Hf – Nb (Hafnium – Niobium)

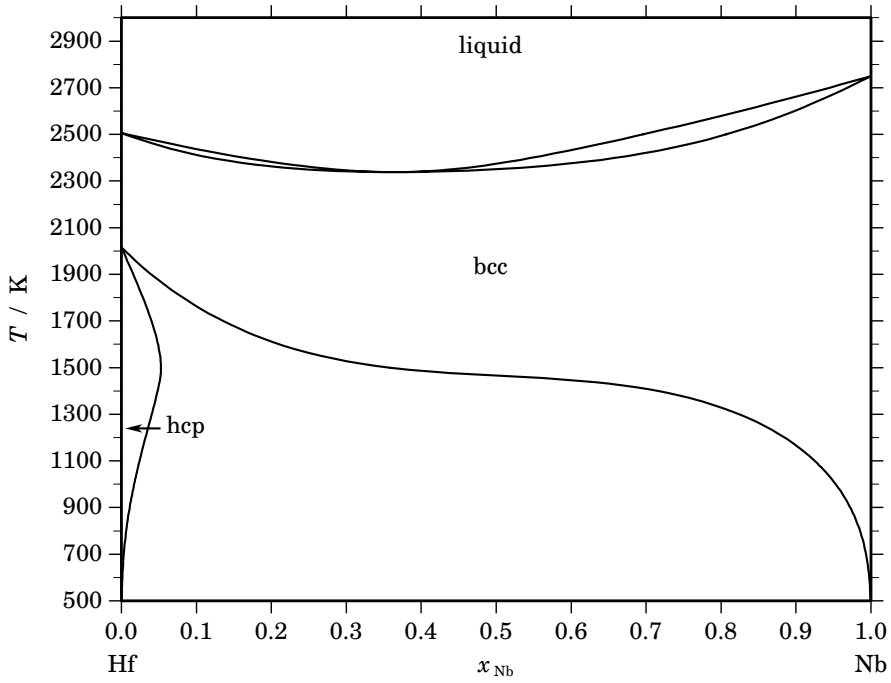

Fig. 1. Calculated phase diagram for the system Hf-Nb.

The Hf-Nb system has been reviewed and a thermodynamic dataset has been optimised in [1996Fer]. The phase diagram consists of three phases only, the liquid and bcc phases with complete miscibility and the hcp phase which has only limited solubility for Nb. The selected data for the assessment determine the melting equilibria [1964Tyl, 1969Rud] and the solid phase equilibria between bcc and hcp [1964Sie, 1964Tyl, 1971Car]. Since no experimental data for the thermodynamic mixing properties have been available various calculations and estimates from the literature have been used to approximate the mixing enthalpy for the liquid and solid alloys.

Table I. Phases, structures and models.

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

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Nb}		$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons$ bcc	congruent	2338.2	0.365	0.365	-24688

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

x_{Nb}	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	−6640	928	2.703	928	0.000	0.000
0.200	−9969	1680	4.161	1680	0.000	0.000
0.300	−11975	2246	5.079	2246	0.000	0.000
0.400	−13055	2613	5.596	2613	0.000	0.000
0.500	−13366	2771	5.763	2771	0.000	0.000
0.600	−12962	2706	5.596	2706	0.000	0.000
0.700	−11813	2409	5.079	2409	0.000	0.000
0.800	−9784	1866	4.161	1866	0.000	0.000
0.900	−6501	1067	2.703	1067	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Hf in the liquid phase at 2800 K.

x_{Hf}	ΔG_{Hf} [J/mol]	ΔH_{Hf} [J/mol]	ΔS_{Hf} [J/(mol·K)]	$G_{\mathrm{Hf}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Hf}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Hf}	γ_{Hf}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2367	86	0.876	86	0.000	0.903	1.004
0.800	−4837	358	1.855	358	0.000	0.812	1.016
0.700	−7463	841	2.966	841	0.000	0.726	1.037
0.600	−10336	1557	4.247	1557	0.000	0.641	1.069
0.500	−13608	2529	5.763	2529	0.000	0.557	1.115
0.400	−17551	3781	7.619	3781	0.000	0.471	1.176
0.300	−22693	5336	10.010	5336	0.000	0.377	1.258
0.200	−30252	7217	13.382	7217	0.000	0.273	1.363
0.100	−44159	9447	19.145	9447	0.000	0.150	1.500
0.000	$-\infty$	12050	∞	12050	0.000	0.000	1.678

Reference state: Hf(liquid)

Table IIIc. 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}
0.000	$-\infty$	10116	∞	10116	0.000	0.000	1.544
0.100	−45098	8507	19.145	8507	0.000	0.144	1.441
0.200	−30500	6969	13.382	6969	0.000	0.270	1.349
0.300	−22504	5525	10.010	5525	0.000	0.380	1.268
0.400	−17133	4199	7.619	4199	0.000	0.479	1.198
0.500	−13125	3012	5.763	3012	0.000	0.569	1.138
0.600	−9903	1990	4.247	1990	0.000	0.654	1.089
0.700	−7150	1154	2.966	1154	0.000	0.736	1.051
0.800	−4667	528	1.855	528	0.000	0.818	1.023
0.900	−2317	136	0.876	136	0.000	0.905	1.006
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Nb(liquid)

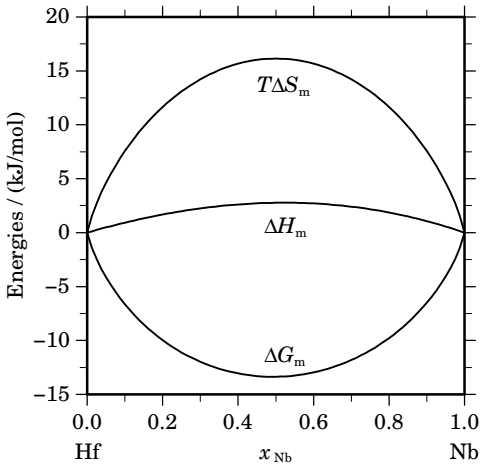

Fig. 2. Integral quantities of the liquid phase at T=2800 K.

