Mg – Zn (Magnesium – Zinc)

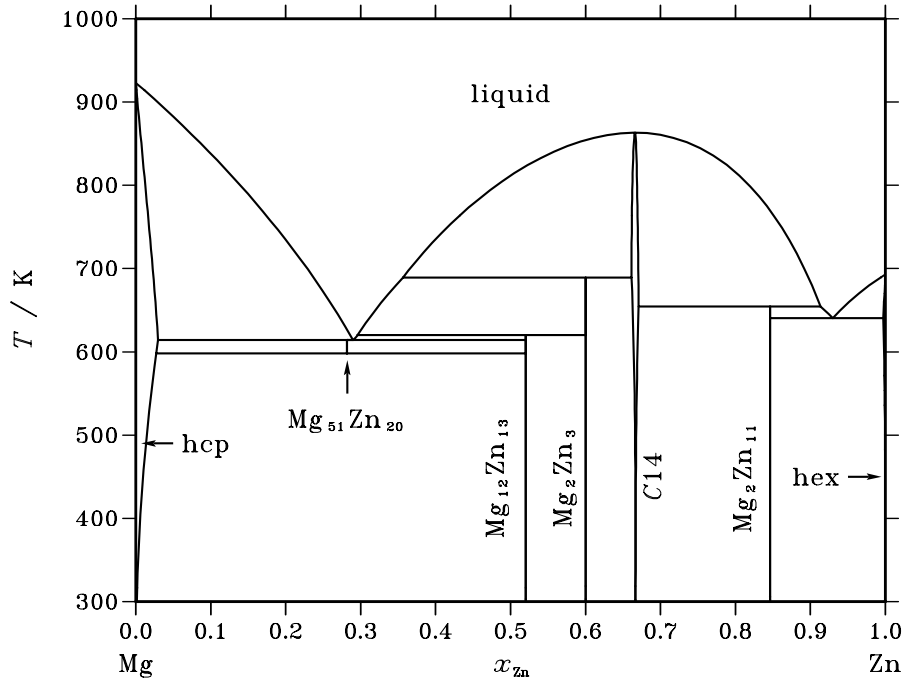

Fig. 1. Calculated phase diagram for the system Mg-Zn.

The Mg-Zn system is of interest for the development of high strength aluminium-base alloys. A compilation of experimental data for the Mg-Zn system has been published by [88Cla]. The thermodynamic parameters of the Mg-Zn system have been first derived by [92Aga]. The subsequent update by [98Lia] is recommended since it reproduces various experimental data such as phase diagram, enthalpy of mixing, heat capacity and chemical potential very well and also takes into account the homogeneity range of the $C14$ Laves phase ($MgZn_2$). The large positive deviation from Neumann-Kopp's rule derived by [92Aga] from the temperature dependence of the enthalpy of mixing of the liquid has been confirmed through the measurement of heat capacity [98Lia] and, very recently by calculations using a statistical thermodynamic theory [01Jha]. However, the description should not be used at temperatures above 3000 K, where an inverse miscibility gap in the liquid phase starts to develop.
The liquid, hcp, and hex-Zn phases are modelled as simple substitutional solutions, the $C14$ Laves phase is described by a two-sublattice model whereas $Mg_{51}Zn_{20}$, $Mg_{12}Zn_{13}$, Mg_2Zn_3, and Mg_2Zn_{11} are treated as stoichiometric phases.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Mg,Zn)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Mg,Zn)_1$
$Mg_{51}Zn_{20}$	$D7_b$	Ta_3B_4	$oI14$	$Immm$	D7B_MG7ZN3	$Mg_{51}Zn_{20}$
$Mg_{12}Zn_{13}$	···	···	···	···	MGZN	$Mg_{12}Zn_{13}$
Mg_2Zn_3	···	···	$mC110$	$C2/m$	MG2ZN3	Mg_2Zn_3
$C14$	$C14$	$MgZn_2$	$hP12$	$P6_3/mmc$	C14_LAVES	$(Mg,Zn)_2(Mg,Zn)_1$
Mg_2Zn_{11}	$D8_c$	Mg_2Zn_{11}	$cP39$	$Pm\overline{3}$	D8C_MG2ZN11	Mg_2Zn_{11}
hex	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_ZN	$(Mg,Zn)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Zn}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons C14$	congruent	863.1	0.666	0.666		−13448
liquid + $C14 \rightleftharpoons Mg_2Zn_3$	peritectic	689.0	0.356	0.661	0.600	−1839
$C14$ + liquid $\rightleftharpoons Mg_2Zn_{11}$	peritectic	654.4	0.671	0.913	0.846	−5687
liquid $\rightleftharpoons Mg_2Zn_{11}$ + hex	eutectic	640.4	0.930	0.846	0.997	−7396
liquid + $Mg_2Zn_3 \rightleftharpoons Mg_{12}Zn_{13}$	peritectic	620.2	0.296	0.600	0.520	−1740
hcp + liquid $\rightleftharpoons Mg_{51}Zn_{20}$	peritectic	614.2	0.030	0.290	0.282	−5793
liquid $\rightleftharpoons Mg_{51}Zn_{20}$ + $Mg_{12}Zn_{13}$	eutectic	614.1	0.290	0.282	0.520	−5989
$Mg_{51}Zn_{20} \rightleftharpoons$ hcp + $Mg_{12}Zn_{13}$	eutectoid	598.2	0.282	0.027	0.520	−204

