Ga – Mg (Gallium – Magnesium)

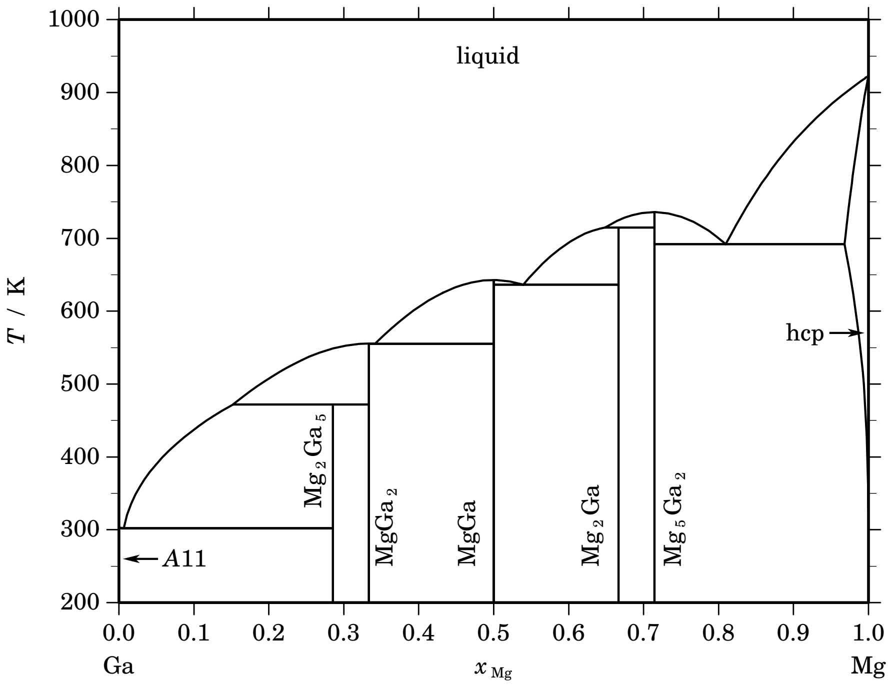

Fig. 1. Calculated phase diagram for the system Ga-Mg.

Magnesium is the major p-type dopant for GaN semiconductors and Ga-Mg melts can be used for this purpose in ion implantation processes. Another interesting applications is the potential use of Ga-based pastes for brazing and soldering Mg-alloys. The Ga-Mg system has been reviewed in [1986Nay] and a new experimental investigation and a thermodynamic optimisation has been reported by [1991Not]. Although this dataset seems to be a good assessment it has not been based on the SGTE description for the element data. Therefore, the system has been re-optimised [2005Fra] using the SGTE element data. For this adjustment the the same selection of experimental data has been used and the same invariant points of the phase diagram as recommended by [1991Not].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Ga,Mg)_1$
$A11$	$A11$	αGa	$oC8$	$Cmca$	ORTHORHOMBIC_CMCA	Ga_1
Mg_2Ga_5	$\cdots$	Mg_2Ga_5	$tI28$	$I4/mmm$	MG2GA5	Mg_2Ga_5
$MgGa_2$	$\cdots$	$MgGa_2$	$oP24$	$Pbam$	MGGA2	Mg_1Ga_2
MgGa	$\cdots$	MgGa	$tI32$	$I4_1/a$	MGGA	Mg_1Ga_1
Mg_2Ga	$\cdots$	Mg_2Ga	$hP18$	$P\overline{6}2c$	MG2GA	Mg_2Ga_1
Mg_5Ga_2	$D8_g$	Mg_5Ga_2	$oI28$	$Ibam$	MG5GA2	Mg_5Ga_2
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Ga,Mg)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Mg}			$\Delta_r H$ / (J/mol)
liquid ⇌ Mg_5Ga_2	congruent	736.0	0.714	0.714		−8726
liquid + Mg_5Ga_2 ⇌ Mg_2Ga	peritectic	714.8	0.649	0.714	0.667	−5944
liquid ⇌ Mg_5Ga_2 + hcp	eutectic	691.9	0.810	0.714	0.968	−7502
liquid ⇌ MgGa	congruent	642.8	0.500	0.500		−8683
liquid ⇌ MgGa + Mg_2Ga	eutectic	636.4	0.540	0.500	0.667	−8284
liquid ⇌ $MgGa_2$	congruent	555.5	0.333	0.333		−7597
liquid ⇌ $MgGa_2$ + MgGa	eutectic	555.3	0.342	0.333	0.500	−7593
liquid + $MgGa_2$ ⇌ Mg_2Ga_5	peritectic	472.1	0.153	0.333	0.286	−2397
liquid ⇌ $A11$ + Mg_2Ga_5	eutectic	302.0	0.006	0.000	0.286	−5619

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

x_{Mg}	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)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−5253	−3129	2.183	−2623	−0.520	0.000
0.200	−8875	−6065	2.888	−4827	−1.273	0.000
0.300	−11507	−8595	2.992	−6565	−2.087	0.000
0.400	−13196	−10470	2.802	−7751	−2.794	0.000
0.500	−13898	−11445	2.521	−8290	−3.243	0.000
0.600	−13541	−11326	2.277	−8096	−3.319	0.000
0.700	−12061	−10006	2.112	−7119	−2.967	0.000
0.800	−9415	−7510	1.958	−5367	−2.203	0.000
0.900	−5559	−4037	1.564	−2929	−1.139	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Ga in the liquid phase at 973 K.

