Mo – Nb (Molybdenum – Niobium)

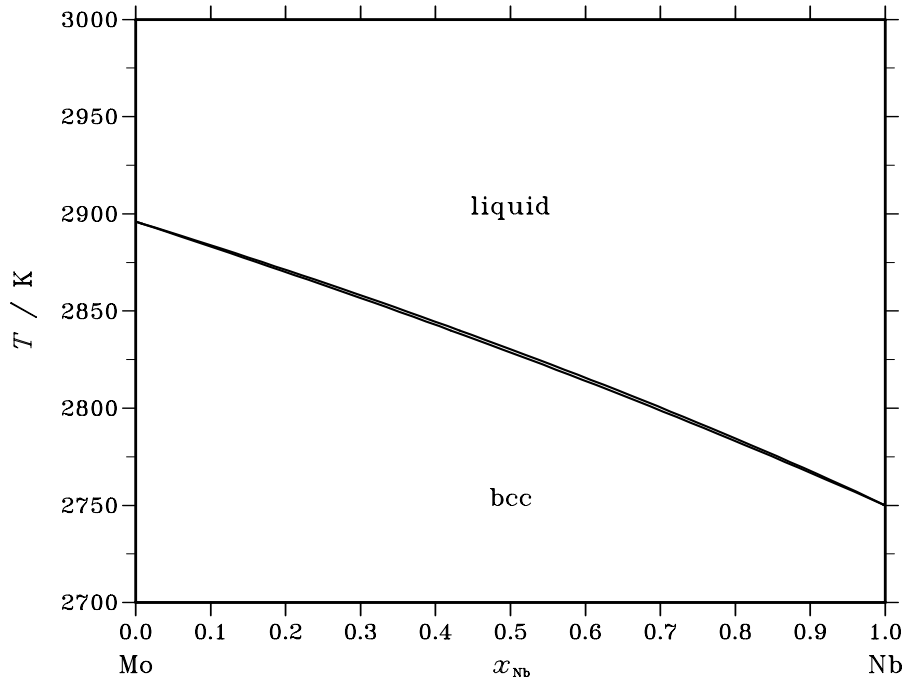

Fig. 1. Calculated phase diagram for the system Mo-Nb.

Molybdenum and niobium are important additions to many alloys, such as superalloys and refractory alloys. The Mo-Nb system is fairly simple with only two condensed stable phases, liquid and bcc. In spite of the high temperatures of the solidus and liquidus, the experimental data are in fairly good agreement. [91Oka] showed that solidus and liquidus can be reproduced by describing both phases as ideal solutions. However, the activities of Nb in the bcc phase that were obtained by [73Sin] from EMF measurements show negative deviations from Raoult's law. These activity data were taken into account in the recommended assessment of [80Che]. The liquidus and solidus obtained from this calculation are very similar to those from [91Oka].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Mo,Nb)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Mo,Nb)_1$

Table IIa. Integral quantities for the liquid phase at 2900 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	−10075	−2924	2.466	−2237	−0.237	0.000
0.200	−16205	−5413	3.721	−4139	−0.439	0.000
0.300	−20376	−7387	4.479	−5647	−0.600	0.000
0.400	−22925	−8765	4.883	−6698	−0.713	0.000
0.500	−23944	−9467	4.992	−7231	−0.771	0.000
0.600	−23414	−9412	4.828	−7186	−0.767	0.000
0.700	−21231	−8518	4.384	−6502	−0.695	0.000
0.800	−17182	−6705	3.613	−5117	−0.548	0.000
0.900	−10808	−3893	2.385	−2970	−0.318	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIb. Partial quantities for Mo in the liquid phase at 2900 K.

