701
βMnTi	0.515	−10387	−14130	−2.514			0.422	
	0.515	−11972	−20106	−5.610			0.370	
bcc	0.293	−11972	−11660	0.215	2811	−9.980	0.370	1.263
	0.200	−15562	−14711	0.587	3842	−12.795	0.275	1.375
	0.100	−22574	−18297	2.950	5186	−16.195	0.154	1.537
	0.000	$-\infty$	−22191	∞	6802	−19.995	0.000	1.758

Reference state: Mn(bcc)

Table IVc. Partial quantities for Ti in the stable phases at 1450 K.

Phase	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}
bcc	0.000	$-\infty$	−24154	∞	4809	−19.974	0.000	1.490
	0.082	−25858	−20100	3.971	4328	−16.848	0.117	1.432
Mn_4Ti	0.185	−25858	−50871	−17.250			0.117	
	0.185	−21999	−32454	−7.210			0.161	
Mn_3Ti	0.250	−21999	−32454	−7.210			0.161	
	0.250	−20343	−35394	−10.380			0.185	
$C14$	0.298	−20343	−30048	−6.693	−5741	−16.763	0.185	0.621
	0.300	−20055	−29569	−6.561	−5540	−16.572	0.189	0.632
	0.398	−5213	7482	8.755	5905	1.087	0.649	1.632
βMnTi	0.485	−5213	−4685	0.366			0.649	
	0.485	−3531	1665	3.583			0.746	
bcc	0.707	−3531	−1840	1.166	657	−1.722	0.746	1.056
	0.800	−2370	−840	1.055	320	−0.800	0.822	1.027
	0.900	−1186	−206	0.676	84	−0.200	0.906	1.007
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(bcc)

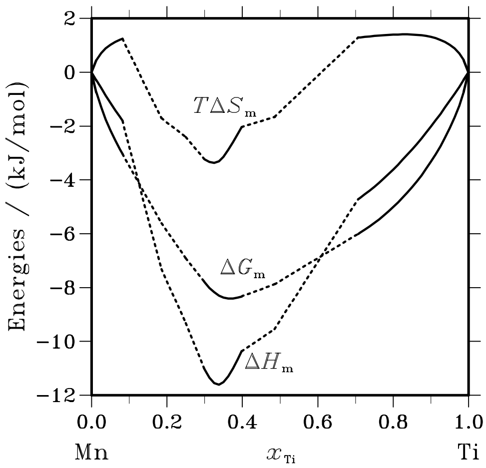

Fig. 4. Integral quantities of the stable phases at T=1450 K.

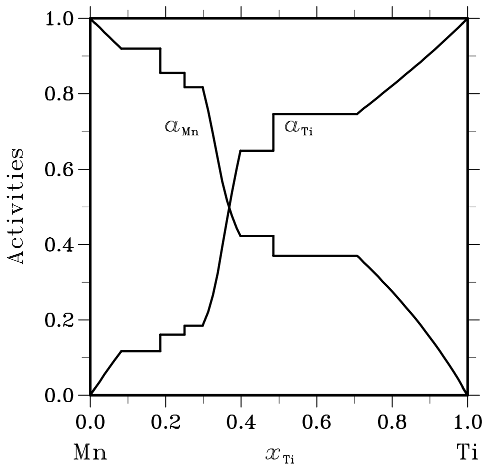

Fig. 5. Activities in the stable phases at T=1450 K.

Table V. 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))	$\Delta_{\mathrm{f}}C^{\circ}_{P}$ / (J/(mol·K))
Mn_4Ti	0.185	−3310	−2445	2.901	−0.004
Mn_3Ti_1	0.250	−5318	−4638	2.281	−0.003
$C14$	0.333	−8799	−8797	0.006	−0.003
βMnTi	0.485	−6223	−5540	2.290	−0.002
αMnTi	0.500	−6335	−5739	2.000	−0.002

References

[87Mur] J.L. Murray, “Phase Diagrams of Binary Titanium Alloys”, ASM, Metals Park, Ohio 44073, 1987.

[93Sau] N. Saunders, unpublished work, 1993.

[98Ans] I. Ansara, A.T. Dinsdale, M.H. Rand (eds.): COST 507, “Thermochemical database for light metal alloys”, Vol. 2, EUR 18499, 1998, 211–214.