Mg – Y (Magnesium – Yttrium)

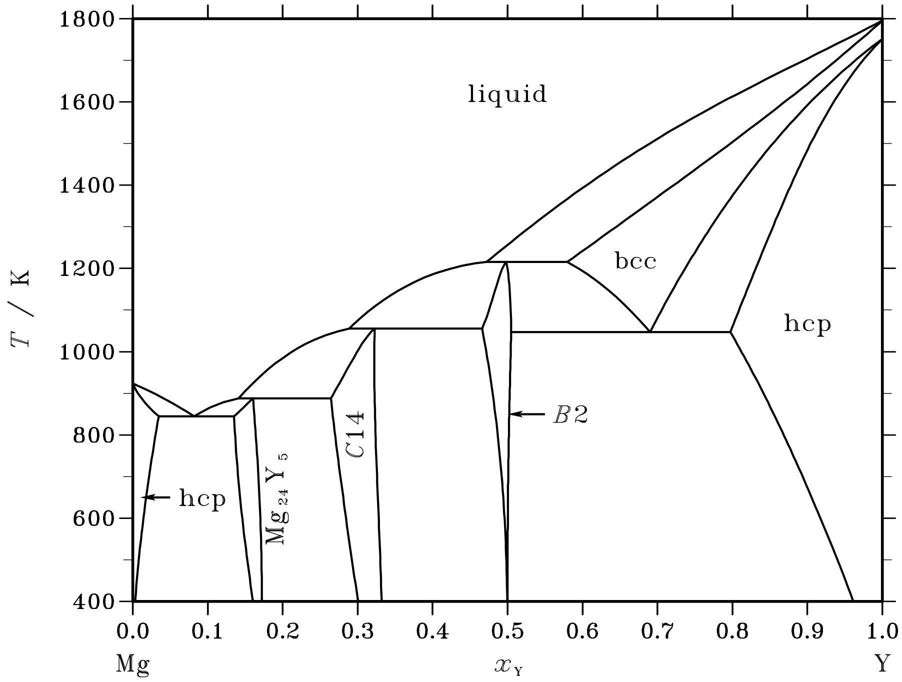

Fig. 1. Calculated phase diagram for the system Mg-Y.

Magnesium alloys are becoming increasingly important due to potential weight saving in comparison with aluminium based alloys. Yttrium additives are of interest because they enhance high-temperature properties and improve casting characteristics. Mg-Y alloys show higher creep resistance, better corrosion resistance, a considerable age hardening response and good strength properties at room temperature as well as at high temperatures. The assessment of thermodynamic data has been performed by [88Ran, 98Luk, 03Fab]. They are based on phase diagram information and thermodynamic data from [65Smi]. The more recent measurements of the enthalpy of mixing of liquid Y in Mg [91Aga, 91Feu, 95Aga], the data of Mg activity in the liquid phase [97Gan] and the enthalpy of formation values of the intermetallic phases from [89Pya, 90Pya] were additionally used by [03Fab]. The new data of [96Bon, 97Fla] on site occupancy in intermetallic compounds were also taken into account by [03Fab]. Therefore, the description of [03Fab] is recommended here. The system Mg-Y is characterised by complete solubility in the liquid state and limited solubility of Mg in solid Y and vice versa. Three intermetallic compounds MgY_{1-x}, Mg_2Y_{1-x} and $Mg_{24}Y_{5-x}$ with limited homogeneity range exist in this system. The MgY_{1-x} phase is described as a highly ordered $B2$ phase originating from the disordered bcc-Y phase. The phases Mg_2Y_{1-x} and $Mg_{24}Y_{5-x}$ are modelled in accordance with experimental site occupancy data [96Bon, 97Fla].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Mg,Y)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Mg,Y)_1$
$Mg_{24}Y_5$	$A12$	αMn	$cI58$	$I\bar{4}3m$	MG24Y5	$Mg_{24}(Mg,Y)_4Y_1$
$C14$	$C14$	$MgZn_2$	$hP12$	$P6_3/mmc$	LAVES_C14	$(Mg,Y)_2(Mg,Y)_1$
$B2$	$B2$	CsCl	$cP2$	$Pm3m$	BCC_B2	$(Mg,Y)_1(Mg,Y)_1$
bcc	$A2$	W	$cI2$	$Im\bar{3}m$	BCC_A2	$(Mg,Y)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_Y			$\Delta_r H$ / (J/mol)
liquid + bcc ⇌ $B2$	peritectic	1215.2	0.472	0.580	0.498	−13794
liquid + $B2$ ⇌ $C14$	peritectic	1055.5	0.289	0.466	0.323	−8869
bcc ⇌ $B2$ + hcp	eutectoid	1047.2	0.690	0.505	0.797	−4142
liquid + $C14$ ⇌ $Mg_{24}Y_5$	peritectic	887.6	0.141	0.264	0.160	−7650
liquid ⇌ hcp + $Mg_{24}Y_5$	eutectic	844.9	0.082	0.035	0.135	−7733

Table IIIa. Integral quantities for the stable phases at 1223 K.

