Gd – Mg (Gadolinium – Magnesium)

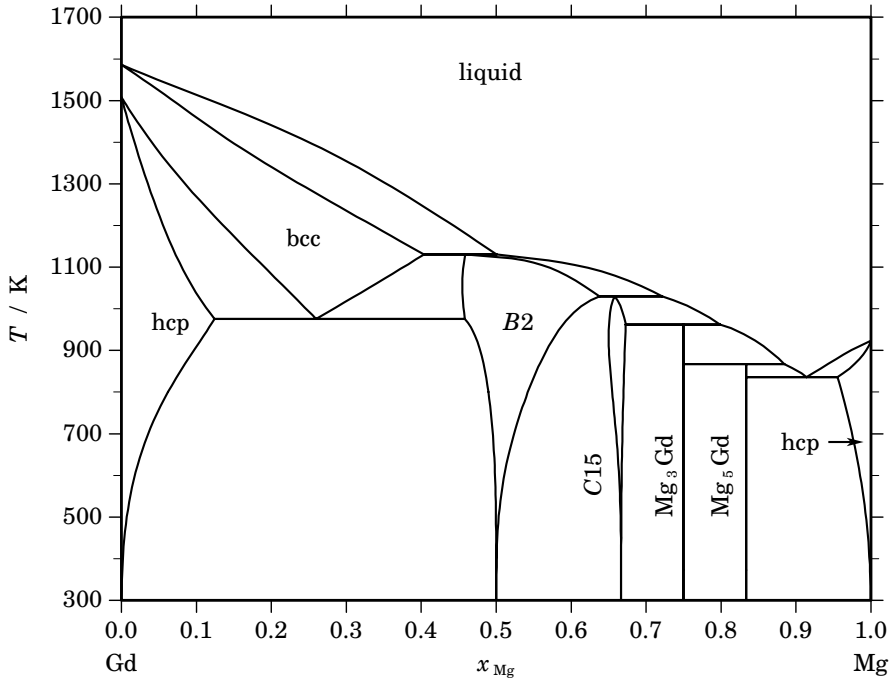

Fig. 1. Calculated phase diagram for the system Gd-Mg.

The rare earth elements have attracted some attention as additives to light metal alloys in the aerospace and automotive industry due to the improvement of mechanical properties of Al- and Mg-alloys at high temperatures. Cacciamani *et al.* [2003Cac] prepared a thermodynamic optimisation of the complete Gd-Mg system, which is mostly based on an experimental investigation of the phase equilibria at elevated temperatures throughout the whole composition range [1986Man]. The solid solubilities have been measured by [1965Jos] for Mg in hcp-Gd and by [1978Rok] for Gd in magnesium. Except for the standard enthalpy of formation of the GdMg phase no other thermodynamic data for the Gd-Mg system have been available. Despite this lack of data, the assessment [2003Cac] can be considered as quite reasonable since other similar systems (Dy-Mg, Ho-Mg) have been evaluated simultaneously and data have been estimated taking advantage of the close relations between the involved rare earth elements.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Gd,Mg)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Gd,Mg)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Gd,Mg)_1$
$B2$	$B2$	CsCl	$cP2$	$Pm3m$	BCC_B2	$(Gd,Mg)_1(Gd,Mg)_1$
$C15$	$C15$	$MgCu_2$	$cF24$	$Fd\overline{3}m$	LAVES_C15	$(Gd,Mg)_2(Gd,Mg)_1$
Mg_3Gd	$D0_3$	BiF_3	$cF16$	$Fm\overline{3}m$	MG3LN	Mg_3Gd_1
Mg_5Gd	$\cdots$	$GdMg_5$	$cF448$	$F\overline{4}3m$	GDMG5	Mg_5Gd_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Mg}			$\Delta_{\mathrm{r}}H$ / (J/mol)
bcc + liquid $\rightleftharpoons$ $B2$	peritectic	1130.4	0.404	0.501	0.459	−7962
$B2$ + liquid $\rightleftharpoons$ $C15$	peritectic	1029.5	0.638	0.722	0.658	−7514
bcc $\rightleftharpoons$ hcp + $B2$	eutectoid	976.0	0.260	0.124	0.458	−5479
$C15$ + liquid $\rightleftharpoons$ Mg_3Gd	peritectic	962.2	0.673	0.798	0.750	−8869
Mg_3Gd + liquid $\rightleftharpoons$ Mg_5Gd	peritectic	867.3	0.750	0.884	0.833	−6828
liquid $\rightleftharpoons$ Mg_5Gd + hcp	eutectic	836.1	0.914	0.833	0.955	−9077

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

x_{Mg}	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	−5952	−551	3.001	−1087	0.298	0.000
0.200	−9916	−1734	4.545	−2427	0.385	0.000
0.300	−12977	−3268	5.394	−3834	0.315	0.000
0.400	−15197	−4867	5.739	−5124	0.143	0.000
0.500	−16485	−6250	5.686	−6111	−0.077	0.000
0.600	−16681	−7133	5.305	−6609	−0.291	0.000
0.700	−15574	−7232	4.634	−6432	−0.445	0.000
0.800	−12885	−6266	3.677	−5395	−0.483	0.000
0.900	−8178	−3949	2.350	−3313	−0.353	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Gd(liquid), Mg(liquid)

