Mo – Ta (Molybdenum – Tantalum)

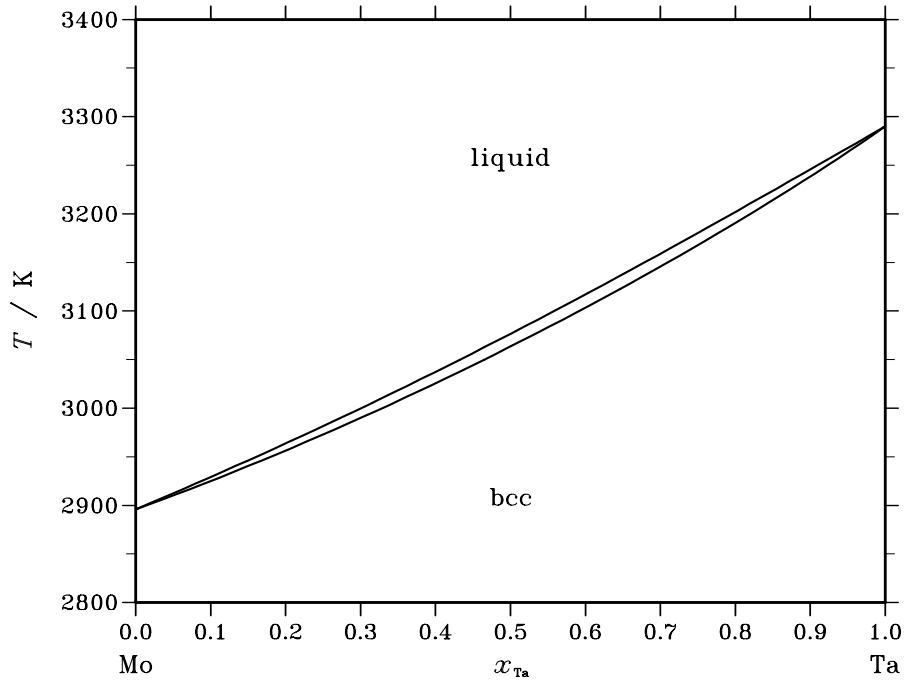

Fig. 1. Calculated phase diagram for the system Mo-Ta.

Molybdenum and tantalum are important additions to many alloys, such as superalloys and refractory alloys. The Mo-Ta system is fairly simple with only two condensed stable phases, liquid and bcc. Two recent thermodynamic assessments used different data sets to derive the Gibbs energy functions. [91Kau] derived the excess Gibbs energy from the semi-empirical prediction of the enthalpy of mixing of the liquid and solid phase by [83Nie]. The assessment of [99Cui] is based on the phase diagram proposed by [86Kri] and the activity data of Ta in the bcc phase reported by [73Sin]. [86Kri] accepted in their evaluation of the calculated phase diagram from [70Kau] although the calculated solidus is consistently lower than the experimental observations. The Ta activities calculated from the [99Cui] description show a more negative deviation from Raoult's law than the experimental values from [73Sin], while those calculated from the [91Kau] description show a less negative deviation than the experimental values. The description of [91Kau] is recommended since it reproduces both the phase diagram and the Ta activities in the bcc phase reasonably well.

Table I. Phases, structures and models.

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

Table IIa. Integral quantities for the liquid phase at 3300 K.

