Mn – Sc (Manganese – Scandium)

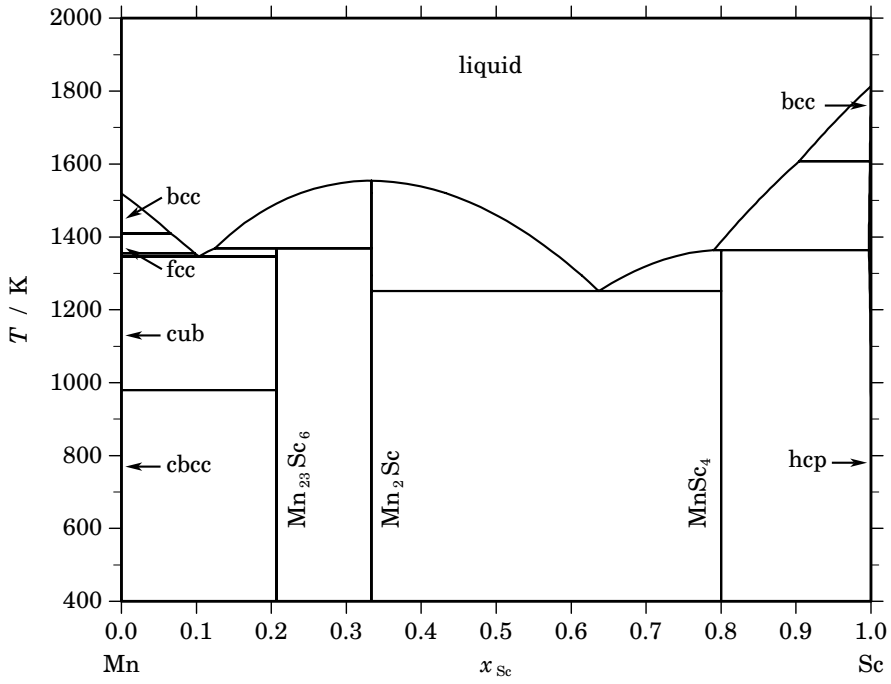

Fig. 1. Calculated phase diagram for the system Mn-Sc.

Manganese and scandium can both be encountered in light metal alloys where Sc improves the mechanical properties at higher temperatures and Mn is added for grain refining. The Mn-Sc system has been investigated by DTA and SEM/EDX across the whole composition range and an optimised thermodynamic dataset has been reported in [1998Pis]. Prior to this study the phase diagram of Mn-Sc has been largely unknown. In addition to the Laves phase Mn_2Sc [1961Dwi] two more intermetallic compounds have been found, $Mn_{23}Sc_6$ and $MnSc_4$ [1998Pis]. The available thermodynamic data have been limited to only 2 values. The enthalpy of mixing in the liquid has been measured by [1985Esi] at a composition of 15 at.% Sc and 1873 K and the enthalpy of formation of Mn_2Sc has been reported by [1983Shi]. Both values are reproduced quite well by the calculations [1998Pis]. The investigation of the phase diagram has been complicated by the sluggish formation of $MnSc_4$ and reactions of the Sc-rich alloys with the crucible in the DTA experiments [1998Pis]. Although the solubility of Sc in solid Mn has been found to be 1 at.% Sc at the eutectic temperature [1998Pis] the calculated value from the optimised dataset is much lower.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Mn,Sc)_1$
cbcc	$A12$	αMn	$cI58$	$I\overline{4}3m$	CBCC_A12	Mn_1
cub	$A13$	βMn	$cP20$	$P4_132$	CUB_A13	Mn_1
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Mn,Sc)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Mn,Sc)_1$
$Mn_{23}Sc_6$	···	···	$cF116$	$Fm\overline{3}m$	MN23SC6	$Mn_{23}Sc_6$
Mn_2Sc	$C14$	$MgZn_2$	$hP12$	$P6_3/mmc$	MN2SC	Mn_2Sc_1
$MnSc_4$	···	···	···	···	MNSC4	Mn_1Sc_4
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Mn,Sc)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Sc}			$\Delta_{\mathrm{r}}H$ / (J/mol)
bcc $\rightleftharpoons$ liquid + hcp	metatectic	1607.3	0.998	0.904	0.999	−3989
liquid $\rightleftharpoons$ Mn_2Sc	congruent	1554.1	0.333	0.333		−25592
bcc $\rightleftharpoons$ fcc + liquid	metatectic	1409.1	0.001	0.000	0.066	−1866
liquid + Mn_2Sc $\rightleftharpoons$ $Mn_{23}Sc_6$	peritectic	1368.6	0.125	0.333	0.207	−12510
liquid + hcp $\rightleftharpoons$ $MnSc_4$	peritectic	1363.6	0.790	0.997	0.800	−17729
fcc $\rightleftharpoons$ cub + liquid	metatectic	1355.3	0.001	0.000	0.098	−2096
liquid $\rightleftharpoons$ cub + $Mn_{23}Sc_6$	eutectic	1346.7	0.103	0.000	0.207	−18856
liquid $\rightleftharpoons$ Mn_2Sc + $MnSc_4$	eutectic	1251.0	0.637	0.333	0.800	−18292
cub $\rightleftharpoons$ cbcc + $Mn_{23}Sc_6$	eutectoid	980.0	0.000	0.000	0.207	−2254

