Mo – V (Molybdenum – Vanadium)

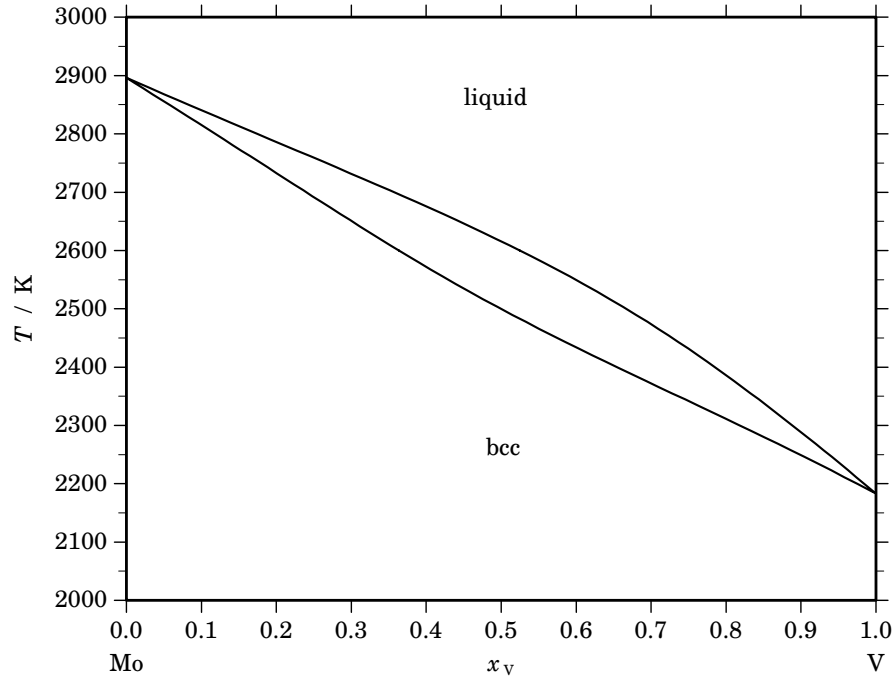

Fig. 1. Calculated phase diagram for the system Mo-V.

Molybdenum and vanadium are important alloying elements for steel and they are added both together in concentrations of some percent to certain hot work tool steels. The phase diagram of the Mo-V system is quite simple consisting of only the liquid and the solid bcc phases each with complete miscibility of the components. The literature on the Mo-V system has been reviewed by [1989Smi, 1999Zhe] and optimised thermodynamic datasets have been reported in [1999Zhe, 2002Bra]. Both reviews conclude that the most reliable data on the phase diagram have been reported by Rudy [1969Rud]. It has also been concluded that no reliable thermodynamic data of mixing have been available which are consistent with the phase diagram data. In order to estimate the thermodynamic excess quantities in the bcc solid solution, [1999Zhe] took account of theoretical considerations given in [1980Bre]. However, under these conditions the calculated two-phase region is clearly more narrow than measured by [1969Rud] although the mixing properties have been described by 4 coefficients for each phase [1999Zhe]. In view of these results [2002Bra] decided to re-assess the system using only reliable experimental data, essentially those of [1969Rud]. In the resulting optimisation these data are well reproduced using a strictly regular solution model for both phases with only one coefficient for each phase. The optimisation of [2002Bra] is recommended here because it provides a better fit to the accepted data with much less parameters. Below 1160 K a miscibility gap in the bcc phase is predicted, however, no experimental evidence is available.

Table I. Phases, structures and models.

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

Table IIa. Integral quantities for the liquid phase at 2900 K.