x_{Ta}	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	−10711	−1791	2.703	−1791	0.000	0.000
0.200	−16898	−3168	4.161	−3168	0.000	0.000
0.300	−20898	−4137	5.079	−4137	0.000	0.000
0.400	−23170	−4704	5.596	−4704	0.000	0.000
0.500	−23894	−4875	5.763	−4875	0.000	0.000
0.600	−23122	−4656	5.596	−4656	0.000	0.000
0.700	−20814	−4053	5.079	−4053	0.000	0.000
0.800	−16802	−3072	4.161	−3072	0.000	0.000
0.900	−10639	−1719	2.703	−1719	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIb. Partial quantities for Mo in the liquid phase at 3300 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	−3099	−208	0.876	−208	0.000	0.893	0.992
0.800	−6947	−824	1.855	−824	0.000	0.776	0.970
0.700	−11622	−1836	2.966	−1836	0.000	0.655	0.935
0.600	−17248	−3232	4.247	−3232	0.000	0.533	0.889
0.500	−24019	−5000	5.763	−5000	0.000	0.417	0.833
0.400	−32269	−7128	7.619	−7128	0.000	0.308	0.771
0.300	−42639	−9604	10.010	−9604	0.000	0.211	0.705
0.200	−56576	−12416	13.382	−12416	0.000	0.127	0.636
0.100	−78730	−15552	19.145	−15552	0.000	0.057	0.567
0.000	$-\infty$	−19000	∞	−19000	0.000	0.000	0.500

Reference state: Mo(liquid)

Table IIc. Partial quantities for Ta in the liquid phase at 3300 K.

x_{Ta}	ΔG_{Ta} [J/mol]	ΔH_{Ta} [J/mol]	ΔS_{Ta} [J/(mol·K)]	$G_{\mathrm{Ta}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Ta}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Ta}	γ_{Ta}
0.000	$-\infty$	−20000	∞	−20000	0.000	0.000	0.482
0.100	−79216	−16038	19.145	−16038	0.000	0.056	0.557
0.200	−56704	−12544	13.382	−12544	0.000	0.127	0.633
0.300	−42541	−9506	10.010	−9506	0.000	0.212	0.707
0.400	−32053	−6912	7.619	−6912	0.000	0.311	0.777
0.500	−23769	−4750	5.763	−4750	0.000	0.421	0.841
0.600	−17024	−3008	4.247	−3008	0.000	0.538	0.896
0.700	−11460	−1674	2.966	−1674	0.000	0.659	0.941
0.800	−6859	−736	1.855	−736	0.000	0.779	0.974
0.900	−3073	−182	0.876	−182	0.000	0.894	0.993
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ta(liquid)

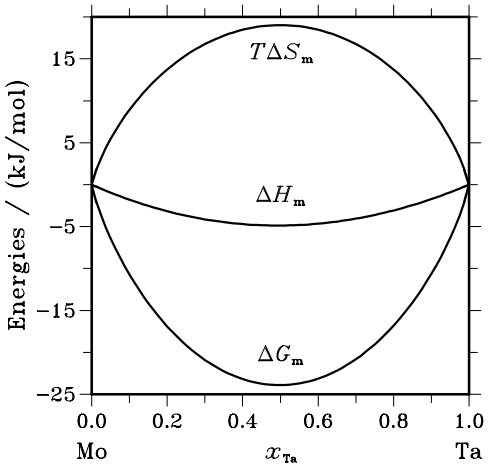

Fig. 2. Integral quantities of the liquid phase at T=3300 K.

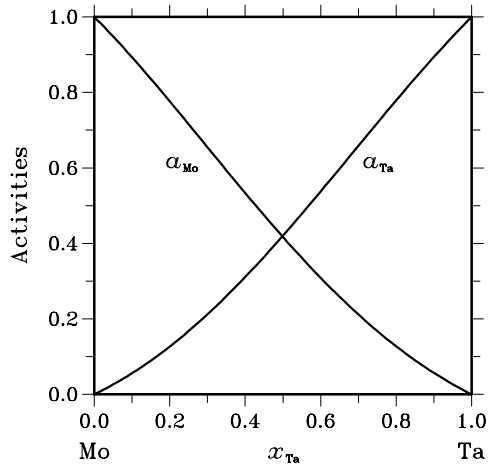

Fig. 3. Activities in the liquid phase at T=3300 K.