Table IIIa. Integral quantities for the liquid phase at 973 K.

x_{Zn}	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	−3650	−1912	1.786	−1020	−0.916	1.544
0.200	−5926	−3445	2.550	−1877	−1.611	2.746
0.300	−7517	−4609	2.989	−2575	−2.090	3.604
0.400	−8545	−5398	3.234	−3100	−2.362	4.118
0.500	−9033	−5791	3.332	−3425	−2.432	4.290
0.600	−8951	−5751	3.289	−3506	−2.307	4.118
0.700	−8228	−5226	3.085	−3286	−1.995	3.604
0.800	−6738	−4150	2.659	−2690	−1.501	2.746
0.900	−4259	−2441	1.869	−1629	−0.834	1.544
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Mg in the liquid phase at 973 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}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−935	−192	0.764	−83	−0.112	0.891	0.990
0.800	−2126	−748	1.416	−321	−0.439	0.769	0.961
0.700	−3616	−1672	1.998	−731	−0.968	0.640	0.914
0.600	−5509	−3015	2.563	−1376	−1.684	0.506	0.844
0.500	−7975	−4872	3.189	−2367	−2.574	0.373	0.746
0.400	−11271	−7385	3.994	−3858	−3.625	0.248	0.621
0.300	−15790	−10741	5.189	−6049	−4.822	0.142	0.473
0.200	−22208	−15173	7.230	−9187	−6.152	0.064	0.321
0.100	−32193	−20960	11.544	−13565	−7.601	0.019	0.187
0.000	$-\infty$	−28426	∞	−19519	−9.155	0.000	0.090

Reference state: Mg(liquid)

Table IIIc. Partial quantities for Zn in the liquid phase at 973 K.

x_{Zn}	ΔG_{Zn} [J/mol]	ΔH_{Zn} [J/mol]	ΔS_{Zn} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Zn}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Zn}}$ [J/(mol·K)]	a_{Zn}	γ_{Zn}
0.000	$-\infty$	−21077	∞	−11057	−10.298	0.000	0.255
0.100	−28080	−17388	10.989	−9452	−8.156	0.031	0.311
0.200	−21125	−14232	7.084	−8104	−6.298	0.073	0.367
0.300	−16619	−11461	5.301	−6879	−4.710	0.128	0.427
0.400	−13099	−8972	4.241	−5686	−3.378	0.198	0.495
0.500	−10090	−6710	3.474	−4483	−2.289	0.287	0.575
0.600	−7404	−4661	2.819	−3272	−1.428	0.400	0.667
0.700	−4987	−2863	2.183	−2101	−0.783	0.540	0.771
0.800	−2870	−1395	1.517	−1065	−0.339	0.701	0.877
0.900	−1155	−383	0.794	−303	−0.082	0.867	0.963
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Zn(liquid)

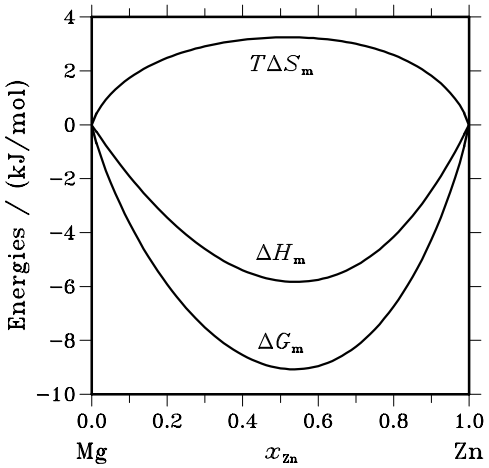

Fig. 2. Integral quantities of the liquid phase at T=973 K.

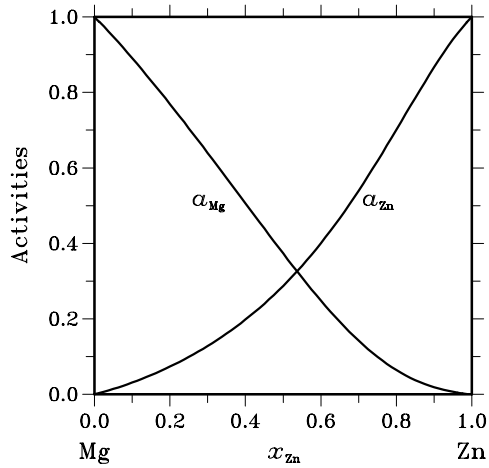

Fig. 3. Activities in the liquid phase at T=973 K.

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

Compound	x_{Zn}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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))
$Mg_{51}Zn_{20}$	0.282	−4580	−4729	−0.500	0.000
$Mg_{12}Zn_{13}$	0.520	−8773	−9479	−2.370	0.000
Mg_2Zn_3	0.600	−10070	−10881	−2.720	0.000
$C14$	0.667	−10906	−11784	−2.944	0.036
Mg_2Zn_{11}	0.846	−5255	−5678	−1.420	0.000

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