Al – Ru (Aluminium – Ruthenium)

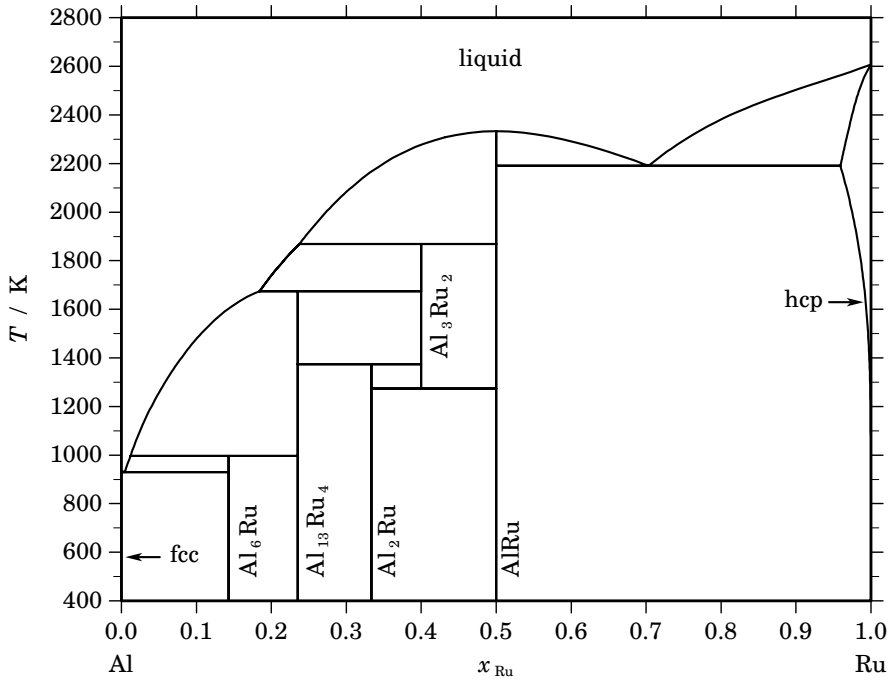

Fig. 1. Calculated phase diagram for the system Al-Ru.

The Al-Ru system contains two components interesting for the nuclear field, aluminium being a major component of the concrete basemat in its oxide form (Al_2O_3) and Ru being one selected component representative of a family of non volatile fission products. The system has been thermodynamically optimised by Chevalier and Fischer [1996Che] and Prins *et al.* [2003Pri] but the latter work is not recommended due to the modelling of the imprecise non-stoichiometry range of $Al_{13}Ru$, Al_2Ru, Al_3Ru_2 and AlRu leading to different temperatures of decomposition of these compounds. The phase diagram reported in the compilation of Moffatt [1981Mof] is based on the phase diagram of Obrowski [1963Obr] which has been obtained from microscopy, X-ray, and DTA experiments, and the investigation of Al-rich alloys by Anlage *et al.* [1988Anl] using scanning electron microscopy, X-ray, and thermal analysis. Five intermetallic compounds were identified, Al_6Ru, $Al_{13}Ru_4$, Al_2Ru, Al_3Ru_2 and AlRu. The three last show a non-negligible stoichiometry range. AlRu melts congruently at about 2323 K. The standard molar enthalpy of formation of AlRu has been determined calorimetrically by Jung and Kleppa [1992Jun]. The excess Gibbs energy of the liquid and hcp solution phases and the Gibbs energy of the intermetallics which have been described as stoichiometric compounds were optimised from the selected experimental information. A sub-regular substitution model was used for the liquid and a regular solution for the hcp phase. The enthalpy of formation was optimised in consistency with other data. The agreement with the experimental information [1963Obr, 1988Anl, 1992Jun] is quite satisfactory. However, a revised phase diagram for Al-rich alloys has been published in [2003Mi] which presents different equilibria at higher temperatures and an additional high-temperature compound, Al_5Ru_2.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Al,Ru)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Al,Ru)_1$
Al_6Ru	$D2_h$	Al_6Mn	$oC28$	$Cmcm$	AL6RU	Al_6Ru_1
$Al_{13}Ru_4$	$\cdots$	$Al_{13}Fe_4$	$mC102$	$C2/m$	AL13RU4	$Al_{13}Ru_4$
Al_2Ru	$C54$	$TiSi_2$	$oF24$	$Fddd$	AL2RU	Al_2Ru_1
Al_3Ru_2	$\cdots$	Al_3Os_2	$tI10$	$I4/mmm$	AL3RU2	Al_3Ru_2
AlRu	$B2$	CsCl	$cP2$	$Pm\overline{3}m$	ALRU	Al_1Ru_1
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Al,Ru)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ru}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ AlRu	congruent	2332.7	0.500	0.500		−63621
liquid $\rightleftharpoons$ AlRu + hcp	eutectic	2191.0	0.703	0.500	0.959	−48684
liquid + AlRu $\rightleftharpoons$ Al_3Ru_2	peritectic	1868.3	0.237	0.500	0.400	−11339
liquid + Al_3Ru_2 $\rightleftharpoons$ $Al_{13}Ru_4$	peritectic	1674.6	0.184	0.400	0.235	−23684
$Al_{13}Ru_4$ + Al_3Ru_2 $\rightleftharpoons$ Al_2Ru	peritectoid	1373.4	0.235	0.400	0.333	−2645
Al_3Ru_2 $\rightleftharpoons$ Al_2Ru + AlRu	eutectoid	1273.1	0.400	0.333	0.500	−3175
liquid + $Al_{13}Ru_4$ $\rightleftharpoons$ Al_6Ru	peritectic	996.0	0.012	0.235	0.143	−7091
liquid $\rightleftharpoons$ fcc + Al_6Ru	eutectic	929.8	0.005	0.000	0.143	−11078