x_{Mo}	ΔG_{Mo} [J/mol]	ΔH_{Mo} [J/mol]	ΔS_{Mo} [J/(mol·K)]	$G_{\mathrm{Mo}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Mo}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Mo}	γ_{Mo}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2697	−204	0.860	−157	−0.016	0.894	0.994
0.800	−6090	−922	1.782	−709	−0.074	0.777	0.971
0.700	−10379	−2318	2.780	−1779	−0.186	0.650	0.929
0.600	−15805	−4551	3.881	−3488	−0.367	0.519	0.865
0.500	−22672	−7784	5.134	−5959	−0.630	0.391	0.781
0.400	−31407	−12179	6.630	−9313	−0.988	0.272	0.680
0.300	−42704	−17896	8.555	−13674	−1.456	0.170	0.567
0.200	−57970	−25098	11.335	−19163	−2.046	0.090	0.452
0.100	−81423	−33945	16.372	−25903	−2.773	0.034	0.342
0.000	$-\infty$	−44600	∞	−34015	−3.650	0.000	0.244

Reference state: Mo(liquid)

Table IIc. Partial quantities for Nb in the liquid phase at 2900 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	$-\infty$	−31137	∞	−23834	−2.518	0.000	0.372
0.100	−76475	−27402	16.922	−20955	−2.223	0.042	0.419
0.200	−56667	−23374	11.480	−17860	−1.901	0.095	0.477
0.300	−43702	−19215	8.444	−14672	−1.567	0.163	0.544
0.400	−33606	−15087	6.386	−11512	−1.233	0.248	0.620
0.500	−25217	−11150	4.851	−8504	−0.913	0.351	0.703
0.600	−18085	−7567	3.627	−5768	−0.620	0.472	0.787
0.700	−12028	−4499	2.596	−3428	−0.369	0.607	0.867
0.800	−6985	−2107	1.682	−1605	−0.173	0.748	0.936
0.900	−2962	−554	0.830	−422	−0.046	0.884	0.983
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Nb(liquid)

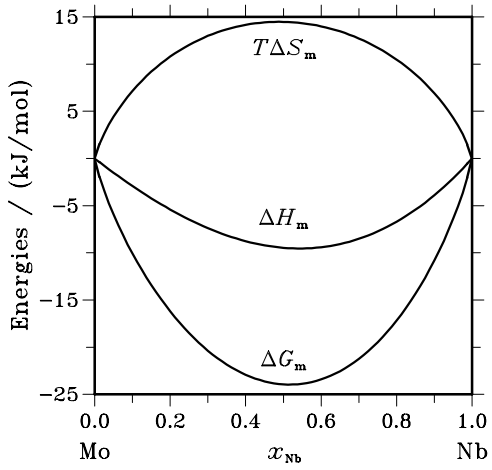

Fig. 2. Integral quantities of the liquid phase at T=2900 K.

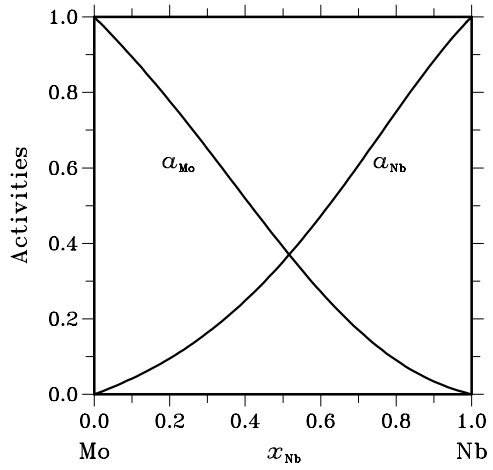

Fig. 3. Activities in the liquid phase at T=2900 K.

Table IIIa. Integral quantities for the stable phases at 2000 K.

Phase	x_{Nb}	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	−7856	−2924	2.466	−2450	−0.237	0.000
	0.200	−12856	−5413	3.721	−4534	−0.439	0.000
	0.300	−16345	−7387	4.479	−6187	−0.600	0.000
	0.400	−18531	−8765	4.883	−7339	−0.713	0.000
	0.500	−19451	−9467	4.992	−7925	−0.771	0.000
	0.600	−19068	−9412	4.828	−7877	−0.767	0.000
	0.700	−17286	−8518	4.384	−7127	−0.695	0.000
	0.800	−13931	−6705	3.613	−5610	−0.548	0.000
	0.900	−8662	−3893	2.385	−3256	−0.318	0.000
	1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Mo in the stable phases at 2000 K.

