Al – Ho (Aluminium – Holmium)

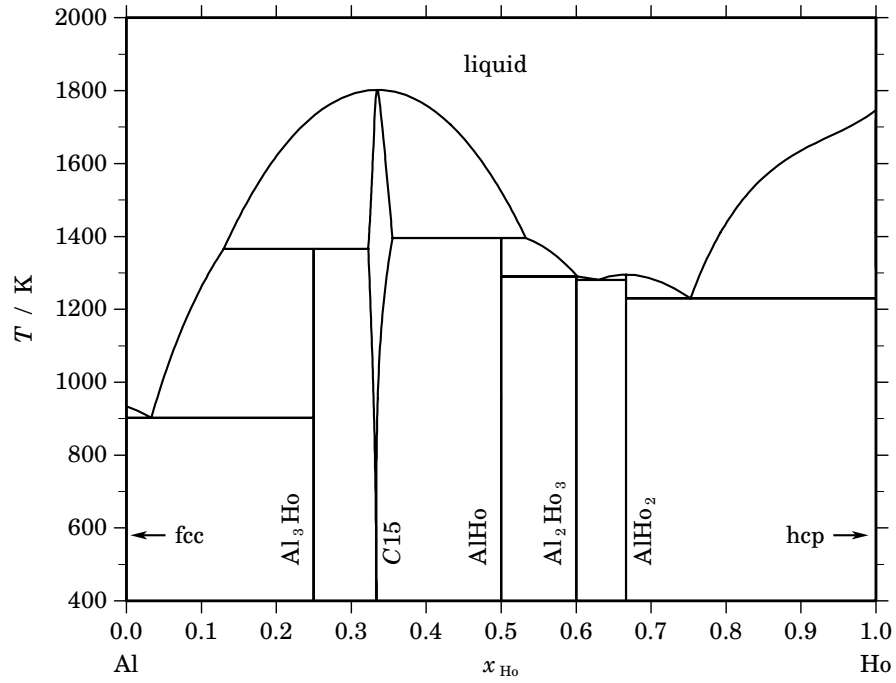

Fig. 1. Calculated phase diagram for the system Al-Ho.

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 Al-Ho system, which is based on an experimental investigation of the phase equilibria involving the liquid [1966Mey] and one datum for the standard enthalpy of formation of the Al_2Ho phase [1985Col]. Although no other thermodynamic data for the system are available, the assessment [2003Cac] can be still considered as reasonable since other similar systems (Al-Dy, Al-Gd) 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	$(Al,Ho)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	Al_1
Al_3Ho	$\cdots$	Al_3Ho	$hR20$	$R\overline{3}m$	AL3LN	Al_3Ho_1
$C15$	$C15$	Cu_2Mg	$cF24$	$Fd\overline{3}m$	C15_LAVES	$(Al,Ho)_2(Al,Ho)_1$
AlHo	$\cdots$	AlEr	$oP16$	$Pmma$	ALLN	Al_1Ho_1
Al_2Ho_3	$\cdots$	Al_2Zr_3	$tP20$	$P4_2/mnm$	AL2LN3	Al_2Ho_3
$AlHo_2$	$C23$	Co_2Si	$oP12$	$Pnma$	ALLN2	Al_1Ho_2
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Al,Ho)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ho}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons C15$	congruent	1802.3	0.334	0.334		−25506
$C15$ + liquid $\rightleftharpoons$ AlHo	peritectic	1396.1	0.355	0.533	0.500	−14730
liquid + $C15$ $\rightleftharpoons$ Al_3Ho	peritectic	1365.6	0.130	0.323	0.250	−5566
liquid $\rightleftharpoons$ $AlHo_2$	congruent	1295.3	0.667	0.667		−15956
AlHo + liquid $\rightleftharpoons$ Al_2Ho_3	peritectic	1290.6	0.500	0.602	0.600	−15536
liquid $\rightleftharpoons$ Al_2Ho_3 + $AlHo_2$	eutectic	1280.8	0.630	0.600	0.667	−15675
liquid $\rightleftharpoons$ $AlHo_2$ + hcp	eutectic	1229.8	0.752	0.667	1.000	−13831
liquid $\rightleftharpoons$ fcc + Al_3Ho	eutectic	902.2	0.033	0.000	0.250	−10736