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

x_{Gd}	ΔG_{Gd} [J/mol]	ΔH_{Gd} [J/mol]	ΔS_{Gd} [J/(mol·K)]	$G_{\mathrm{Gd}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Gd}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Gd}	γ_{Gd}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1419	364	0.990	158	0.114	0.910	1.011
0.800	−2957	1077	2.241	383	0.385	0.821	1.026
0.700	−5033	1573	3.670	305	0.705	0.714	1.021
0.600	−8093	1286	5.211	−448	0.963	0.582	0.971
0.500	−12619	−350	6.816	−2245	1.053	0.430	0.861
0.400	−19173	−3902	8.484	−5460	0.865	0.278	0.694
0.300	−28481	−9937	10.302	−10462	0.292	0.149	0.497
0.200	−41710	−19021	12.605	−17623	−0.776	0.062	0.308
0.100	−61775	−31720	16.698	−27314	−2.447	0.016	0.161
0.000	$-\infty$	−48600	∞	−39906	−4.830	0.000	0.069

Reference state: Gd(liquid)

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

x_{Mg}	ΔG_{Mg} [J/mol]	ΔH_{Mg} [J/mol]	ΔS_{Mg} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Mg}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Mg}}$ [J/(mol·K)]	a_{Mg}	γ_{Mg}
0.000	$-\infty$	−1400	∞	−8982	4.212	0.000	0.549
0.100	−46746	−8780	21.092	−12285	1.947	0.044	0.440
0.200	−37752	−12979	13.763	−13665	0.381	0.080	0.401
0.300	−31512	−14563	9.416	−13493	−0.594	0.122	0.406
0.400	−25853	−14098	6.531	−12140	−1.088	0.178	0.444
0.500	−20350	−12150	4.556	−9977	−1.207	0.257	0.513
0.600	−15020	−9286	3.185	−7375	−1.062	0.367	0.611
0.700	−10043	−6073	2.205	−4705	−0.760	0.511	0.730
0.800	−5678	−3077	1.445	−2338	−0.410	0.684	0.855
0.900	−2223	−864	0.755	−646	−0.121	0.862	0.958
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Mg(liquid)

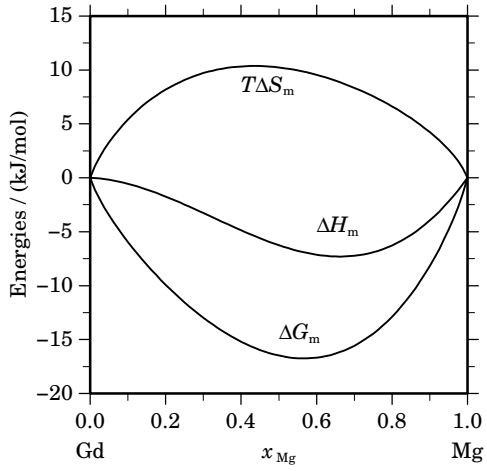

Fig. 2. Integral quantities of the liquid phase at T=1800 K.

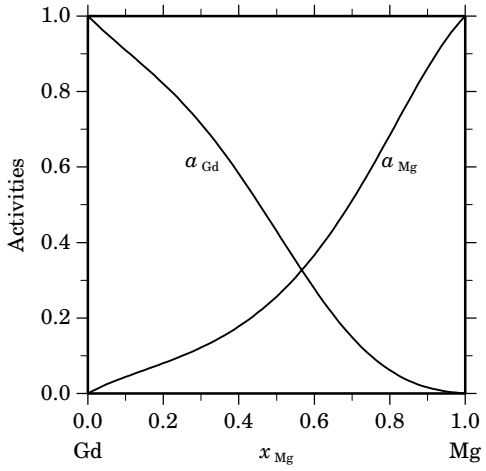

Fig. 3. Activities in the liquid phase at T=1800 K.

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

Compound	x_{Mg}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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))
$B2$	0.500	−14191	−15138	−3.176	−6.456
$C15$	0.667	−13962	−14750	−2.643	−4.322
Mg_3Gd_1	0.750	−11732	−12313	−1.949	−3.244
Mg_5Gd_1	0.833	−8274	−8659	−1.290	−2.163

References

[1965Jos] R.R. Joseph, K.A. Gschneidner jr.: Trans. Metall. Soc. AIME **233** (1965) 2063–2069.

[1978Rok] L.L. Rokhlin in: "Probl. Metalloved. Tsvetn. Splavov", N.M. Zhavoronkov (Ed.), Izd. Nauka, Moscow, 1978, pp. 59–70.

[2003Cac] G. Cacciamani, S. de Negri, A. Saccone, R. Ferro: Intermetallics **11** (2003) 1135–1151.