Mo – Ti (Molybdenum – Titanium)

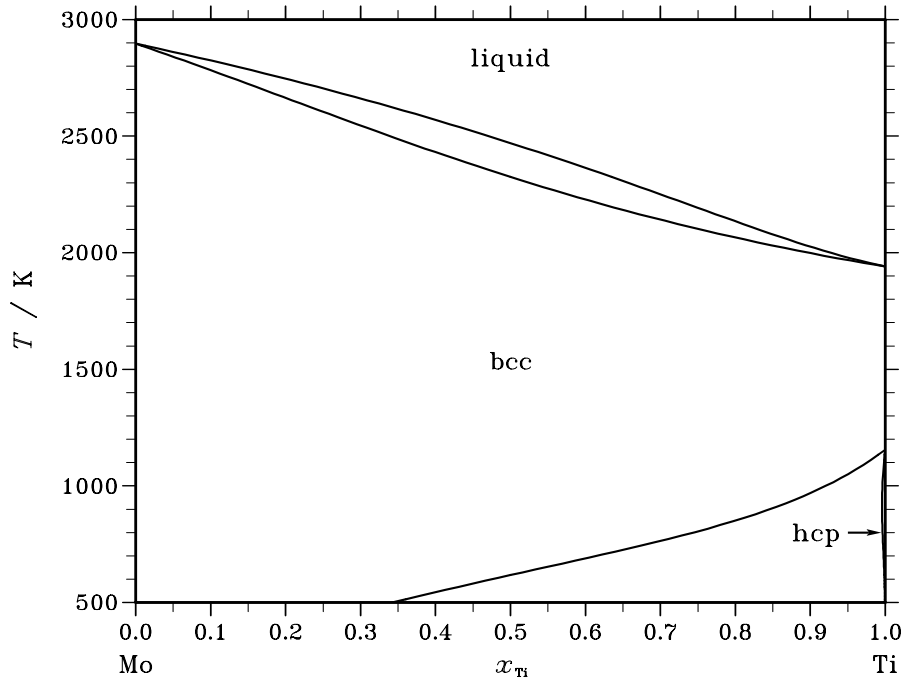

Fig. 1. Calculated phase diagram for the system Mo-Ti.

Molybdenum and titanium are important additions to many alloys, such as superalloys and refractory alloys. The Mo-Ti system is fairly simple with only three condensed stable phases, liquid, bcc and hcp. According to the critical evaluation of the available experimental information [87Mur], the bcc phase shows a miscibility gap and a monotectic reaction. However, [87Mur] also points out that the experimental evidence is somewhat ambiguous. Based on first principles calculations, [95Rub] doubts the existence of such a miscibility gap. A number of thermodynamic descriptions have been developed for this system. The description of [98Sau] is in qualitative agreement with the first principles results and reproduces well the established phases boundaries, i.e. liquidus and the boundaries of the hcp+bcc two-phase region, thus is recommended.

Table I. Phases, structures and models.

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

Table IIa. Integral quantities for the liquid phase at 2900 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	−8126	−810	2.523	−288	−0.180	0.000
0.200	−12578	−1440	3.841	−512	−0.320	0.000
0.300	−15401	−1890	4.659	−672	−0.420	0.000
0.400	−16996	−2160	5.116	−768	−0.480	0.000
0.500	−17513	−2250	5.263	−800	−0.500	0.000
0.600	−16996	−2160	5.116	−768	−0.480	0.000
0.700	−15401	−1890	4.659	−672	−0.420	0.000
0.800	−12578	−1440	3.841	−512	−0.320	0.000
0.900	−8126	−810	2.523	−288	−0.180	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Mo(liquid), Ti(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	−2572	−90	0.856	−32	−0.020	0.899	0.999
0.800	−5508	−360	1.775	−128	−0.080	0.796	0.995
0.700	−8888	−810	2.786	−288	−0.180	0.692	0.988
0.600	−12829	−1440	3.927	−512	−0.320	0.587	0.979
0.500	−17513	−2250	5.263	−800	−0.500	0.484	0.967
0.400	−23246	−3240	6.899	−1152	−0.720	0.381	0.953
0.300	−30598	−4410	9.030	−1568	−0.980	0.281	0.937
0.200	−40855	−5760	12.102	−2048	−1.280	0.184	0.919
0.100	−58112	−7290	17.525	−2592	−1.620	0.090	0.898
0.000	$-\infty$	−9000	∞	−3200	−2.000	0.000	0.876

Reference state: Mo(liquid)

Table IIc. Partial quantities for Ti in the liquid phase at 2900 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	$-\infty$	−9000	∞	−3200	−2.000	0.000	0.876
0.100	−58112	−7290	17.525	−2592	−1.620	0.090	0.898
0.200	−40855	−5760	12.102	−2048	−1.280	0.184	0.919
0.300	−30598	−4410	9.030	−1568	−0.980	0.281	0.937
0.400	−23246	−3240	6.899	−1152	−0.720	0.381	0.953
0.500	−17513	−2250	5.263	−800	−0.500	0.484	0.967
0.600	−12829	−1440	3.927	−512	−0.320	0.587	0.979
0.700	−8888	−810	2.786	−288	−0.180	0.692	0.988
0.800	−5508	−360	1.775	−128	−0.080	0.796	0.995
0.900	−2572	−90	0.856	−32	−0.020	0.899	0.999
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(liquid)

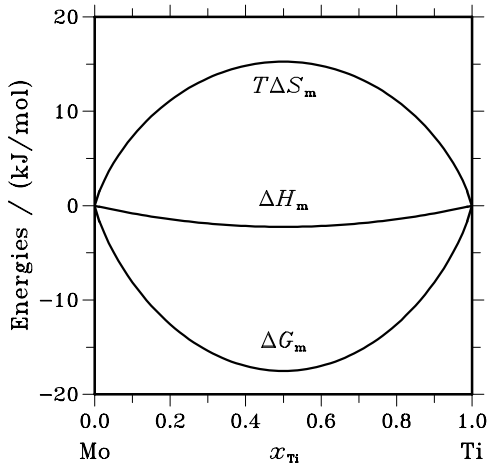

Fig. 2. Integral quantities of the liquid phase at T=2900 K.

