Al – Sc (Aluminium – Scandium)

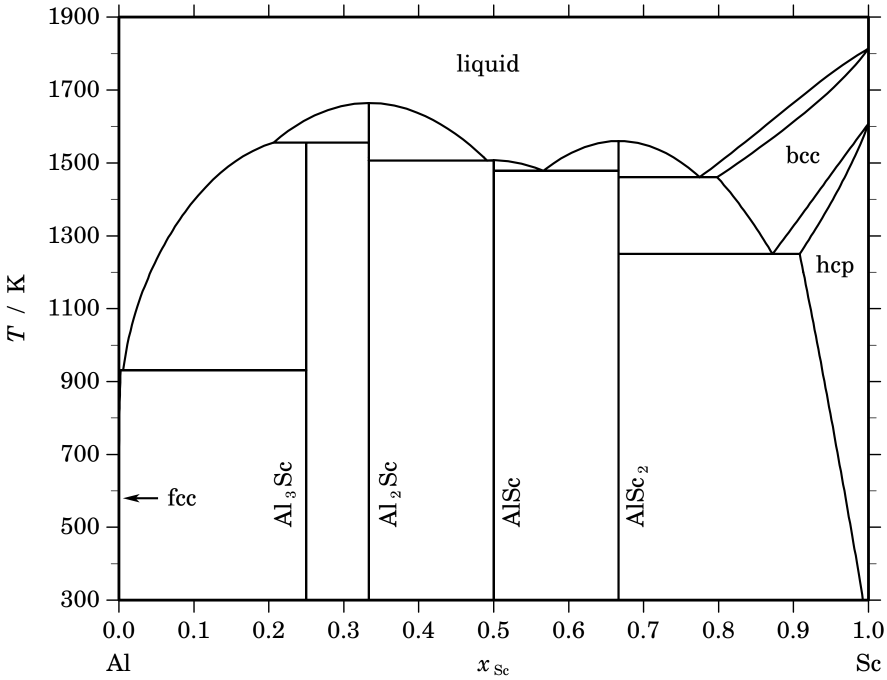

Fig. 1. Calculated phase diagram for the system Al-Sc.

Additions of Sc to Al- and Mg-alloys are of potential interest for the aerospace and automotive industry because the mechanical properties of the alloys can be improved at higher temperatures. Thermodynamic assessments and reviews of the literature of the Al-Sc system have been reported in [1998Mur, 1999Cac]. The assessment of [1999Cac] is selected here, because it includes a set of additional experimental data which are reported in that paper. The optimisation takes into account data for the phase equilibria from several literature sources as well as new DTA investigations [1999Cac]. According to these results, the solubility of Al in bcc-Sc and hcp-Sc is much higher than in previous reports. Furthermore, the assessment takes account of investigations of mixing enthalpies in the liquid [1986Lit] and heats of formation for the intermetallic compounds from the literature as well as from new experiments [1999Cac].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Al,Sc)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Al,Sc)_1$
Al_3Sc	$L1_2$	$AuCu_3$	$cP4$	$Pm\overline{3}m$	AL3SC	Al_3Sc_1
Al_2Sc	$C15$	Cu_2Mg	$cF24$	$Fd\overline{3}m$	AL2SC	Al_2Sc_1
AlSc	$B2$	CsCl	$cP2$	$Pm\overline{3}m$	ALSC	Al_1Sc_1
$AlSc_2$	$B8_2$	Ni_2In	$hP6$	$P6_3/mmc$	ALSC2	Al_1Sc_2
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Al,Sc)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Al,Sc)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Sc}			$\Delta_r H$ / (J/mol)
liquid ⇌ Al_2Sc	congruent	1664.8	0.333	0.333		−33033
liquid ⇌ $AlSc_2$	congruent	1560.3	0.667	0.667		−24360
liquid + Al_2Sc ⇌ Al_3Sc	peritectic	1556.1	0.207	0.333	0.250	−19839
liquid ⇌ AlSc	congruent	1507.3	0.500	0.500		−28477
liquid ⇌ Al_2Sc + AlSc	eutectic	1506.8	0.491	0.333	0.500	−28528
liquid ⇌ AlSc + $AlSc_2$	eutectic	1478.3	0.566	0.500	0.667	−25832
liquid ⇌ $AlSc_2$ + bcc	eutectic	1460.8	0.775	0.667	0.798	−9058
bcc ⇌ $AlSc_2$ + hcp	eutectoid	1250.3	0.872	0.667	0.908	−5731
liquid ⇌ fcc + Al_3Sc	eutectic	930.9	0.006	0.002	0.250	−10819

Table IIIa. Integral quantities for the liquid phase at 1873 K.