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

Phase	x_{Ta}	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	−7152	−1746	2.703	−1746	0.000	0.000
	0.200	−11409	−3088	4.161	−3088	0.000	0.000
	0.300	−14190	−4032	5.079	−4032	0.000	0.000
	0.400	−15776	−4584	5.596	−4584	0.000	0.000
	0.500	−16276	−4750	5.763	−4750	0.000	0.000
	0.600	−15728	−4536	5.596	−4536	0.000	0.000
	0.700	−14106	−3948	5.079	−3948	0.000	0.000
	0.800	−11313	−2992	4.161	−2992	0.000	0.000
	0.900	−7080	−1674	2.703	−1674	0.000	0.000
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Mo(bcc), Ta(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	−1955	−203	0.876	−203	0.000	0.889	0.988
	0.800	−4515	−804	1.855	−804	0.000	0.762	0.953
	0.700	−7722	−1791	2.966	−1791	0.000	0.629	0.898
	0.600	−11647	−3152	4.247	−3152	0.000	0.496	0.827
	0.500	−16401	−4875	5.763	−4875	0.000	0.373	0.746
	0.400	−22185	−6948	7.619	−6948	0.000	0.263	0.658
	0.300	−29380	−9359	10.010	−9359	0.000	0.171	0.570
	0.200	−38859	−12096	13.382	−12096	0.000	0.097	0.483
	0.100	−53437	−15147	19.145	−15147	0.000	0.040	0.402
	0.000	$-\infty$	−18500	∞	−18500	0.000	0.000	0.329

Reference state: Mo(bcc)

Table IIIc. Partial quantities for Ta in the stable phases at 2000 K.

Phase	x_{Ta}	ΔG_{Ta} [J/mol]	ΔH_{Ta} [J/mol]	ΔS_{Ta} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ta}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ta}}$ [J/(mol·K)]	a_{Ta}	γ_{Ta}
bcc	0.000	$-\infty$	−19500	∞	−19500	0.000	0.000	0.310
	0.100	−53923	−15633	19.145	−15633	0.000	0.039	0.391
	0.200	−38987	−12224	13.382	−12224	0.000	0.096	0.479
	0.300	−29282	−9261	10.010	−9261	0.000	0.172	0.573
	0.400	−21969	−6732	7.619	−6732	0.000	0.267	0.667
	0.500	−16151	−4625	5.763	−4625	0.000	0.379	0.757
	0.600	−11423	−2928	4.247	−2928	0.000	0.503	0.839
	0.700	−7560	−1629	2.966	−1629	0.000	0.635	0.907
	0.800	−4427	−716	1.855	−716	0.000	0.766	0.958
	0.900	−1929	−177	0.876	−177	0.000	0.890	0.989
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ta(bcc)

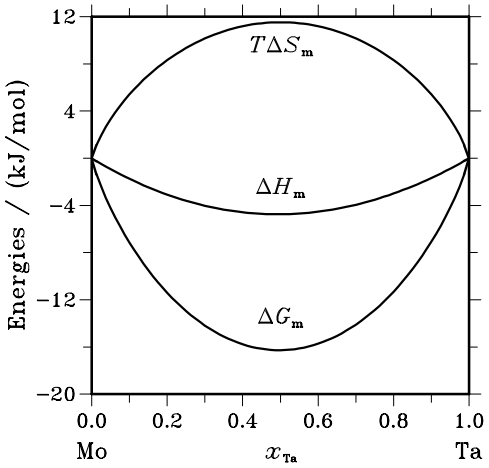

Fig. 4. Integral quantities of the stable phases at T=2000 K.

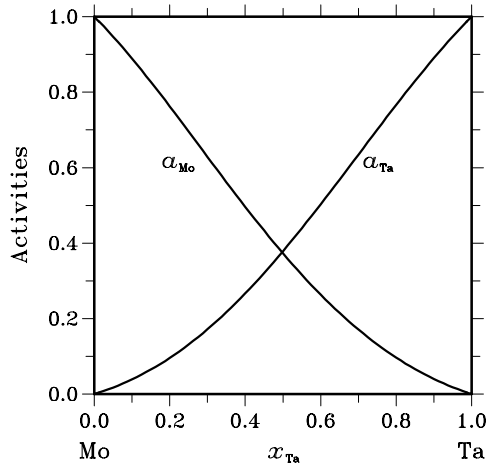

Fig. 5. Activities in the stable phases at T=2000 K.

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