x_{V}	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	−6238	1601	2.703	1601	0.000	0.000
0.200	−9220	2845	4.161	2845	0.000	0.000
0.300	−10995	3735	5.079	3735	0.000	0.000
0.400	−11960	4268	5.596	4268	0.000	0.000
0.500	−12267	4446	5.763	4446	0.000	0.000
0.600	−11960	4268	5.596	4268	0.000	0.000
0.700	−10995	3735	5.079	3735	0.000	0.000
0.800	−9220	2845	4.161	2845	0.000	0.000
0.900	−6238	1601	2.703	1601	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Mo(liquid), V(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	−2363	178	0.876	178	0.000	0.907	1.007
0.800	−4669	711	1.855	711	0.000	0.824	1.030
0.700	−7000	1601	2.966	1601	0.000	0.748	1.069
0.600	−9472	2845	4.247	2845	0.000	0.675	1.125
0.500	−12267	4446	5.763	4446	0.000	0.601	1.202
0.400	−15691	6402	7.619	6402	0.000	0.522	1.304
0.300	−20316	8714	10.010	8714	0.000	0.431	1.435
0.200	−27425	11382	13.382	11382	0.000	0.321	1.603
0.100	−41115	14405	19.145	14405	0.000	0.182	1.817
0.000	$-\infty$	17784	∞	17784	0.000	0.000	2.091

Reference state: Mo(liquid)

Table IIc. Partial quantities for V in the liquid phase at 2900 K.

x_{V}	ΔG_{V} [J/mol]	ΔH_{V} [J/mol]	ΔS_{V} [J/(mol·K)]	$G_{\mathrm{V}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{V}}^{\mathrm{E}}$ [J/(mol·K)]	a_{V}	γ_{V}
0.000	$-\infty$	17784	∞	17784	0.000	0.000	2.091
0.100	−41115	14405	19.145	14405	0.000	0.182	1.817
0.200	−27425	11382	13.382	11382	0.000	0.321	1.603
0.300	−20316	8714	10.010	8714	0.000	0.431	1.435
0.400	−15691	6402	7.619	6402	0.000	0.522	1.304
0.500	−12267	4446	5.763	4446	0.000	0.601	1.202
0.600	−9472	2845	4.247	2845	0.000	0.675	1.125
0.700	−7000	1601	2.966	1601	0.000	0.748	1.069
0.800	−4669	711	1.855	711	0.000	0.824	1.030
0.900	−2363	178	0.876	178	0.000	0.907	1.007
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: V(liquid)

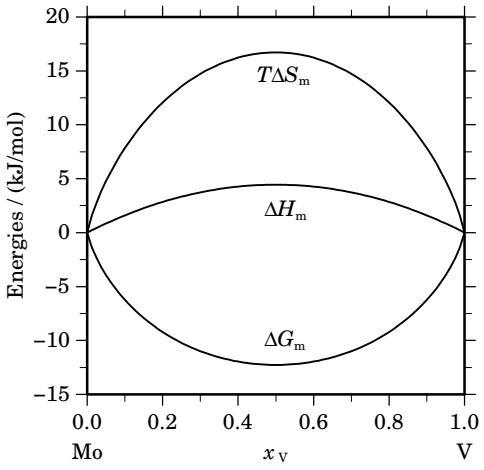

Fig. 2. Integral quantities of the liquid phase at T=2900 K.

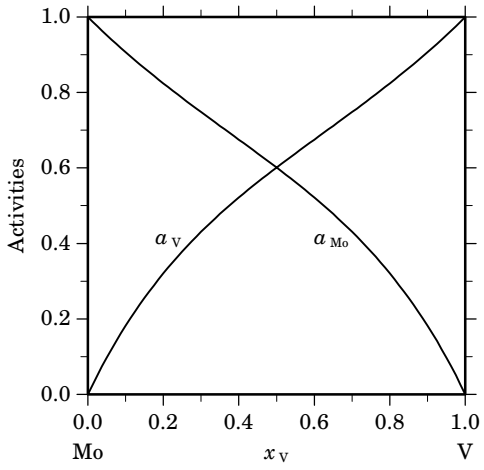

Fig. 3. Activities in the liquid phase at T=2900 K.

