Al – Gd (Aluminium – Gadolinium)

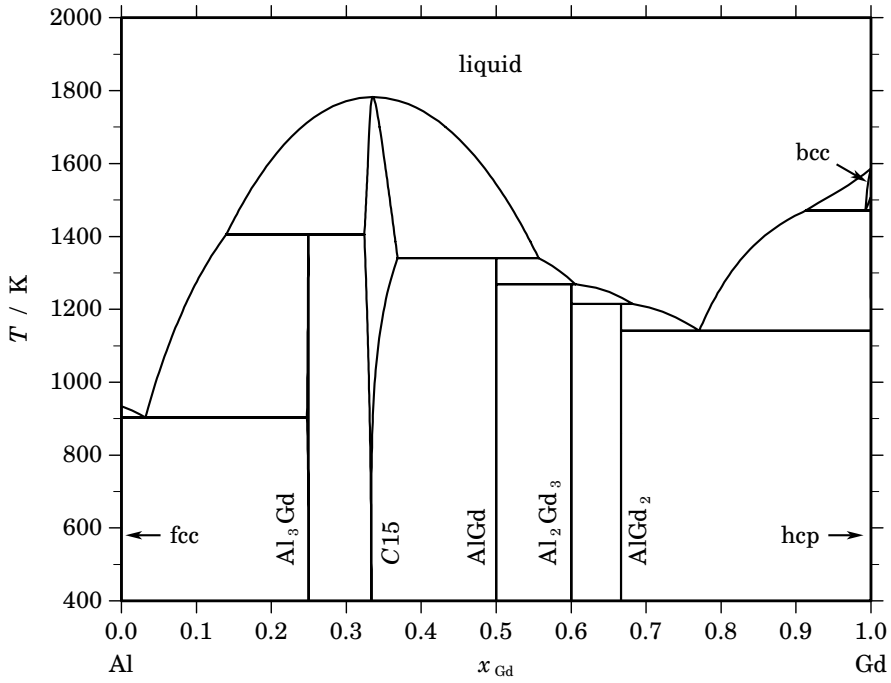

Fig. 1. Calculated phase diagram for the system Al-Gd.

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. For the Al-Gd system two thermodynamic optimisations have been reported in the literature [2001Grö, 2003Cac], however, no parameters have been given in [2001Grö]. The optimisation of Cacciamani *et al.* [2003Cac] is based on an experimental revision of the phase equilibria in the concentration range from 0 to 67 at.% Al [2000Sac] and for the Al-rich part on the review [1988Gsc]. In addition, the assessment takes into account the standard enthalpies of formation for the five intermetallic compounds from the literature [1987Som, 1988Col]. The dataset should not be used at too high temperatures because an artificial inverse miscibility gap opens in the liquid above 3900 K.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Al,Gd)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Al,Gd)_1$
Al_3Gd	$D0_{19}$	Ni_3Sn	$hP8$	$P6_3/mmc$	AL3LN	$Al_3(Al,Gd)_1$
$C15$	$C15$	Cu_2Mg	$cF24$	$Fd\overline{3}m$	C15_LAVES	$(Al,Gd)_2(Al,Gd)_1$
AlGd	$\cdots$	AlEr	$oP16$	$Pmma$	ALLN	Al_1Gd_1
Al_2Gd_3	$\cdots$	Al_2Zr_3	$tP20$	$P4_2/mnm$	AL2LN3	Al_2Gd_3
$AlGd_2$	$C23$	Co_2Si	$oP12$	$Pnma$	ALLN2	Al_1Gd_2
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Al,Gd)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Al,Gd)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Gd}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons C15$	congruent	1782.9	0.335	0.335		−25768
bcc $\rightleftharpoons$ liquid + hcp	metatectic	1471.0	0.993	0.913	1.000	−2797
liquid + $C15 \rightleftharpoons$ Al_3Gd	peritectic	1405.0	0.140	0.324	0.249	−6300
$C15$ + liquid $\rightleftharpoons$ AlGd	peritectic	1341.0	0.368	0.557	0.500	−14046
AlGd + liquid $\rightleftharpoons$ Al_2Gd_3	peritectic	1268.6	0.500	0.606	0.600	−16460
Al_2Gd_3 + liquid $\rightleftharpoons$ $AlGd_2$	peritectic	1214.3	0.600	0.682	0.667	−12817
liquid $\rightleftharpoons$ $AlGd_2$ + hcp	eutectic	1141.0	0.771	0.667	1.000	−12777
liquid $\rightleftharpoons$ fcc + Al_3Gd	eutectic	903.0	0.032	0.000	0.248	−10769

