Ni – Ti (Nickel – Titanium)

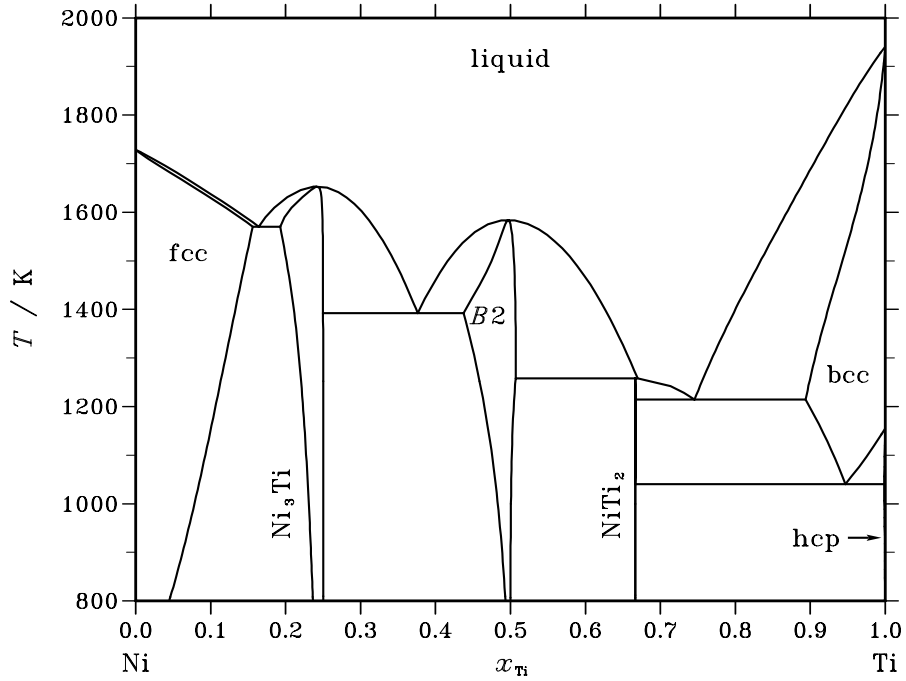

Fig. 1. Calculated phase diagram for the system Ni-Ti.

Ni and Ti are both alloying elements in steels and other alloys. Ti is a strong carbide former and also promotes the ordered Ni_3Al phase in Ni-based superalloys. In the binary Ni-Ti diagram the hexagonal $D0_{24}$ is more stable than the $L1_2$ phase and there is an ordered $B2$ phase stable in the middle. The assessment has been reported in [96Bel].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Ni,Ti)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Ni,Ti)_1$
Ni_3Ti	$D0_{24}$	Ni_3Ti	$hP16$	$P6_3/mmc$	D024_NI3TI	$Ni_3(Ni,Ti)_1$
$B2$	$B2$	CsCl	$cP2$	$Pm3m$	BCC_B2	$(Ni,Ti,\Box)_1(Ni,Ti,\Box)_1$
$NiTi_2$	$\cdots$	$NiTi_2$	$cF96$	$Fd\overline{3}m$	MTI2	$(Ni,Ti)_1(Ni,Ti)_2$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_B2	$(Ni,Ti)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Ni,Ti)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ti}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons$ Ni_3Ti	congruent	1652.9	0.242	0.242		−17460
liquid $\rightleftharpoons$ $B2$	congruent	1583.8	0.497	0.497		−12917
liquid $\rightleftharpoons$ fcc + Ni_3Ti	eutectic	1570.3	0.164	0.156	0.193	−6507
liquid $\rightleftharpoons$ Ni_3Ti + $B2$	eutectic	1392.5	0.376	0.250	0.438	−10333
$B2$ + liquid $\rightleftharpoons$ $NiTi_2$	peritectic	1257.8	0.507	0.670	0.667	−12899
liquid $\rightleftharpoons$ $NiTi_2$ + bcc	eutectic	1214.7	0.746	0.667	0.894	−10562
bcc $\rightleftharpoons$ $NiTi_2$ + hcp	eutectoid	1040.1	0.947	0.667	0.998	−5782