Phase	x_{Mo}	ΔG_{Mo} [J/mol]	ΔH_{Mo} [J/mol]	ΔS_{Mo} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Mo}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Mo}}$ [J/(mol·K)]	a_{Mo}	γ_{Mo}
bcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1923	−204	0.860	−171	−0.016	0.891	0.990
	0.800	−4486	−922	1.782	−775	−0.074	0.764	0.954
	0.700	−7877	−2318	2.780	−1946	−0.186	0.623	0.890
	0.600	−12312	−4551	3.881	−3818	−0.367	0.477	0.795
	0.500	−18052	−7784	5.134	−6525	−0.630	0.338	0.675
	0.400	−25440	−12179	6.630	−10203	−0.988	0.217	0.541
	0.300	−35005	−17896	8.555	−14984	−1.456	0.122	0.406
	0.200	−47768	−25098	11.335	−21005	−2.046	0.057	0.283
	0.100	−66688	−33945	16.372	−28399	−2.773	0.018	0.181
	0.000	$-\infty$	−44600	∞	−37300	−3.650	0.000	0.106

Reference state: Mo(bcc)

Table IIIc. Partial quantities for Nb in the stable phases at 2000 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	$-\infty$	−31137	∞	−26101	−2.518	0.000	0.208
	0.100	−61246	−27402	16.922	−22956	−2.223	0.025	0.251
	0.200	−46335	−23374	11.480	−19571	−1.901	0.062	0.308
	0.300	−36103	−19215	8.444	−16082	−1.567	0.114	0.380
	0.400	−27859	−15087	6.386	−12622	−1.233	0.187	0.468
	0.500	−20851	−11150	4.851	−9325	−0.913	0.285	0.571
	0.600	−14821	−7567	3.627	−6326	−0.620	0.410	0.684
	0.700	−9691	−4499	2.596	−3760	−0.369	0.558	0.798
	0.800	−5471	−2107	1.682	−1761	−0.173	0.720	0.900
	0.900	−2215	−554	0.830	−463	−0.046	0.875	0.973
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Nb(bcc)

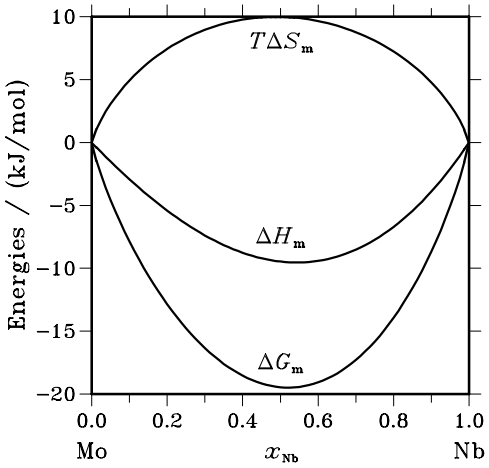

Fig. 4. Integral quantities of the stable phases at T=2000 K.

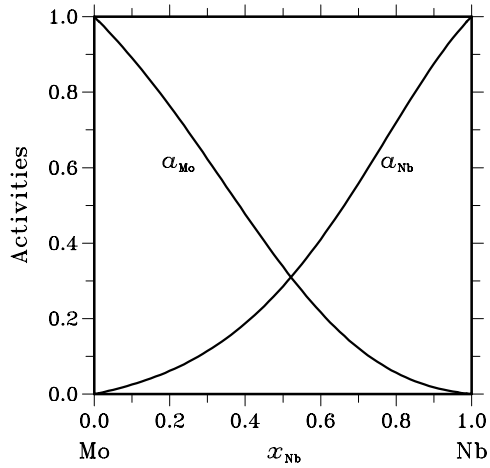

Fig. 5. Activities in the stable phases at T=2000 K.

References

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