Nb – Ti (Niobium – Titanium)

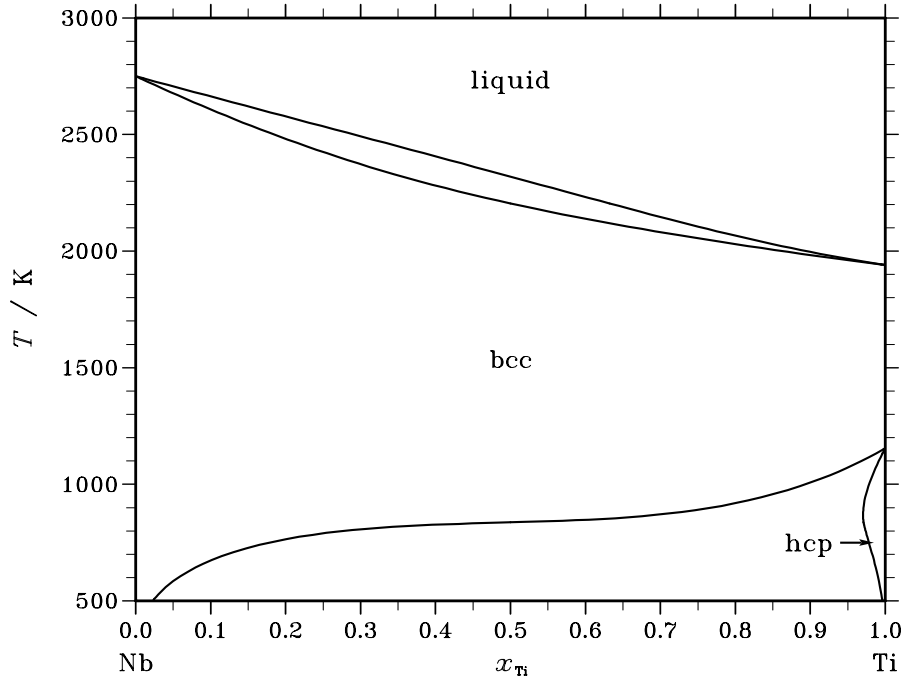

Fig. 1. Calculated phase diagram for the system Nb-Ti.

Niobium and titanium are important additions to many alloys, such as superalloys and refractory alloys. The Nb-Ti system is fairly simple with only three condensed stable phases, liquid, bcc and hcp. According to the critical evaluation of [87Mur], there is some experimental evidence of the existence of a metastable miscibility gap in the bcc phase. However, the interpretation of experimental results may be complicated by the formation of the metastable omega phase. Several thermodynamic descriptions for this system have been developed. The most recent descriptions of [94Har, 98Sau, 01Zha] reproduce the experimental data very well. The major differences between these descriptions are the calculated properties of the metastable equilibria. The description of [94Har] produces a hcp/bcc T_0 curve below the experimental M_S temperatures, an unrealistic result. [01Zha] used stable as well as the metastable equilibria for the development of the thermodynamic description. Therefore, this description is recommended.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Nb,Ti)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Nb,Ti)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Nb,Ti)_1$

Table IIa. Integral quantities for the liquid phase at 2800 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	−6902	667	2.703	667	0.000	0.000
0.200	−10465	1185	4.161	1185	0.000	0.000
0.300	−12666	1555	5.079	1555	0.000	0.000
0.400	−13891	1777	5.596	1777	0.000	0.000
0.500	−14285	1852	5.763	1852	0.000	0.000
0.600	−13891	1777	5.596	1777	0.000	0.000
0.700	−12666	1555	5.079	1555	0.000	0.000
0.800	−10465	1185	4.161	1185	0.000	0.000
0.900	−6902	667	2.703	667	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIb. Partial quantities for Nb in the liquid phase at 2800 K.