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

Phase	x_V	ΔG_m [J/mol]	ΔH_m [J/mol]	ΔS_m [J/(mol·K)]	G_m^E [J/mol]	S_m^E [J/(mol·K)]	ΔC_P [J/(mol·K)]
bcc	0.000	0	0	0.000	0	0.000	0.000
	0.100	−3674	1732	2.703	1732	0.000	0.000
	0.200	−5242	3079	4.161	3079	0.000	0.000
	0.300	−6117	4041	5.079	4041	0.000	0.000
	0.400	−6573	4619	5.596	4619	0.000	0.000
	0.500	−6715	4811	5.763	4811	0.000	0.000
	0.600	−6573	4619	5.596	4619	0.000	0.000
	0.700	−6117	4041	5.079	4041	0.000	0.000
	0.800	−5242	3079	4.161	3079	0.000	0.000
	0.900	−3674	1732	2.703	1732	0.000	0.000
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Mo(bcc), V(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_{Mo}^E [J/mol]	S_{Mo}^E [J/(mol·K)]	a_{Mo}	γ_{Mo}
bcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1560	192	0.876	192	0.000	0.910	1.012
	0.800	−2941	770	1.855	770	0.000	0.838	1.047
	0.700	−4199	1732	2.966	1732	0.000	0.777	1.110
	0.600	−5415	3079	4.247	3079	0.000	0.722	1.203
	0.500	−6715	4811	5.763	4811	0.000	0.668	1.336
	0.400	−8309	6928	7.619	6928	0.000	0.607	1.517
	0.300	−10591	9430	10.010	9430	0.000	0.529	1.763
	0.200	−14447	12317	13.382	12317	0.000	0.419	2.097
	0.100	−22701	15589	19.145	15589	0.000	0.255	2.553
	0.000	$-\infty$	19245	∞	19245	0.000	0.000	3.181

Reference state: Mo(bcc)

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

Phase	x_V	ΔG_V [J/mol]	ΔH_V [J/mol]	ΔS_V [J/(mol·K)]	G_V^E [J/mol]	S_V^E [J/(mol·K)]	a_V	γ_V
bcc	0.000	$-\infty$	19245	∞	19245	0.000	0.000	3.181
	0.100	−22701	15588	19.145	15588	0.000	0.255	2.553
	0.200	−14447	12317	13.382	12317	0.000	0.419	2.097
	0.300	−10591	9430	10.010	9430	0.000	0.529	1.763
	0.400	−8309	6928	7.619	6928	0.000	0.607	1.517
	0.500	−6715	4811	5.763	4811	0.000	0.668	1.336
	0.600	−5415	3079	4.247	3079	0.000	0.722	1.203
	0.700	−4199	1732	2.966	1732	0.000	0.777	1.110
	0.800	−2941	770	1.855	770	0.000	0.838	1.047
	0.900	−1560	192	0.876	192	0.000	0.910	1.012
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: V(bcc)

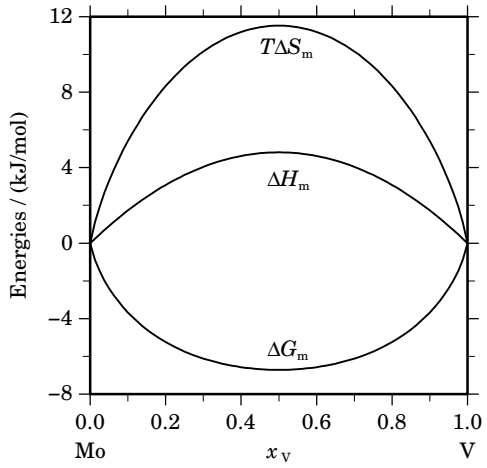

Fig. 4. Integral quantities of the stable phases at T=2000 K.

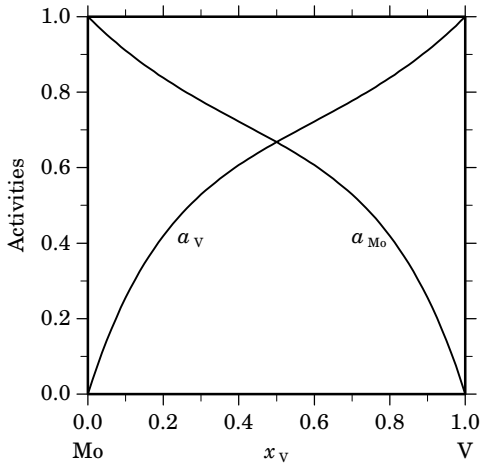

Fig. 5. Activities in the stable phases at T=2000 K.

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