Table IIIa. Integral quantities for the liquid phase at 2700 K.

x_{Ru}	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	−19011	−11713	2.703	−11713	0.000	0.000
0.200	−30522	−19288	4.161	−19288	0.000	0.000
0.300	−37015	−23302	5.079	−23302	0.000	0.000
0.400	−39437	−24329	5.596	−24329	0.000	0.000
0.500	−38505	−22945	5.763	−22945	0.000	0.000
0.600	−34834	−19725	5.596	−19725	0.000	0.000
0.700	−28959	−15245	5.079	−15245	0.000	0.000
0.800	−21315	−10081	4.161	−10081	0.000	0.000
0.900	−12105	−4807	2.703	−4807	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Al in the liquid phase at 2700 K.

x_{Al}	ΔG_{Al} [J/mol]	ΔH_{Al} [J/mol]	ΔS_{Al} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Al}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Al}}$ [J/(mol·K)]	a_{Al}	γ_{Al}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−4530	−2165	0.876	−2165	0.000	0.817	0.908
0.800	−12901	−7891	1.855	−7891	0.000	0.563	0.704
0.700	−24036	−16029	2.966	−16029	0.000	0.343	0.490
0.600	−36894	−25427	4.247	−25427	0.000	0.193	0.322
0.500	−50494	−34933	5.763	−34933	0.000	0.105	0.211
0.400	−63969	−43399	7.619	−43399	0.000	0.058	0.145
0.300	−76699	−49671	10.010	−49671	0.000	0.033	0.109
0.200	−88730	−52600	13.382	−52600	0.000	0.019	0.096
0.100	−102725	−51034	19.145	−51034	0.000	0.010	0.103
0.000	−∞	−43823	∞	−43823	0.000	0.000	0.142

Reference state: Al(liquid)

Table IIIc. Partial quantities for Ru in the liquid phase at 2700 K.

x_{Ru}	ΔG_{Ru} [J/mol]	ΔH_{Ru} [J/mol]	ΔS_{Ru} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ru}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ru}}$ [J/(mol·K)]	a_{Ru}	γ_{Ru}
0.000	−∞	−139734	∞	−139734	0.000	0.000	0.002
0.100	−149338	−97647	19.145	−97647	0.000	0.001	0.013
0.200	−101007	−64876	13.382	−64876	0.000	0.011	0.056
0.300	−67300	−40272	10.010	−40272	0.000	0.050	0.166
0.400	−43252	−22682	7.619	−22682	0.000	0.146	0.364
0.500	−26516	−10956	5.763	−10956	0.000	0.307	0.614
0.600	−15410	−3943	4.247	−3943	0.000	0.503	0.839
0.700	−8498	−491	2.966	−491	0.000	0.685	0.978
0.800	−4460	549	1.855	549	0.000	0.820	1.025
0.900	−2036	329	0.876	329	0.000	0.913	1.015
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ru(liquid)

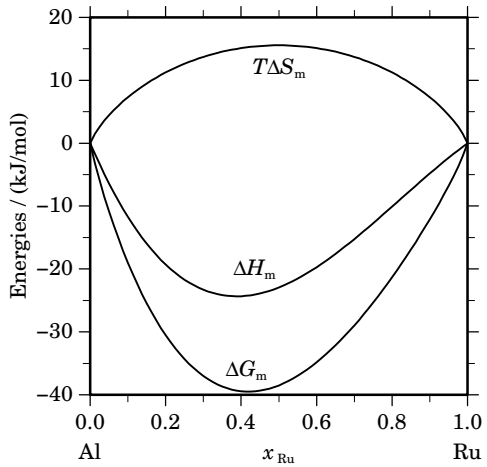

Fig. 2. Integral quantities of the liquid phase at T=2700 K.

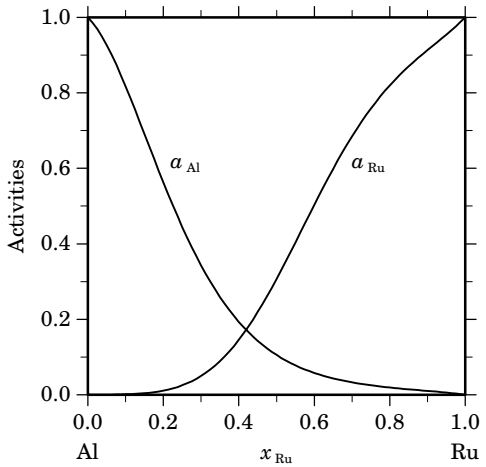

Fig. 3. Activities in the liquid phase at T=2700 K.

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

Compound	x_{Ru}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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))
Al_6Ru_1	0.143	−26312	−28000	−5.660	0.000
$Al_{13}Ru_4$	0.235	−40494	−42300	−6.056	0.000
Al_2Ru_1	0.333	−48062	−51000	−9.854	4.971
Al_3Ru_2	0.400	−50011	−52245	−7.494	4.474
Al_1Ru_1	0.500	−59012	−62050	−10.188	3.728

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