Nb – Ni (Niobium – Nickel)

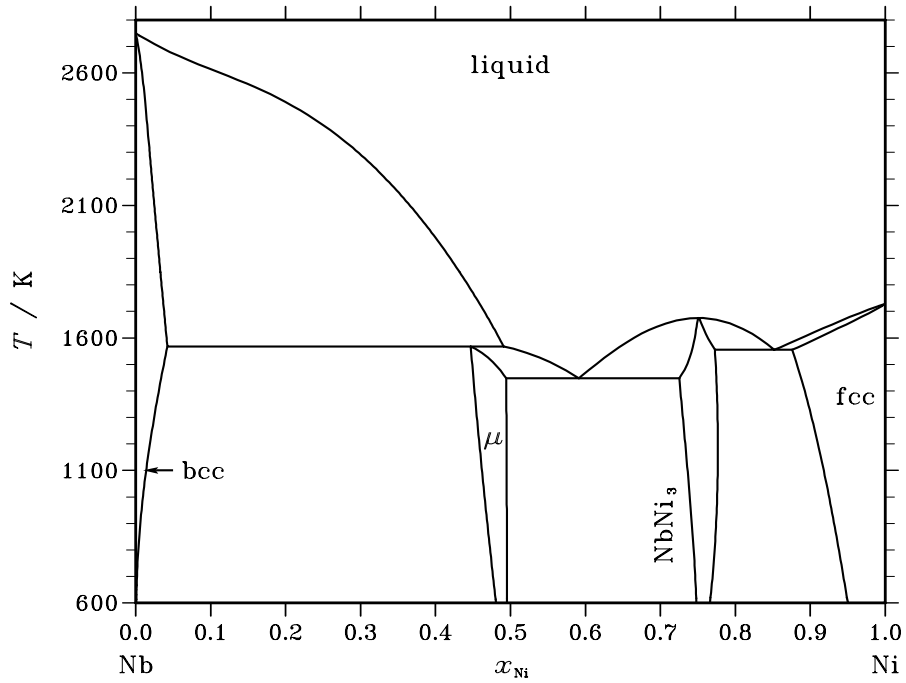

Fig. 1. Calculated phase diagram for the system Nb-Ni.

Nb-Ni is an important binary system for Ni-base superalloys. Many of the intermetallic phases encountered in these alloys contain not only Ni but also a significant amount of Nb. In order to predict the stable and metastable phase equilibria in multicomponent superalloys by extrapolation of thermodynamic parameters from the constituent alloy systems, an accurate description of the Nb-Ni phase diagram with respect to the experimentally determined phase boundaries is necessary. The Nb-Ni system is characterised by two intermetallic compounds: $NbNi_3$ which melts congruently at 1675 K and a μ-phase which decomposes peritectically at 1568 K. The Nb solution in solid Ni can reach up to 12.4 at.% Nb at the fcc-Ni+Ni_3Nb eutectic. The solubility of Ni in solid Nb is more limited with a value of 4.2 at.% Ni at the peritectic invariant. There are five different thermodynamic assessments in the literature. Kaufman and Nesor [78Kau], Chevalier [81Che] and Camus [89Cam] used simplified, stoichiometric descriptions for the intermetallic phases. Zeng *et al.* [92Zen1, 92Zen2] transformed these into solution models, but the optimised parameters do not agree with the available thermodynamic measurements. Bolcavage and Kattner [96Bol] performed the most recent modelling and their optimised parameters have been chosen. Their assessment is in good agreement with the literature review of the available data by Nash *et al.* [86Nash].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Nb,Ni)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Nb,Ni)_1$
μ	$D8_5$	Fe_7W_6	$hR13$	$R\overline{3}m$	D85_NI7NB6	$Nb_6(Nb,Ni)_7$
$NbNi_3$	$D0_a$	βCu_3Ti	$oP8$	$Pmmm$	D0A_NBNI3	$(Nb,Ni)_1(Nb,Ni)_3$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Nb,Ni)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ni}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons$ $NbNi_3$	congruent	1675.0	0.751	0.751		−31766
bcc + liquid $\rightleftharpoons$ μ	peritectic	1568.0	0.042	0.491	0.447	−22830
liquid $\rightleftharpoons$ $NbNi_3$ + fcc	eutectic	1555.1	0.852	0.773	0.876	−18658
liquid $\rightleftharpoons$ μ + $NbNi_3$	eutectic	1448.0	0.591	0.494	0.725	−25455