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	−16301	−19725	−1.712	−10895	−4.415	0.000
0.200	−25820	−32448	−3.314	−17499	−7.475	0.000
0.300	−31010	−39152	−4.071	−20852	−9.150	0.000
0.400	−32992	−40817	−3.913	−21801	−9.508	0.000
0.500	−32524	−38427	−2.952	−20997	−8.715	0.000
0.600	−30092	−32962	−1.435	−18901	−7.031	0.000
0.700	−25936	−25405	0.265	−15778	−4.814	0.000
0.800	−20021	−16738	1.641	−11700	−2.519	0.000
0.900	−11951	−7942	2.004	−6545	−0.699	0.000
1.000	0	0	0.000	0	0.000	0.000

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

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

x_{Ni}	ΔG_{Ni} [J/mol]	ΔH_{Ni} [J/mol]	ΔS_{Ni} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ni}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ni}}$ [J/(mol·K)]	a_{Ni}	γ_{Ni}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−4087	−3665	0.211	−2335	−0.665	0.782	0.869
0.800	−11566	−13349	−0.891	−7856	−2.747	0.499	0.623
0.700	−20705	−27089	−3.192	−14774	−6.158	0.288	0.411
0.600	−30376	−42922	−6.273	−21881	−10.520	0.161	0.268
0.500	−40075	−58883	−9.404	−28548	−15.167	0.090	0.180
0.400	−49965	−73009	−11.522	−34728	−19.140	0.050	0.124
0.300	−60975	−83335	−11.180	−40954	−21.191	0.026	0.085
0.200	−75102	−87899	−6.399	−48338	−19.780	0.011	0.055
0.100	−96865	−84736	6.065	−58576	−13.080	0.003	0.030
0.000	$-\infty$	−71883	∞	−73939	1.028	0.000	0.012

Reference state: Ni(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	$-\infty$	−235532	∞	−134349	−50.591	0.000	0.000
0.100	−126224	−164270	−19.023	−87935	−38.168	0.001	0.005
0.200	−82834	−108846	−13.006	−56071	−26.388	0.007	0.034
0.300	−55055	−67298	−6.122	−35034	−16.132	0.036	0.122
0.400	−36917	−37661	−0.372	−21680	−7.990	0.109	0.272
0.500	−24972	−17971	3.501	−13446	−2.262	0.223	0.445
0.600	−16844	−6264	5.290	−8349	1.042	0.363	0.605
0.700	−10919	−578	5.170	−4988	2.205	0.519	0.741
0.800	−6250	1052	3.651	−2540	1.796	0.687	0.858
0.900	−2516	590	1.553	−764	0.677	0.860	0.955
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(liquid)

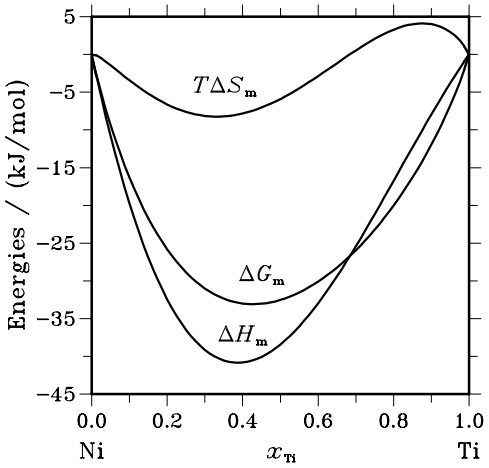

Fig. 2. Integral quantities of the liquid phase at T=2000 K.

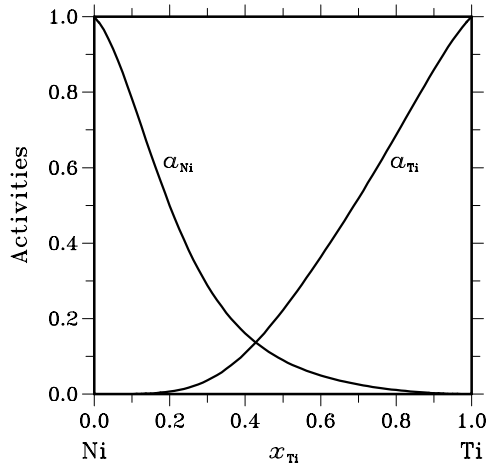

Fig. 3. Activities in the liquid phase at T=2000 K.

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))	$\Delta_{\mathrm{f}}C^{\circ}_{P}$ / (J/(mol·K))
Ni_3Ti	0.250	−36322	−37272	−3.185	−0.573
$B2$	0.500	−34126	−34052	0.250	4.207
$NiTi_2$	0.667	−26371	−26901	−1.778	−0.255

References

[96Bel] P. Bellen, K.C. Hari Kumar, P. Wollants: Z. Metallkd. **87** (1996) 972–978.