Mn – Y (Manganese – Yttrium)

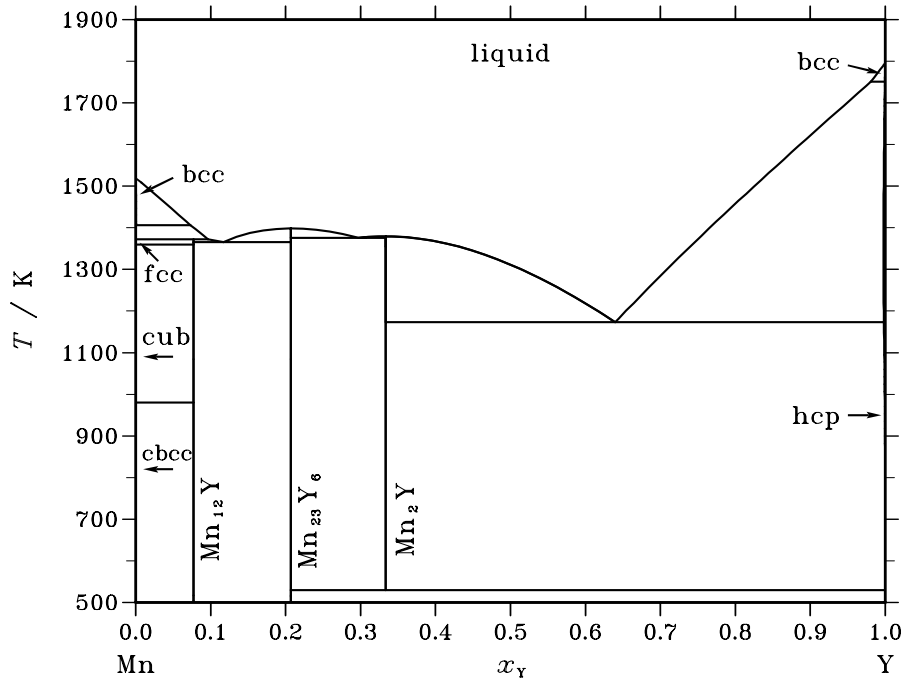

Fig. 1. Calculated phase diagram for the system Mn-Y.

Manganese and rare-earth metals are important alloying elements for magnesium alloys because they enhance their corrosion resistance and mechanical properties. A thermodynamic modelling of the binary Mn-Y system has been performed by Flandorfer *et al.* [97Fla] and more recently by Gröbner *et al.* [01Grö]. The phase diagram is characterised by three stoichiometric intermetallic compounds: $Mn_{12}Y$, $Mn_{23}Y_6$ and Mn_2Y. $Mn_{23}Y_6$ and Mn_2Y melt congruently at 1398 K and 1379 K, respectively. Mn_2Y decomposes at lower temperature, in agreement with the calorimetric data from Pisch *et al.* [01Pis]. The third intermetallic, $Mn_{12}Y$, forms peritectically at 1372 K. The phase diagram is further characterised by negligible mutual solubility of solid Mn and Y and by a deep eutectic Mn_2Y+Y at the Y-rich side of the diagram. The thermodynamic modelling of Gröbner *et al.* [01Grö] has been selected because it is based on calorimetric data and the agreement to the phase diagram data from Myklebust and Daane [62Myk] is good.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Mn,Y)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Mn,Y)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Mn,Zr)_1$
cbcc	$A12$	αMn	$cI58$	$I\overline{4}3m$	CBCC_A12	Mn_1
cub	$A13$	βMn	$cP20$	$P4_132$	CUB_A13	Mn_1
$Mn_{12}Y$	$D2_h$	$Mn_{12}Th$	$tI26$	$I4/mmm$	MN12Y	$Mn_{12}Y_1$
$Mn_{23}Y_6$	$D8_a$	$Mn_{23}Th_6$	$cF116$	$Fm\overline{3}m$	MN23Y6	$Mn_{23}Y_6$
Mn_2Y	$C15$	Cu_2Mg	$cF116$	$Fd\overline{3}m$	MN2Y	Mn_2Y_1
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Mn,Y)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Y}			$\Delta_{\mathrm{r}}H$ / (J/mol)
bcc $\rightleftharpoons$ liquid + hcp	metatectic	1750.9	1.000	0.981	1.000	−4856
bcc $\rightleftharpoons$ fcc + liquid	metatectic	1406.0	0.001	0.000	0.073	−1813
liquid $\rightleftharpoons$ $Mn_{23}Y_6$	congruent	1398.4	0.207	0.207		−20600
liquid $\rightleftharpoons$ Mn_2Y	congruent	1379.4	0.333	0.333		−17373
liquid $\rightleftharpoons$ $Mn_{23}Y_6$ + Mn_2Y	eutectic	1375.7	0.298	0.207	0.333	−18218
fcc + liquid $\rightleftharpoons$ $Mn_{12}Y$	peritectic	1372.2	0.000	0.096	0.077	−16168
liquid $\rightleftharpoons$ $Mn_{12}Y$ + $Mn_{23}Y_6$	eutectic	1365.8	0.117	0.077	0.207	−19460
fcc $\rightleftharpoons$ cub + $Mn_{12}Y$	eutectoid	1359.8	0.000	0.000	0.077	−2170
liquid $\rightleftharpoons$ Mn_2Y + hcp	eutectic	1173.0	0.640	0.333	0.998	−14149
cub $\rightleftharpoons$ cbcc + $Mn_{12}Y$	eutectoid	980.0	0.000	0.000	0.077	−2254
Mn_2Y $\rightleftharpoons$ $Mn_{23}Y_6$ + hcp	eutectoid	529.9	0.333	0.207	1.000	−1397