x_{Ga}	ΔG_{Ga} [J/mol]	ΔH_{Ga} [J/mol]	ΔS_{Ga} [J/(mol·K)]	G_{Ga}^E [J/mol]	S_{Ga}^E [J/(mol·K)]	a_{Ga}	γ_{Ga}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1058	−66	1.019	−205	0.143	0.877	0.975
0.800	−2667	−519	2.207	−862	0.352	0.719	0.899
0.700	−5016	−1861	3.243	−2131	0.277	0.538	0.768
0.600	−8369	−4618	3.855	−4236	−0.392	0.355	0.592
0.500	−12974	−9172	3.908	−7367	−1.855	0.201	0.402
0.400	−18996	−15595	3.496	−11583	−4.123	0.096	0.239
0.300	−26464	−23481	3.066	−16724	−6.945	0.038	0.127
0.200	−35333	−31782	3.650	−22313	−9.732	0.013	0.063
0.100	−46089	−38633	7.663	−27461	−11.481	0.003	0.034
0.000	$-\infty$	−41193	∞	−30777	−10.705	0.000	0.022

Reference state: Ga(liquid)

Table IIIc. 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}
0.000	$-\infty$	−31717	∞	−28295	−3.517	0.000	0.030
0.100	−43007	−30697	12.652	−24380	−6.493	0.005	0.049
0.200	−33709	−28249	5.612	−20689	−7.770	0.016	0.078
0.300	−26650	−24308	2.407	−16910	−7.603	0.037	0.124
0.400	−20436	−19247	1.222	−13023	−6.397	0.080	0.200
0.500	−14821	−13719	1.133	−9214	−4.630	0.160	0.320
0.600	−9904	−8480	1.464	−5772	−2.783	0.294	0.490
0.700	−5888	−4231	1.704	−3003	−1.262	0.483	0.690
0.800	−2935	−1442	1.535	−1130	−0.321	0.696	0.870
0.900	−1055	−193	0.886	−203	0.010	0.878	0.975
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Mg(liquid)

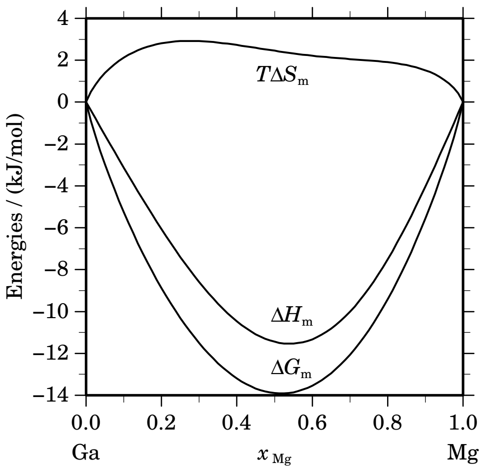

Fig. 2. Integral quantities of the liquid phase at T=973 K.

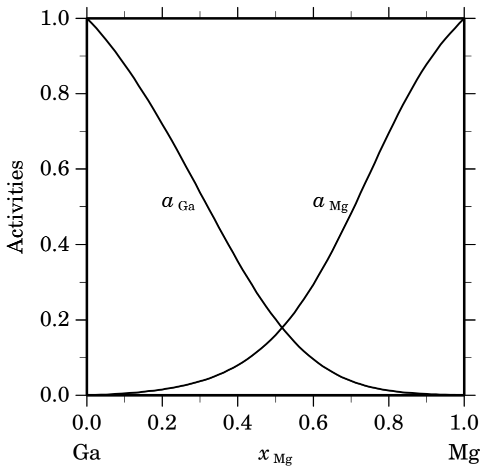

Fig. 3. Activities in the liquid phase at T=973 K.

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

Compound	x_{Mg}	$\Delta_{\mathrm{f}}G^\circ$ / (J/mol)	$\Delta_{\mathrm{f}}H^\circ$ / (J/mol)	$\Delta_{\mathrm{f}}S^\circ$ / (J/(mol·K))	$\Delta_{\mathrm{f}}C_P^\circ$ / (J/(mol·K))
Mg_2Ga_5	0.286	−10766	−9695	3.594	0.000
Mg_1Ga_2	0.333	−11783	−10388	4.680	0.000
Mg_1Ga_1	0.500	−14015	−13183	2.790	0.000
Mg_2Ga_1	0.667	−12293	−11463	2.785	0.000
Mg_5Ga_2	0.714	−11508	−10927	1.950	0.000

References

[1988Nay] A.A. Nayeb-Hashemi, J.B. Clark in: "Phase Diagrams of Binary Magnesium Alloys", A.A. Nayeb-Hashemi, J.B. Clark, Eds., ASM Intl., Metals Park, OH, 1988, pp. 122–128.

[1991Not] M. Notin, E. Belbacha, J. Charles, J. Hertz: J. Alloys Comp. **176** (1991) 25–38.

[2005Fra] P. Franke: unpublished optimisation, 2005.