Phase	x_Y	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)]
liquid	0.000	0	0	0.000	0	0.000	0.000
	0.100	−5346	−3555	1.464	−2041	−1.238	0.606
	0.200	−8298	−5533	2.261	−3209	−1.900	1.211
	0.300	−9837	−6121	3.039	−3625	−2.040	1.817
	0.400	−10252	−5508	3.879	−3408	−1.717	2.422
	0.477	−9922	−4336	4.568	−2884	−1.187	2.889
bcc	0.586	−9096	−9757	−0.540	−2198	−6.181	−1.349
	0.600	−8979	−9426	−0.365	−2135	−5.961	−1.379
	0.700	−7731	−6632	0.899	−1519	−4.180	−1.588
	0.745	−6929	−5117	1.482	−1151	−3.242	−1.681
hcp	0.836	−5122	−4802	0.261	−589	−3.445	−0.020
	0.900	−3682	−3058	0.510	−376	−2.193	−0.012
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Mg(liquid), Y(hcp)

Table IIIb. Partial quantities for Mg in the stable phases at 1223 K.

Phase	x_{Mg}	ΔG_{Mg} [J/mol]	ΔH_{Mg} [J/mol]	ΔS_{Mg} [J/(mol·K)]	G_{Mg}^E [J/mol]	S_{Mg}^E [J/(mol·K)]	a_{Mg}	γ_{Mg}
liquid	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1528	−821	0.578	−456	−0.298	0.861	0.956
	0.800	−3934	−3031	0.739	−1665	−1.117	0.679	0.849
	0.700	−7014	−6253	0.623	−3387	−2.343	0.502	0.717
	0.600	−10578	−10109	0.383	−5383	−3.864	0.353	0.589
	0.523	−13549	−13275	0.224	−6957	−5.166	0.264	0.505
bcc	0.414	−13549	−22847	−7.603	−4591	−14.928	0.264	0.637
	0.400	−14199	−23604	−7.690	−4882	−15.308	0.247	0.619
	0.300	−19116	−29141	−8.197	−6874	−18.207	0.153	0.509
	0.255	−21603	−31748	−8.296	−7724	−19.644	0.119	0.468
hcp	0.164	−21603	−26601	−4.087	−3201	−19.133	0.119	0.730
	0.100	−26979	−28851	−1.531	−3565	−20.676	0.070	0.704
	0.000	$-\infty$	−32450	∞	−3923	−23.326	0.000	0.680

Reference state: Mg(liquid)

Table IIIc. Partial quantities for Y in the stable phases at 1223 K.

Phase	x_{Y}	ΔG_{Y} [J/mol]	ΔH_{Y} [J/mol]	ΔS_{Y} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Y}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Y}}$ [J/(mol·K)]	a_{Y}	γ_{Y}
liquid	0.000	$-\infty$	−44075	∞	−25169	−15.459	0.000	0.084
	0.100	−39717	−28170	9.442	−16303	−9.703	0.020	0.201
	0.200	−25753	−15541	8.349	−9387	−5.032	0.079	0.397
	0.300	−16423	−5812	8.676	−4180	−1.334	0.199	0.663
	0.400	−9762	1395	9.123	−445	1.504	0.383	0.957
	0.477	−5946	5465	9.330	1581	3.176	0.557	1.168
bcc	0.586	−5946	−494	4.458	−505	0.009	0.557	0.952
	0.600	−5499	26	4.517	−304	0.270	0.582	0.971
	0.700	−2851	3015	4.797	776	1.831	0.755	1.079
	0.745	−1896	4018	4.836	1103	2.384	0.830	1.115
hcp	0.836	−1896	−535	1.113	−78	−0.374	0.830	0.992
	0.900	−1093	−192	0.737	−22	−0.139	0.898	0.998
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Y(hcp)

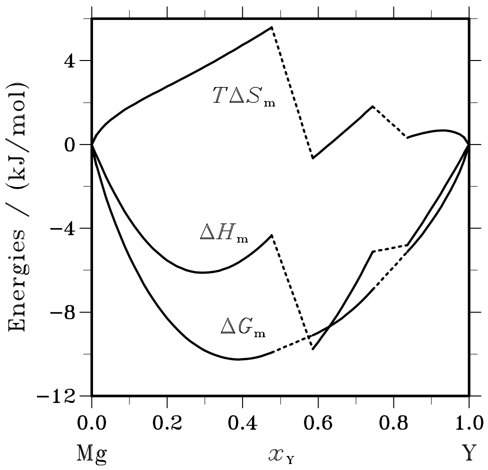

Fig. 2. Integral quantities of the stable phases at T=1223 K.

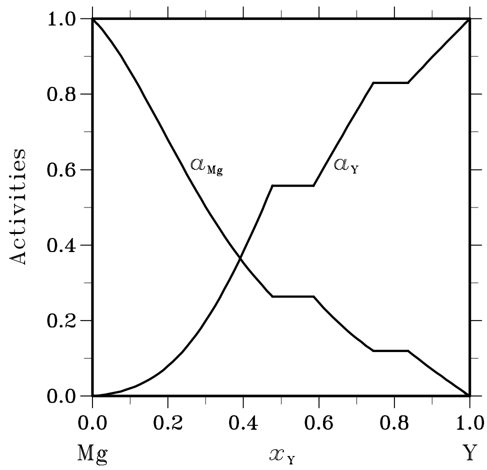

Fig. 3. Activities in the stable phases at T=1223 K.

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))	$\Delta_{\mathrm{f}}C^{\circ}_{P}$ / (J/(mol·K))
$Mg_{24}Si_5$	0.170	−7368	−7707	−1.137	0.000
$C14$	0.320	−11645	−12165	−1.743	0.000
$B2$	0.500	−14473	−15580	−3.716	0.023

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