x_{Nb}	ΔG_{Nb} [J/mol]	ΔH_{Nb} [J/mol]	ΔS_{Nb} [J/(mol·K)]	$G_{\mathrm{Nb}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Nb}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Nb}	γ_{Nb}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2379	74	0.876	74	0.000	0.903	1.003
0.800	−4899	296	1.855	296	0.000	0.810	1.013
0.700	−7637	667	2.966	667	0.000	0.720	1.029
0.600	−10707	1185	4.247	1185	0.000	0.631	1.052
0.500	−14285	1852	5.763	1852	0.000	0.541	1.083
0.400	−18666	2666	7.619	2666	0.000	0.449	1.121
0.300	−24400	3629	10.010	3629	0.000	0.351	1.169
0.200	−32729	4740	13.382	4740	0.000	0.245	1.226
0.100	−47607	5999	19.145	5999	0.000	0.129	1.294
0.000	$-\infty$	7406	∞	7406	0.000	0.000	1.375

Reference state: Nb(liquid)

Table IIc. Partial quantities for Ti in the liquid phase at 2800 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	$-\infty$	7406	∞	7406	0.000	0.000	1.375
0.100	−47607	5999	19.145	5999	0.000	0.129	1.294
0.200	−32729	4740	13.382	4740	0.000	0.245	1.226
0.300	−24400	3629	10.010	3629	0.000	0.351	1.169
0.400	−18666	2666	7.619	2666	0.000	0.449	1.121
0.500	−14285	1852	5.763	1852	0.000	0.541	1.083
0.600	−10707	1185	4.247	1185	0.000	0.631	1.052
0.700	−7637	667	2.966	667	0.000	0.720	1.029
0.800	−4899	296	1.855	296	0.000	0.810	1.013
0.900	−2379	74	0.876	74	0.000	0.903	1.003
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(liquid)

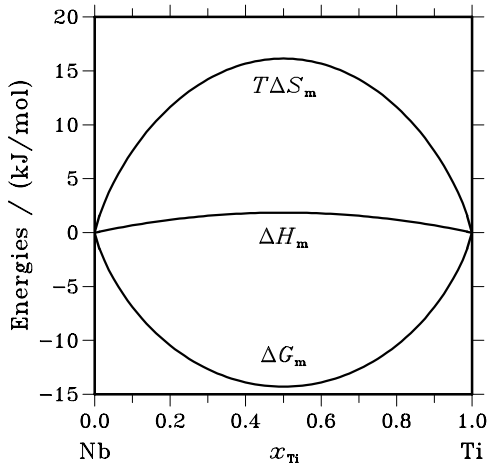

Fig. 2. Integral quantities of the liquid phase at T=2800 K.

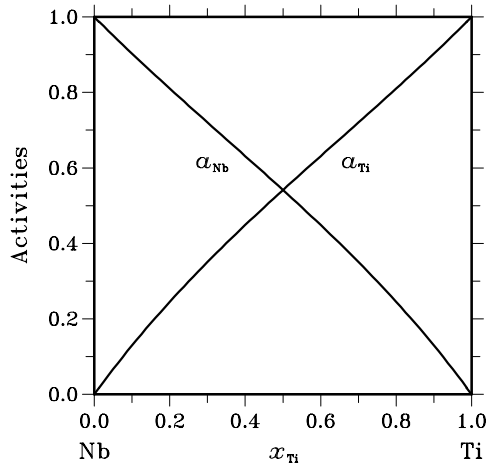

Fig. 3. Activities in the liquid phase at T=2800 K.

Table IIIa. Integral quantities for the stable phases at 1500 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
	0.100	−2880	1174	2.703	1174	0.000	0.000
	0.200	−4154	2087	4.161	2087	0.000	0.000
	0.300	−4879	2740	5.079	2740	0.000	0.000
	0.400	−5263	3131	5.596	3131	0.000	0.000
	0.500	−5383	3261	5.763	3261	0.000	0.000
	0.600	−5263	3131	5.596	3131	0.000	0.000
	0.700	−4879	2740	5.079	2740	0.000	0.000
	0.800	−4154	2087	4.161	2087	0.000	0.000
	0.900	−2880	1174	2.703	1174	0.000	0.000
	1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Nb in the stable phases at 1500 K.