Table IIIa. Integral quantities for the liquid phase at 2000 K.

x_{Sc}	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	−7982	−3298	2.342	−2576	−0.361	0.000
0.200	−12901	−5863	3.519	−4580	−0.642	0.000
0.300	−16170	−7696	4.237	−6012	−0.842	0.000
0.400	−18062	−8795	4.633	−6870	−0.962	0.000
0.500	−18683	−9162	4.761	−7157	−1.003	0.000
0.600	−18062	−8795	4.633	−6870	−0.962	0.000
0.700	−16170	−7696	4.237	−6012	−0.842	0.000
0.800	−12901	−5863	3.519	−4580	−0.642	0.000
0.900	−7982	−3298	2.342	−2576	−0.361	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Mn(liquid), Sc(liquid)

Table IIIb. Partial quantities for Mn in the liquid phase at 2000 K.

x_{Mn}	ΔG_{Mn} [J/mol]	ΔH_{Mn} [J/mol]	ΔS_{Mn} [J/(mol·K)]	$G_{\mathrm{Mn}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Mn}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Mn}	γ_{Mn}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2038	−366	0.836	−286	−0.040	0.885	0.983
0.800	−4856	−1466	1.695	−1145	−0.160	0.747	0.933
0.700	−8508	−3298	2.605	−2576	−0.361	0.600	0.856
0.600	−13075	−5863	3.606	−4580	−0.642	0.456	0.759
0.500	−18683	−9162	4.761	−7157	−1.003	0.325	0.650
0.400	−25543	−13193	6.175	−10306	−1.444	0.215	0.538
0.300	−34048	−17957	8.046	−14027	−1.965	0.129	0.430
0.200	−45084	−23454	10.815	−18321	−2.566	0.066	0.332
0.100	−61477	−29684	15.897	−23188	−3.248	0.025	0.248
0.000	$-\infty$	−36647	∞	−28627	−4.010	0.000	0.179

Reference state: Mn(liquid)

Table IIIc. Partial quantities for Sc in the liquid phase at 2000 K.

x_{Sc}	ΔG_{Sc} [J/mol]	ΔH_{Sc} [J/mol]	ΔS_{Sc} [J/(mol·K)]	G^E_{Sc} [J/mol]	S^E_{Sc} [J/(mol·K)]	a_{Sc}	γ_{Sc}
0.000	$-\infty$	−36647	∞	−28627	−4.010	0.000	0.179
0.100	−61477	−29684	15.897	−23188	−3.248	0.025	0.248
0.200	−45084	−23454	10.815	−18321	−2.566	0.066	0.332
0.300	−34048	−17957	8.046	−14027	−1.965	0.129	0.430
0.400	−25543	−13193	6.175	−10306	−1.444	0.215	0.538
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0.700	−8508	−3298	2.605	−2576	−0.361	0.600	0.856
0.800	−4856	−1466	1.695	−1145	−0.160	0.747	0.933
0.900	−2038	−366	0.836	−286	−0.040	0.885	0.983
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Sc(liquid)

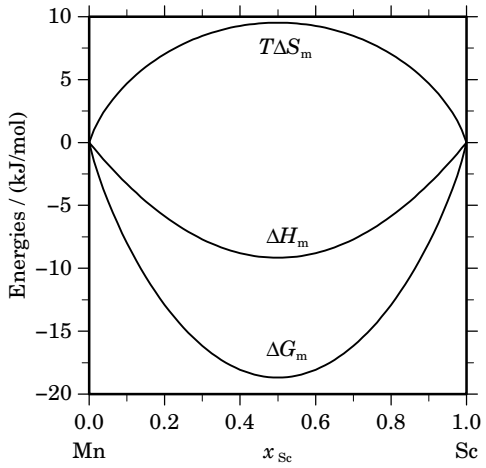

Fig. 2. Integral quantities of the liquid phase at T=2000 K.

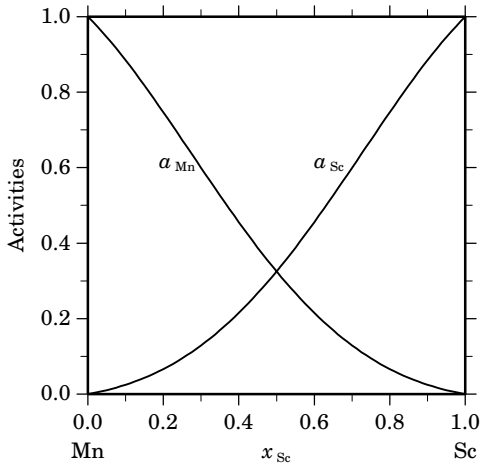

Fig. 3. Activities in the liquid phase at T=2000 K.

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

Compound	x_{Sc}	$\Delta_f G^\circ$ / (J/mol)	$\Delta_f H^\circ$ / (J/mol)	$\Delta_f S^\circ$ / (J/(mol·K))	$\Delta_f C^\circ_P$ / (J/(mol·K))
$Mn_{23}Sc_6$	0.207	−10172	−10172	0.001	0.000
Mn_2Sc_1	0.333	−15500	−15500	0.001	0.000
Mn_1Sc_4	0.800	−7344	−7344	0.000	0.000

References

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