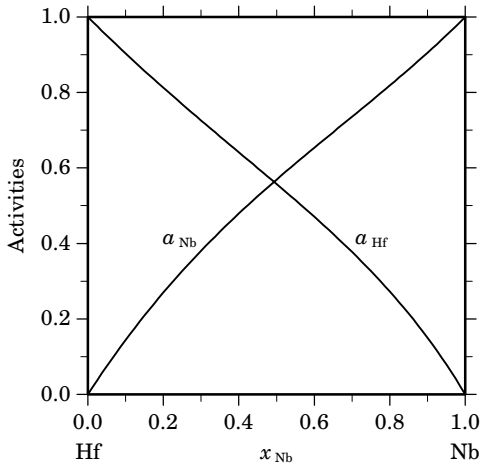

Fig. 3. Activities in the liquid phase at T=2800 K.

Table IVa. Integral quantities for the stable phases at 2200 K.

Phase	x_{Nb}	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)]
bcc	0.000	0	0	0.000	0	0.000	0.000
	0.100	−3889	2057	2.703	2057	0.000	0.000
	0.200	−5501	3652	4.161	3652	0.000	0.000
	0.300	−6389	4785	5.079	4785	0.000	0.000
	0.400	−6851	5460	5.596	5460	0.000	0.000
	0.500	−7001	5678	5.763	5678	0.000	0.000
	0.600	−6868	5442	5.596	5442	0.000	0.000
	0.700	−6420	4754	5.079	4754	0.000	0.000
	0.800	−5537	3616	4.161	3616	0.000	0.000
	0.900	−3915	2031	2.703	2031	0.000	0.000
	1.000	0	0	0.000	0	0.000	0.000

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

Table IVb. Partial quantities for Hf in the stable phases at 2200 K.

Phase	x_{Hf}	ΔG_{Hf} [J/mol]	ΔH_{Hf} [J/mol]	ΔS_{Hf} [J/(mol·K)]	$G_{\mathrm{Hf}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Hf}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Hf}	γ_{Hf}
bcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1695	232	0.876	232	0.000	0.911	1.013
	0.800	−3157	925	1.855	925	0.000	0.841	1.052
	0.700	−4450	2074	2.966	2074	0.000	0.784	1.120
	0.600	−5669	3675	4.247	3675	0.000	0.734	1.223
	0.500	−6955	5724	5.763	5724	0.000	0.684	1.367
	0.400	−8544	8217	7.619	8217	0.000	0.627	1.567
	0.300	−10875	11148	10.010	11148	0.000	0.552	1.839
	0.200	−14927	14513	13.382	14513	0.000	0.442	2.211
	0.100	−23810	18309	19.145	18309	0.000	0.272	2.721
	0.000	$-\infty$	22529	∞	22529	0.000	0.000	3.427

Reference state: Hf(bcc)

Table IVc. Partial quantities for Nb in the stable phases at 2200 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	0.000	$-\infty$	22898	∞	22898	0.000	0.000	3.497
	0.100	−23631	18487	19.145	18487	0.000	0.275	2.747
	0.200	−14880	14560	13.382	14560	0.000	0.443	2.217
	0.300	−10911	11112	10.010	11112	0.000	0.551	1.836
	0.400	−8624	8137	7.619	8137	0.000	0.624	1.560
	0.500	−7047	5632	5.763	5632	0.000	0.680	1.361
	0.600	−5751	3593	4.247	3593	0.000	0.730	1.217
	0.700	−4510	2014	2.966	2014	0.000	0.781	1.116
	0.800	−3189	892	1.855	892	0.000	0.840	1.050
	0.900	−1705	222	0.876	222	0.000	0.911	1.012
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Nb(bcc)

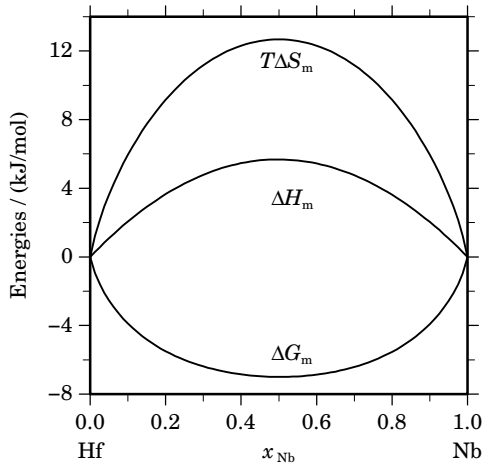

Fig. 4. Integral quantities of the stable phases at T=2200 K.

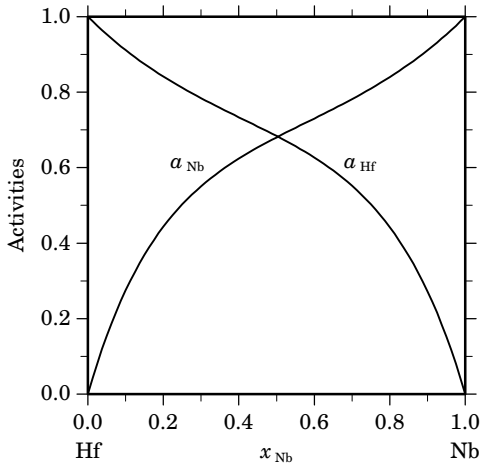

Fig. 5. Activities in the stable phases at T=2200 K.

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