Fe – Ti (Iron – Titanium)

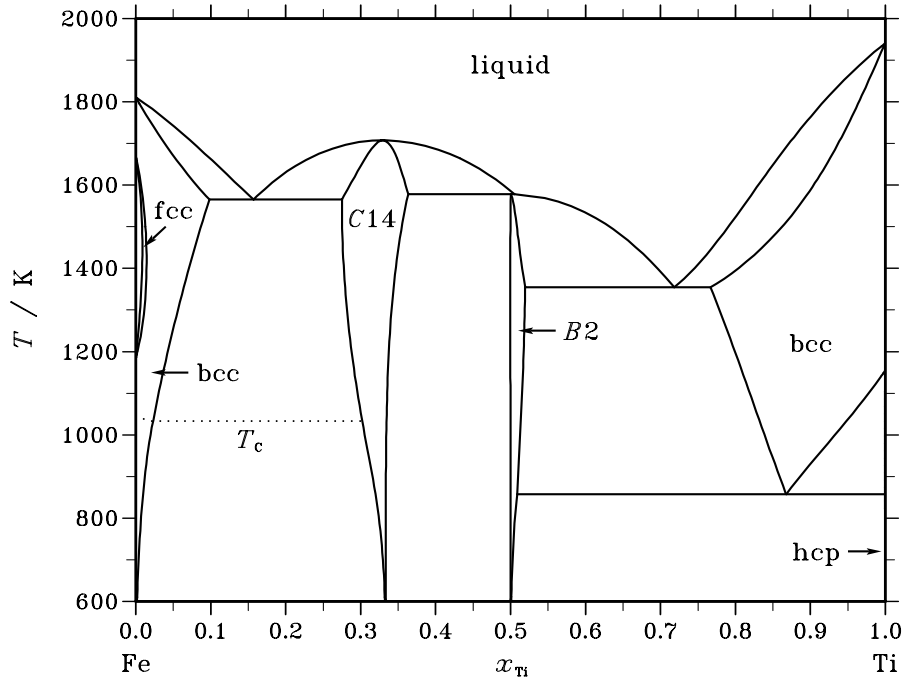

Fig. 1. Calculated phase diagram for the system Fe-Ti.

The system has complete solubility in the liquid and there are two compounds, a Laves phase ($C14$) and a $B2$ ordered bcc phase. Both Fe and Ti are stable as bcc but the transition from bcc to the ordered $B2$ is of first order. The fcc phase is stable in a narrow "gamma-loop" close to pure Fe and the hcp-Ti phase has almost no solubility of Fe. Ti is used as carbide former in steels. The current assessment [98Kum] was selected as it has the best modelling of the intermetallic phases.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Fe,Ti)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Fe,Ti)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Fe,Ti,\Box)_1$
$C14$	$C14$	$MgZn_2$	$hP12$	$P6_3/mmc$	LAVES_C14	$(Fe,Ti)_2(Fe,Ti)_1$
$B2$	$B2$	CsCl	$cP2$	$Pm3m$	BCC_B2	$(Fe,Ti)_1(Fe,Ti)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Fe,Ti)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ti}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons C14$	congruent	1707.3	0.330	0.330		−26370
$C14$ + liquid $\rightleftharpoons B2$	peritectic	1577.7	0.363	0.505	0.500	−24468
liquid $\rightleftharpoons$ bcc + $C14$	eutectic	1565.0	0.157	0.098	0.275	−14167
liquid $\rightleftharpoons B2$ + bcc	eutectic	1354.2	0.718	0.519	0.767	−9387
bcc $\rightleftharpoons B2$ + hcp	eutectoid	857.5	0.868	0.509	1.000	−5843

Table IIIa. Integral quantities for the liquid phase at 2200 K.

x_{Ti}	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	−9431	−6037	1.697	−4025	−1.006	0.000
0.200	−15284	−11182	2.051	−6963	−2.110	0.000
0.300	−19067	−15195	1.936	−8909	−3.143	0.000
0.400	−21136	−17874	1.631	−9945	−3.965	0.000
0.500	−21666	−19062	1.302	−10139	−4.461	0.000
0.600	−20740	−18641	1.049	−9548	−4.546	0.000
0.700	−18373	−16537	0.918	−8215	−4.161	0.000
0.800	−14491	−12716	0.888	−6170	−3.273	0.000
0.900	−8836	−7187	0.824	−3430	−1.878	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Fe in the liquid phase at 2200 K.