Phase	x_{Nb}	ΔG_{Nb} [J/mol]	ΔH_{Nb} [J/mol]	ΔS_{Nb} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Nb}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Nb}}$ [J/(mol·K)]	a_{Nb}	γ_{Nb}
bcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1184	130	0.876	130	0.000	0.909	1.011
	0.800	−2261	522	1.855	522	0.000	0.834	1.043
	0.700	−3274	1174	2.966	1174	0.000	0.769	1.099
	0.600	−4284	2087	4.247	2087	0.000	0.709	1.182
	0.500	−5383	3261	5.763	3261	0.000	0.649	1.299
	0.400	−6731	4696	7.619	4696	0.000	0.583	1.457
	0.300	−8623	6392	10.010	6392	0.000	0.501	1.670
	0.200	−11724	8349	13.382	8349	0.000	0.391	1.953
	0.100	−18151	10567	19.145	10567	0.000	0.233	2.333
	0.000	$-\infty$	13045	∞	13045	0.000	0.000	2.846

Reference state: Nb(bcc)

Table IIIc. Partial quantities for Ti in the stable phases at 1500 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	$-\infty$	13045	∞	13045	0.000	0.000	2.846
	0.100	−18151	10567	19.145	10567	0.000	0.233	2.333
	0.200	−11724	8349	13.382	8349	0.000	0.391	1.953
	0.300	−8623	6392	10.010	6392	0.000	0.501	1.670
	0.400	−6731	4696	7.619	4696	0.000	0.583	1.457
	0.500	−5383	3261	5.763	3261	0.000	0.649	1.299
	0.600	−4284	2087	4.247	2087	0.000	0.709	1.182
	0.700	−3274	1174	2.966	1174	0.000	0.769	1.099
	0.800	−2261	522	1.855	522	0.000	0.834	1.043
	0.900	−1184	130	0.876	130	0.000	0.909	1.011
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(bcc)

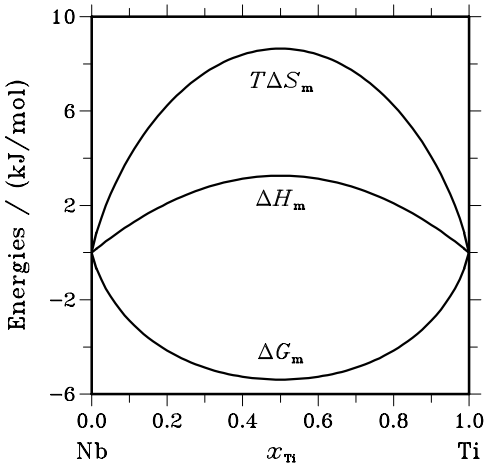

Fig. 4. Integral quantities of the stable phases at T=1500 K.

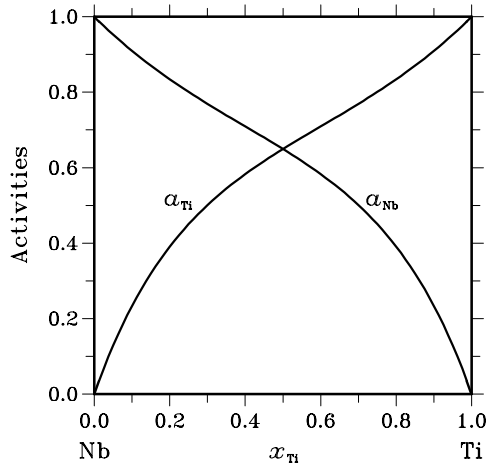

Fig. 5. Activities in the stable phases at T=1500 K.

References

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