Fe – Mo (Iron – Molybdenum)

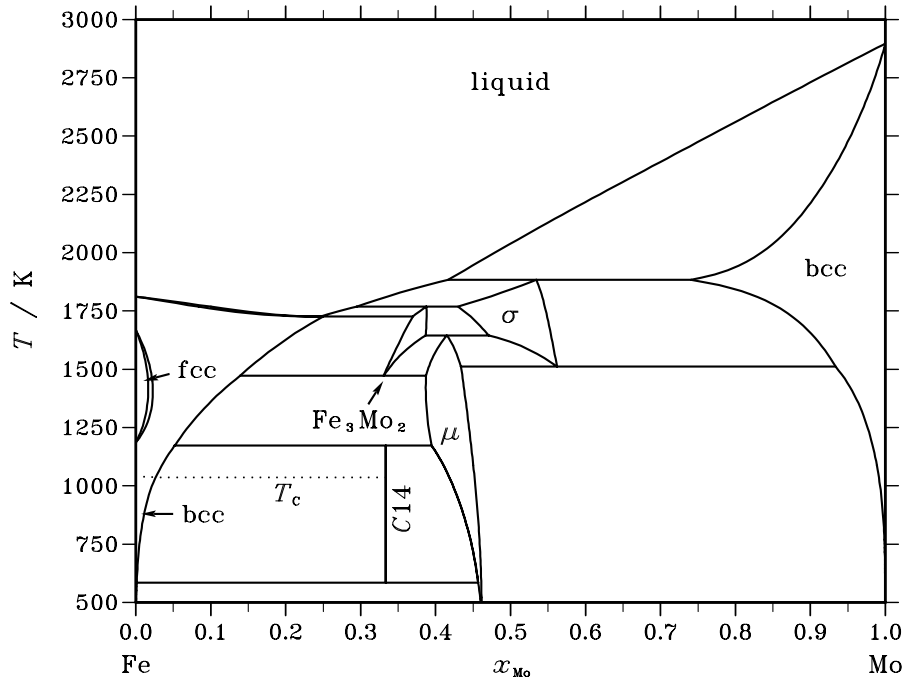

Fig. 1. Calculated phase diagram for the system Fe-Mo.

There are four intermetallic phases in the Fe-Mo system. The σ-phase and R-phase (Fe_3Mo_2) are stable at high temperature in contact with the liquid. At lower temperature they are replaced by the μ-phase which is stable below room temperature. There is also a Laves phase ($C14$) formed at 1173 K for Fe-rich systems. In the present assessment from [88And] the Laves phase is not stable below 600 K but there is no experimental evidence for that. Mo stabilises the bcc phase and a characteristic closed "gamma-loop" is formed for the fcc phase on the Fe-rich side. The original assessment by [82Fer] used a different model for the σ-phase than used later by [88And] but the original model with 3 sublattices and 10:4:16 sites has recently been restored. Mo is an important alloying element in stainless steels to prevent corrosion in salt water but also a strong carbide former in tool steels and other hard materials.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Fe,Mo)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Fe,Mo)_1$
bcc	$A2$	W	$cI24$	$Im\overline{3}m$	BCC_A2	$(Fe,Mo)_1$
$C14$	$C14$	$MgZn_2$	$hP12$	$P6_3/mmc$	LAVES_C14	Fe_2Mo_1
Fe_3Mo_2	$\cdots$	R-(Co,Cr,Mo)	$hR53$	$\cdots$	R_PHASE	$Fe_{27}Mo_{14}(Fe,Mo)_{12}$
μ	$D8_5$	Fe_7W_6	$hR13$	$R\overline{3}m$	D85_MU	$Fe_7Mo_2(Fe,Mo)_4$
σ	$D8_b$	σCrFe	$tP30$	$P4_2/mnm$	D8B_SIGMA	$Fe_{10}Mo_4(Fe,Mo)_{16}$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Mo}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid + bcc $\rightleftharpoons \sigma$	peritectic	1883.2	0.417	0.741	0.534	−14328
liquid + $\sigma \rightleftharpoons Fe_3Mo_2$	peritectic	1768.7	0.295	0.430	0.388	−6797
liquid + $Fe_3Mo_2 \rightleftharpoons$ bcc	peritectic	1726.4	0.247	0.370	0.250	−10766
liquid $\rightleftharpoons$ bcc	congruent	1726.2	0.240	0.240		−11257
Fe_3Mo_2 + $\sigma \rightleftharpoons \mu$	peritectoid	1644.4	0.387	0.471	0.415	−5734
$\sigma \rightleftharpoons \mu$ + bcc	eutectoid	1511.7	0.562	0.434	0.934	−5057
$Fe_3Mo_2 \rightleftharpoons$ bcc + μ	eutectoid	1472.5	0.331	0.139	0.387	−1263
bcc + $\mu \rightleftharpoons C14$	peritectoid	1172.4	0.052	0.395	0.333	−2039
$C14 \rightleftharpoons$ bcc + μ	eutectoid	584.9	0.333	0.001	0.457	−1015

Table IIIa. Integral quantities for the stable phases at 1823 K.