x_{Fe}	ΔG_{Fe} [J/mol]	ΔH_{Fe} [J/mol]	ΔS_{Fe} [J/(mol·K)]	$G_{\mathrm{Fe}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Fe}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Fe}	γ_{Fe}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2312	−402	0.955	−560	0.079	0.870	0.967
0.800	−5819	−1951	1.934	−2108	0.079	0.705	0.881
0.700	−10405	−5067	2.669	−4474	−0.297	0.535	0.764
0.600	−16020	−10048	2.986	−7526	−1.261	0.382	0.636
0.500	−22698	−17064	2.817	−11171	−2.947	0.255	0.511
0.400	−30594	−26161	2.216	−15357	−5.402	0.159	0.397
0.300	−40088	−37259	1.414	−20067	−8.596	0.090	0.299
0.200	−52088	−50155	0.967	−25325	−12.415	0.044	0.218
0.100	−69483	−64517	2.483	−31193	−16.662	0.015	0.153
0.000	$-\infty$	−79892	∞	−37772	−21.060	0.000	0.103

Reference state: Fe(liquid)

Table IIIc. Partial quantities for Ti in the liquid phase at 2200 K.

x_{Ti}	ΔG_{Ti} [J/mol]	ΔH_{Ti} [J/mol]	ΔS_{Ti} [J/(mol·K)]	$G_{\mathrm{Ti}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Ti}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Ti}	γ_{Ti}
0.000	$-\infty$	−63912	∞	−46028	−8.942	0.000	0.063
0.100	−73495	−56751	8.372	−35206	−10.773	0.012	0.120
0.200	−53145	−48109	2.518	−26382	−10.864	0.041	0.205
0.300	−39279	−38825	0.227	−19258	−9.784	0.094	0.314
0.400	−28811	−29613	−0.401	−13574	−8.020	0.177	0.442
0.500	−20634	−21059	−0.213	−9107	−5.976	0.289	0.578
0.600	−14171	−13628	0.271	−5676	−3.976	0.426	0.711
0.700	−9067	−7656	0.706	−3136	−2.260	0.580	0.828
0.800	−5092	−3357	0.868	−1382	−0.988	0.736	0.920
0.900	−2098	−817	0.640	−346	−0.236	0.881	0.979
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(liquid)

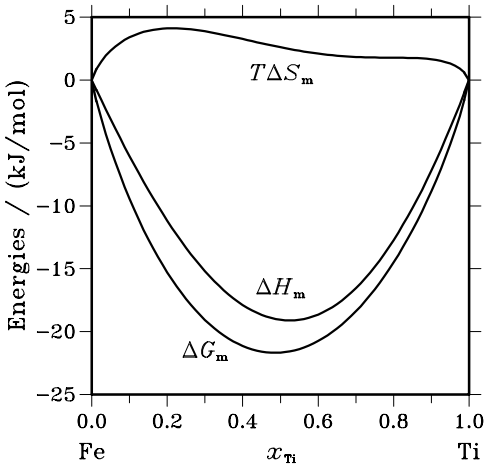

Fig. 2. Integral quantities of the liquid phase at T=2200 K.

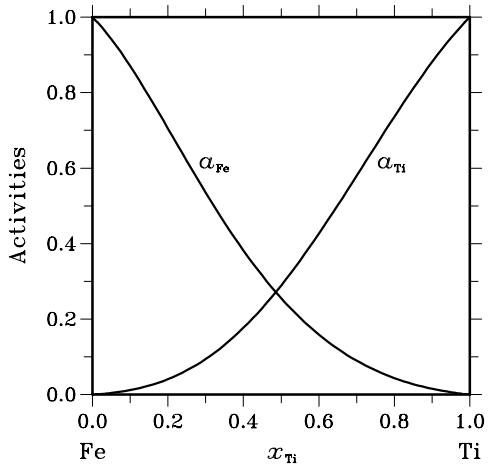

Fig. 3. Activities in the liquid phase at T=2200 K.

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))
$C14$	0.333	−20141	−19128	3.399	0.597
$B2$	0.500	−24649	−24589	0.203	−1.054

References

[98Har] K.C. Hari Kumar: unpublished assessment, 1998.