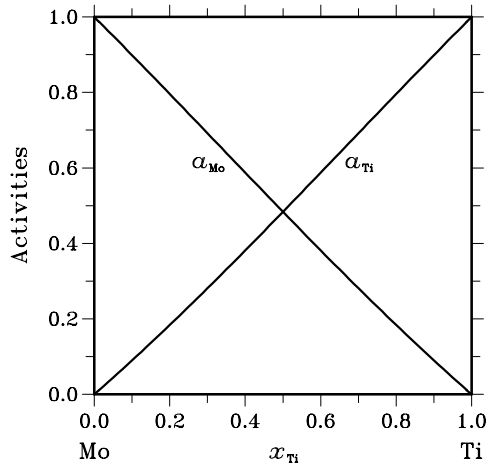

Fig. 3. Activities in the liquid phase at T=2900 K.

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	−4018	36	2.703	36	0.000	0.000
	0.200	−6113	128	4.161	128	0.000	0.000
	0.300	−7367	252	5.079	252	0.000	0.000
	0.400	−8010	384	5.596	384	0.000	0.000
	0.500	−8145	500	5.763	500	0.000	0.000
	0.600	−7818	576	5.596	576	0.000	0.000
	0.700	−7031	588	5.079	588	0.000	0.000
	0.800	−5729	512	4.161	512	0.000	0.000
	0.900	−3730	324	2.703	324	0.000	0.000
	1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Mo in the stable phases at 1500 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	−1346	−32	0.876	−32	0.000	0.898	0.997
	0.800	−2879	−96	1.855	−96	0.000	0.794	0.992
	0.700	−4592	−144	2.966	−144	0.000	0.692	0.989
	0.600	−6499	−128	4.247	−128	0.000	0.594	0.990
	0.500	−8645	0	5.763	0	0.000	0.500	1.000
	0.400	−11140	288	7.619	288	0.000	0.409	1.023
	0.300	−14232	784	10.010	784	0.000	0.319	1.065
	0.200	−18537	1536	13.382	1536	0.000	0.226	1.131
	0.100	−26125	2592	19.145	2592	0.000	0.123	1.231
	0.000	$-\infty$	4000	∞	4000	0.000	0.000	1.378

Reference state: Mo(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	$-\infty$	0	∞	0	0.000	0.000	1.000
	0.100	−28069	648	19.145	648	0.000	0.105	1.053
	0.200	−19049	1024	13.382	1024	0.000	0.217	1.086
	0.300	−13840	1176	10.010	1176	0.000	0.330	1.099
	0.400	−10276	1152	7.619	1152	0.000	0.439	1.097
	0.500	−7645	1000	5.763	1000	0.000	0.542	1.083
	0.600	−5603	768	4.247	768	0.000	0.638	1.064
	0.700	−3944	504	2.966	504	0.000	0.729	1.041
	0.800	−2527	256	1.855	256	0.000	0.817	1.021
	0.900	−1242	72	0.876	72	0.000	0.905	1.006
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(bcc)

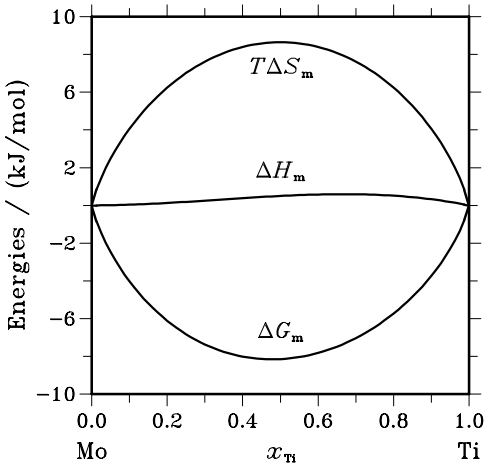

Fig. 4. Integral quantities of the stable phases at T=1500 K.

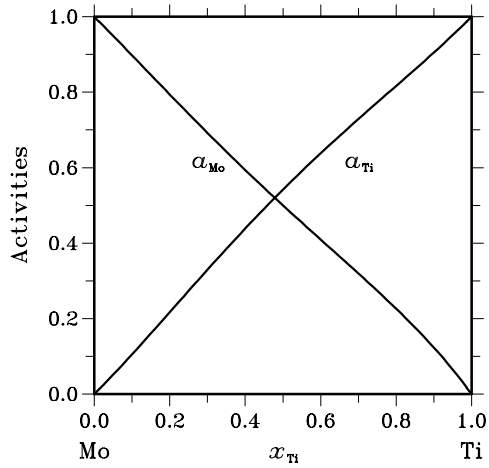

Fig. 5. Activities in the stable phases at T=1500 K.

References

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