Phase	x_{Mo}	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)]
liquid	0.000	0	0	0.000	0	0.000	0.000
	0.100	−4196	2860	3.871	731	1.168	−0.065
	0.200	−5911	6312	6.705	1674	2.544	−0.131
	0.300	−6446	10242	9.154	2813	4.075	−0.196
	0.347	−6373	12219	10.198	3411	4.831	−0.227
σ	0.483	−5886	−3506	1.306	4611	−4.453	−3.000
	0.500	−5815	−3387	1.332	4692	−4.431	−2.913
	0.541	−5539	−3158	1.306	4916	−4.429	−2.704
bcc	0.819	−3129	3045	3.387	4036	−0.544	−0.922
	0.900	−2320	1988	2.363	2607	−0.340	−0.510
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Fe(liquid), Mo(bcc)

Table IIIb. Partial quantities for Fe in the stable phases at 1823 K.

Phase	x_{Fe}	ΔG_{Fe} [J/mol]	ΔH_{Fe} [J/mol]	ΔS_{Fe} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Fe}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Fe}}$ [J/(mol·K)]	a_{Fe}	γ_{Fe}
liquid	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1705	−315	0.763	−108	−0.113	0.894	0.993
	0.800	−3795	−1108	1.474	−413	−0.381	0.778	0.973
	0.700	−6292	−2154	2.270	−885	−0.696	0.660	0.943
	0.653	−7614	−2668	2.713	−1156	−0.829	0.605	0.927
σ	0.517	−7614	−7122	0.270	2387	−5.216	0.605	1.171
	0.500	−8259	−6692	0.859	2248	−4.904	0.580	1.160
	0.459	−10231	−5587	2.547	1576	−3.929	0.509	1.110
bcc	0.181	−10231	11258	11.788	15687	−2.430	0.509	2.815
	0.100	−13167	16486	16.266	21734	−2.878	0.419	4.195
	0.000	$-\infty$	23668	∞	31113	−4.084	0.000	7.788

Reference state: Fe(liquid)

Table IIIc. Partial quantities for Mo in the stable phases at 1823 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}
liquid	0.000	$-\infty$	25264	∞	6207	10.454	0.000	1.506
	0.100	−26616	31433	31.842	8285	12.698	0.173	1.727
	0.200	−14374	35992	27.628	10021	14.246	0.387	1.937
	0.300	−6806	39168	25.219	11443	15.208	0.638	2.127
	0.347	−4037	40245	24.291	12010	15.488	0.766	2.209
σ	0.483	−4037	364	2.414	6992	−3.636	0.766	1.586
	0.500	−3370	−81	1.804	7136	−3.959	0.801	1.601
	0.541	−1561	−1099	0.253	7748	−4.853	0.902	1.667
bcc	0.819	−1561	1232	1.532	1464	−0.127	0.902	1.101
	0.900	−1115	378	0.819	482	−0.057	0.929	1.032
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Mo(bcc)

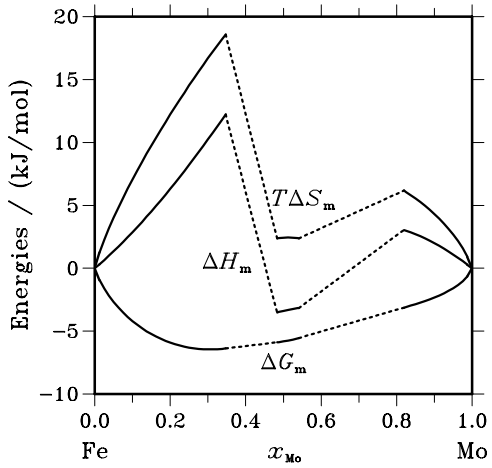

Fig. 2. Integral quantities of the stable phases at T=1823 K.

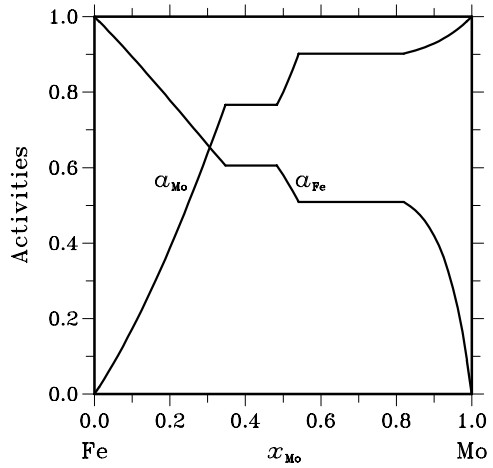

Fig. 3. Activities in the stable phases at T=1823 K.

Table IV. Standard reaction quantities at 298.15 K for the compounds per mole of atoms.

Compound	x_{Mo}	$\Delta_{\mathrm{f}}G^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}H^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}S^{\circ}$ / (J/(mol·K))	$\Delta_{\mathrm{f}}C^{\circ}_{P}$ / (J/(mol·K))
$C14$	0.333	−11	1716	5.792	0.234
μ	0.462	−816	704	5.096	0.192

References

[82Fer] A. Fernández Guillermet: Calphad **6** (1982) 127–140.
[88And] J.O. Andersson: Calphad **12** (1988) 9–23.