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

x_{Gd}	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	−12014	−15631	−2.009	−7149	−4.712	0.000
0.200	−20267	−27857	−4.217	−12777	−8.378	0.000
0.300	−25691	−36341	−5.917	−16549	−10.996	0.000
0.400	−28377	−40924	−6.971	−18305	−12.566	0.000
0.500	−28437	−41625	−7.327	−18063	−13.090	0.000
0.600	−26093	−38640	−6.971	−16021	−12.566	0.000
0.700	−21695	−32344	−5.917	−12552	−10.996	0.000
0.800	−15699	−23289	−4.217	−8210	−8.378	0.000
0.900	−8588	−12205	−2.009	−3723	−4.712	0.000
1.000	0	0	0.000	0	0.000	0.000

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

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

x_{Al}	ΔG_{Al} [J/mol]	ΔH_{Al} [J/mol]	ΔS_{Al} [J/(mol·K)]	$G_{\mathrm{Al}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Al}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Al}	γ_{Al}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2266	−1632	0.352	−689	−0.524	0.859	0.955
0.800	−6634	−7065	−0.239	−3295	−2.094	0.642	0.802
0.700	−13561	−16706	−1.747	−8223	−4.712	0.404	0.577
0.600	−22994	−30428	−4.130	−15348	−8.378	0.215	0.359
0.500	−34384	−47573	−7.327	−24011	−13.090	0.101	0.201
0.400	−46730	−66946	−11.231	−33016	−18.850	0.044	0.110
0.300	−58658	−86820	−15.646	−40639	−25.656	0.020	0.066
0.200	−68706	−104937	−20.129	−44619	−33.510	0.010	0.051
0.100	−76623	−118503	−23.267	−42162	−42.412	0.006	0.060
0.000	$-\infty$	−124190	∞	−29942	−52.360	0.000	0.135

Reference state: Al(liquid)

Table IIIc. 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)]	$G^{\mathrm{E}}_{\mathrm{Gd}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Gd}}$ [J/(mol·K)]	a_{Gd}	γ_{Gd}
0.000	$-\infty$	−171770	∞	−77522	−52.360	0.000	0.006
0.100	−99746	−141627	−23.267	−65286	−42.412	0.001	0.013
0.200	−74796	−111027	−20.129	−50709	−33.510	0.007	0.034
0.300	−53995	−82158	−15.646	−35976	−25.656	0.027	0.090
0.400	−36452	−56668	−11.231	−22739	−18.850	0.088	0.219
0.500	−22489	−35678	−7.327	−12116	−13.090	0.223	0.445
0.600	−12336	−19770	−4.130	−4691	−8.378	0.439	0.731
0.700	−5853	−8998	−1.747	−515	−4.712	0.676	0.966
0.800	−2447	−2877	−0.239	892	−2.094	0.849	1.061
0.900	−1029	−395	0.352	548	−0.524	0.934	1.037
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Gd(liquid)

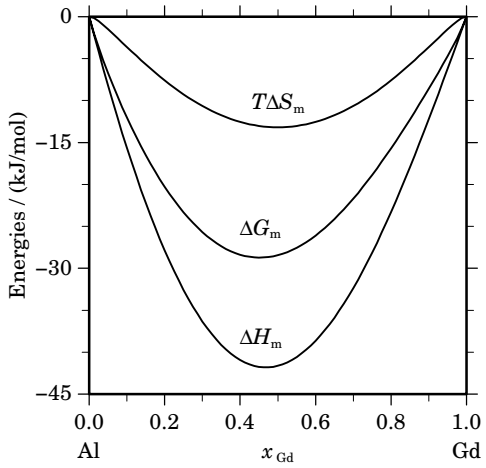

Fig. 2. Integral quantities of the liquid phase at T=1800 K.

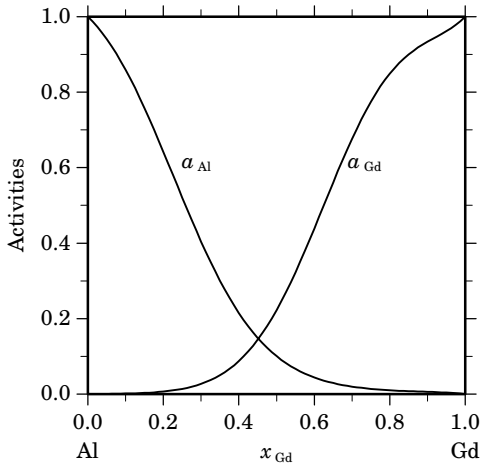

Fig. 3. Activities in the liquid phase at T=1800 K.

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

Compound	x_{Gd}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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))
Al_3Gd	0.250	−39008	−41063	−6.892	−3.243
$C15$	0.333	−50043	−53084	−10.200	−4.326
AlGd	0.500	−45501	−48626	−10.480	−6.489
Al_2Gd_3	0.600	−40583	−43551	−9.953	−7.786
Al_1Gd_2	0.667	−35386	−38001	−8.773	−8.652

References

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