Table IIIa. Integral quantities for the liquid phase at 1800 K.

x_{Y}	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)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−5700	−982	2.621	−835	−0.082	0.000
0.200	−8895	−1654	4.023	−1406	−0.138	0.000
0.300	−10885	−2051	4.908	−1743	−0.171	0.000
0.400	−11947	−2205	5.412	−1875	−0.184	0.000
0.500	−12204	−2153	5.584	−1830	−0.179	0.000
0.600	−11712	−1929	5.435	−1640	−0.161	0.000
0.700	−10474	−1567	4.948	−1332	−0.131	0.000
0.800	−8426	−1102	4.069	−937	−0.092	0.000
0.900	−5348	−568	2.656	−483	−0.047	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Mn in the liquid phase at 1800 K.

x_{Mn}	ΔG_{Mn} [J/mol]	ΔH_{Mn} [J/mol]	ΔS_{Mn} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Mn}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Mn}}$ [J/(mol·K)]	a_{Mn}	γ_{Mn}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1714	−161	0.863	−137	−0.013	0.892	0.991
0.800	−3848	−598	1.806	−508	−0.050	0.773	0.967
0.700	−6393	−1241	2.862	−1055	−0.103	0.652	0.932
0.600	−9364	−2023	4.079	−1719	−0.169	0.535	0.891
0.500	−12816	−2873	5.524	−2442	−0.239	0.425	0.849
0.400	−16878	−3723	7.308	−3164	−0.310	0.324	0.809
0.300	−21846	−4503	9.635	−3827	−0.375	0.232	0.774
0.200	−28460	−5145	12.953	−4373	−0.429	0.149	0.747
0.100	−39203	−5579	18.680	−4742	−0.465	0.073	0.728
0.000	$-\infty$	−5736	∞	−4876	−0.478	0.000	0.722

Reference state: Mn(liquid)

Table IIIc. Partial quantities for Y in the liquid phase at 1800 K.

x_{Y}	ΔG_{Y} [J/mol]	ΔH_{Y} [J/mol]	ΔS_{Y} [J/(mol·K)]	$G_{\mathrm{Y}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Y}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Y}	γ_{Y}
0.000	$-\infty$	−11492	∞	−9768	−0.958	0.000	0.521
0.100	−41580	−8376	18.447	−7119	−0.698	0.062	0.621
0.200	−29086	−5881	12.892	−4999	−0.490	0.143	0.716
0.300	−21367	−3939	9.682	−3348	−0.328	0.240	0.800
0.400	−15821	−2479	7.412	−2107	−0.207	0.347	0.869
0.500	−11593	−1434	5.644	−1219	−0.120	0.461	0.922
0.600	−8269	−734	4.186	−624	−0.061	0.576	0.959
0.700	−5601	−309	2.940	−263	−0.026	0.688	0.983
0.800	−3417	−91	1.848	−78	−0.008	0.796	0.995
0.900	−1586	−11	0.875	−10	−0.001	0.899	0.999
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Y(liquid)

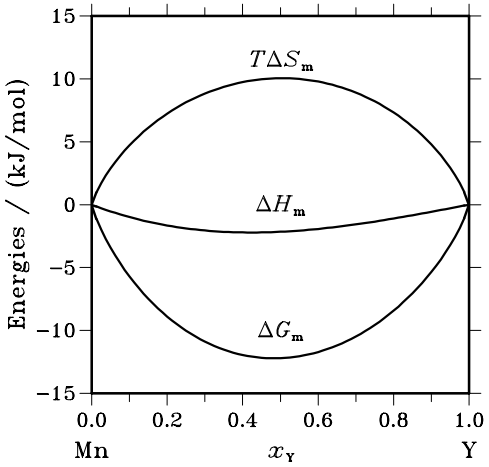

Fig. 2. Integral quantities of the liquid phase at T=1800 K.

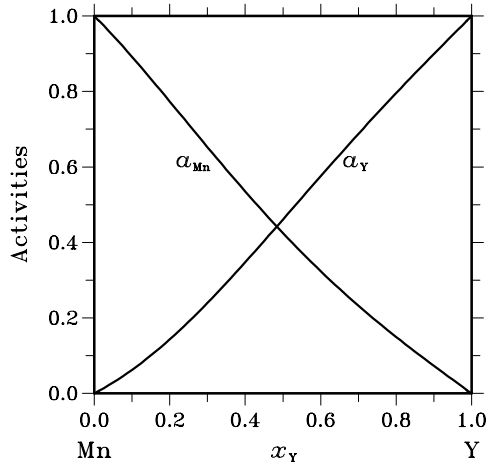

Fig. 3. Activities in the liquid phase at T=1800 K.

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

Compound	x_{Y}	$\Delta_{\mathrm{f}}G^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}H^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}S^{\circ}$ / (J/(mol·K))	$\Delta_{\mathrm{f}}C_P^{\circ}$ / (J/(mol·K))
$\mathrm{Mn_{12}Y_1}$	0.077	−2310	−2092	0.732	0.000
$\mathrm{Mn_{23}Y_6}$	0.207	−5368	−5027	1.143	0.000
$\mathrm{Mn_2Y_1}$	0.333	−3901	−2828	3.597	0.000

References

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