Table IIIa. Integral quantities for the liquid phase at 2800 K.

x_{Ni}	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	−12572	420	4.640	−5004	1.937	0.000
0.200	−22422	−2833	6.996	−10772	2.835	0.000
0.300	−30655	−8250	8.002	−16434	2.923	0.000
0.400	−36881	−14415	8.024	−21213	2.428	0.000
0.500	−40567	−20009	7.342	−24430	1.579	0.000
0.600	−41168	−23811	6.199	−25500	0.603	0.000
0.700	−38157	−24694	4.808	−23936	−0.271	0.000
0.800	−30996	−21627	3.346	−19346	−0.815	0.000
0.900	−19002	−13675	1.902	−11434	−0.800	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. 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	−1917	2097	1.433	536	0.557	0.921	1.023
0.800	−4262	6324	3.781	933	1.926	0.833	1.041
0.700	−8712	9806	6.614	−409	3.648	0.688	0.983
0.600	−16693	9952	9.516	−4800	5.269	0.488	0.814
0.500	−29403	4462	12.095	−13266	6.331	0.283	0.566
0.400	−47873	−8678	13.998	−26542	6.380	0.128	0.320
0.300	−73104	−31194	14.968	−45074	4.957	0.043	0.144
0.200	−106493	−64521	14.990	−69024	1.608	0.010	0.052
0.100	−151869	−109810	15.021	−98263	−4.124	0.001	0.015
0.000	$-\infty$	−167922	∞	−132374	−12.696	0.000	0.003

Reference state: Nb(liquid)

Table IIIc. Partial quantities for Ni in the liquid phase at 2800 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}
0.000	$-\infty$	27848	∞	−43064	25.326	0.000	0.157
0.100	−108464	−14666	33.499	−54858	14.354	0.009	0.095
0.200	−95061	−39463	19.857	−57593	6.475	0.017	0.084
0.300	−81856	−50379	11.242	−53827	1.231	0.030	0.099
0.400	−67164	−50965	5.786	−45832	−1.833	0.056	0.140
0.500	−51731	−44481	2.589	−35594	−3.174	0.108	0.217
0.600	−36698	−33900	0.999	−24806	−3.248	0.207	0.345
0.700	−23181	−21909	0.454	−14877	−2.511	0.369	0.528
0.800	−12121	−10903	0.435	−6926	−1.420	0.594	0.743
0.900	−4239	−2993	0.445	−1786	−0.431	0.834	0.926
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ni(liquid)

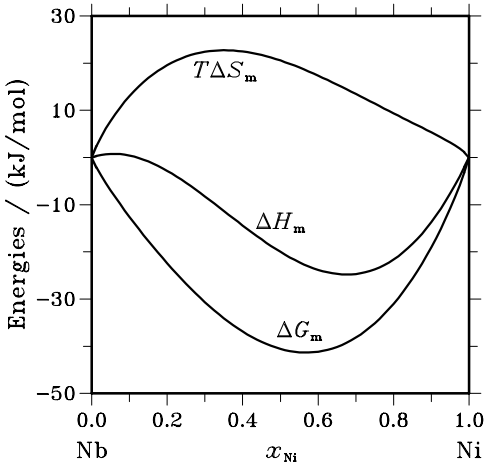

Fig. 2. Integral quantities of the liquid phase at T=2800 K.

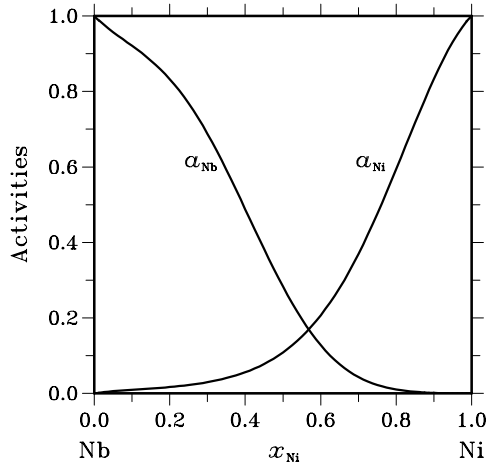

Fig. 3. Activities in the liquid phase at T=2800 K.

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

Compound	x_{Ni}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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))
μ	0.500	−22257	−21588	2.245	−0.382
$NbNi_3$	0.750	−33202	−33921	−2.413	−0.573

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