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

x_{Ho}	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	−12708	−16944	−2.353	−7843	−5.056	0.000
0.200	−21753	−30444	−4.828	−14264	−8.989	0.000
0.300	−27915	−40009	−6.719	−18773	−11.798	0.000
0.400	−31163	−45361	−7.887	−21091	−13.483	0.000
0.500	−31523	−46430	−8.282	−21149	−14.045	0.000
0.600	−29164	−43362	−7.887	−19092	−13.483	0.000
0.700	−24418	−36511	−6.719	−15275	−11.798	0.000
0.800	−17756	−26446	−4.828	−10267	−8.989	0.000
0.900	−9710	−13946	−2.353	−4845	−5.056	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Al(liquid), Ho(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	−2188	−1622	0.314	−611	−0.562	0.864	0.960
0.800	−6545	−7250	−0.392	−3205	−2.247	0.646	0.807
0.700	−13784	−17548	−2.091	−8446	−5.056	0.398	0.569
0.600	−24010	−32544	−4.742	−16365	−8.989	0.201	0.335
0.500	−36728	−51635	−8.282	−26354	−14.045	0.086	0.172
0.400	−50888	−73579	−12.606	−37174	−20.225	0.033	0.083
0.300	−64969	−96501	−17.518	−46950	−27.528	0.013	0.043
0.200	−77257	−117889	−22.573	−53170	−35.955	0.006	0.029
0.100	−87150	−134599	−26.361	−52689	−45.506	0.003	0.030
0.000	$-\infty$	−142850	∞	−41726	−56.180	0.000	0.062

Reference state: Al(liquid)

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

x_{Ho}	ΔG_{Ho} [J/mol]	ΔH_{Ho} [J/mol]	ΔS_{Ho} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ho}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ho}}$ [J/(mol·K)]	a_{Ho}	γ_{Ho}
0.000	$-\infty$	−184490	∞	−83366	−56.180	0.000	0.004
0.100	−107387	−154836	−26.361	−72926	−45.506	0.001	0.008
0.200	−82587	−123219	−22.573	−58500	−35.955	0.004	0.020
0.300	−60888	−92420	−17.518	−42869	−27.528	0.017	0.057
0.400	−41893	−64585	−12.606	−28180	−20.225	0.061	0.152
0.500	−26318	−41225	−8.282	−15944	−14.045	0.172	0.345
0.600	−14682	−23217	−4.742	−7037	−8.989	0.375	0.625
0.700	−7039	−10802	−2.091	−1701	−5.056	0.625	0.893
0.800	−2880	−3586	−0.392	459	−2.247	0.825	1.031
0.900	−1105	−540	0.314	472	−0.562	0.929	1.032
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ho(liquid)

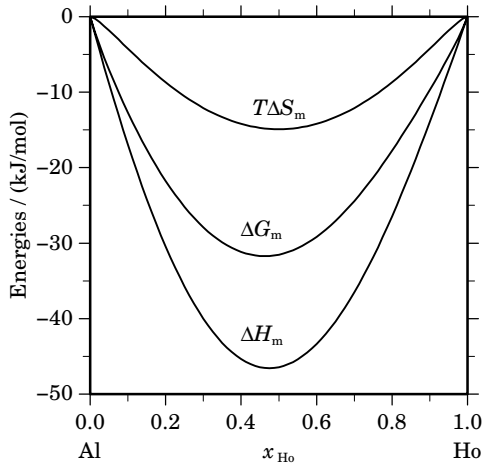

Fig. 2. Integral quantities of the liquid phase at T=1800 K.

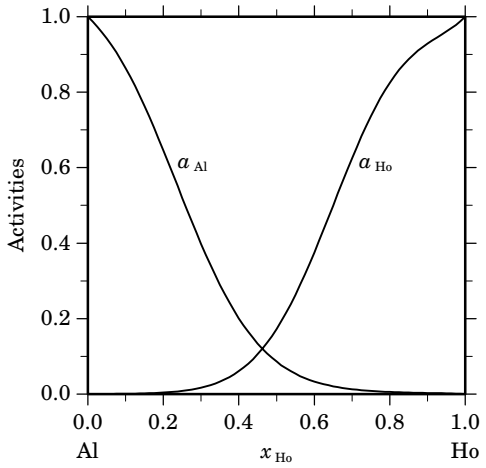

Fig. 3. Activities in the liquid phase at T=1800 K.

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

Compound	x_{Ho}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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_3Ho	0.250	−40754	−43000	−7.532	0.000
$C15$	0.333	−52687	−56000	−11.113	0.000
AlHo	0.500	−47389	−50500	−10.435	0.000
Al_2Ho_3	0.600	−41638	−44500	−9.600	0.000
Al_1Ho_2	0.667	−37302	−40000	−9.050	0.000

References

[1966Mey] A. Meyer: J. Less-Common Met. **10** (1966) 121–129.
[1985Col] C. Colinet, A. Pasturel, K.H.J. Buschow: J. Chem. Thermodyn. **17** (1985) 1133–1139.
[2003Cac] G. Cacciamani, S. de Negri, A. Saccone, R. Ferro: Intermetallics **11** (2003) 1135–1151.