x_{Sc}	ΔG_m [J/mol]	ΔH_m [J/mol]	ΔS_m [J/(mol·K)]	G^E_m [J/mol]	S^E_m [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−13456	−11364	1.117	−8393	−1.586	0.000
0.200	−22715	−20203	1.341	−14922	−2.820	0.000
0.300	−29098	−26517	1.378	−19585	−3.701	0.000
0.400	−32863	−30305	1.366	−22383	−4.230	0.000
0.500	−34110	−31568	1.357	−23315	−4.406	0.000
0.600	−32863	−30305	1.366	−22383	−4.230	0.000
0.700	−29098	−26517	1.378	−19585	−3.701	0.000
0.800	−22715	−20203	1.341	−14922	−2.820	0.000
0.900	−13456	−11364	1.117	−8393	−1.586	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Al in the liquid phase at 1873 K.

x_{Al}	ΔG_{Al} [J/mol]	ΔH_{Al} [J/mol]	ΔS_{Al} [J/(mol·K)]	G^E_{Al} [J/mol]	S^E_{Al} [J/(mol·K)]	a_{Al}	γ_{Al}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2573	−1263	0.700	−933	−0.176	0.848	0.942
0.800	−7205	−5051	1.150	−3730	−0.705	0.630	0.787
0.700	−13948	−11364	1.379	−8393	−1.586	0.408	0.583
0.600	−22877	−20203	1.427	−14922	−2.820	0.230	0.384
0.500	−34110	−31568	1.357	−23315	−4.406	0.112	0.224
0.400	−47843	−45457	1.274	−33574	−6.345	0.046	0.116
0.300	−64447	−61873	1.375	−45698	−8.636	0.016	0.053
0.200	−84751	−80813	2.102	−59687	−11.279	0.004	0.022
0.100	−111399	−102279	4.869	−75541	−14.276	0.001	0.008
0.000	$-\infty$	−126270	∞	−93260	−17.624	0.000	0.003

Reference state: Al(liquid)

Table IIIc. Partial quantities for Sc in the liquid phase at 1873 K.

x_{Sc}	ΔG_{Sc} [J/mol]	ΔH_{Sc} [J/mol]	ΔS_{Sc} [J/(mol·K)]	G^E_{Sc} [J/mol]	S^E_{Sc} [J/(mol·K)]	a_{Sc}	γ_{Sc}
0.000	$-\infty$	−126270	∞	−93261	−17.624	0.000	0.003
0.100	−111399	−102279	4.869	−75541	−14.276	0.001	0.008
0.200	−84751	−80813	2.102	−59687	−11.279	0.004	0.022
0.300	−64447	−61873	1.375	−45698	−8.636	0.016	0.053
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0.800	−7205	−5051	1.150	−3730	−0.705	0.630	0.787
0.900	−2573	−1263	0.700	−933	−0.176	0.848	0.942
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Sc(liquid)

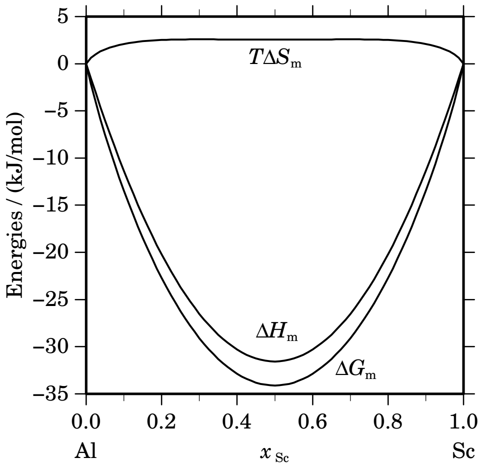

Fig. 2. Integral quantities of the liquid phase at T=1873 K.

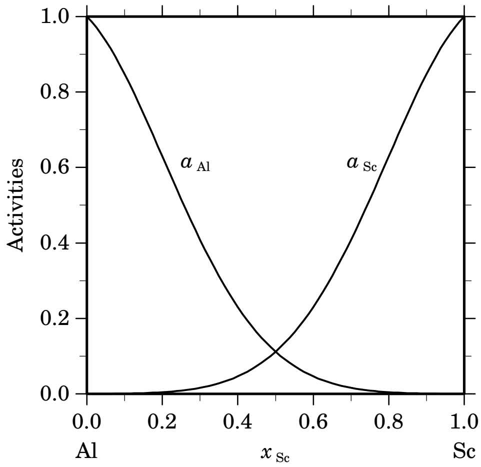

Fig. 3. Activities in the liquid phase at T=1873 K.

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

Compound	x_{Sc}	$\Delta_f G°$ / (J/mol)	$\Delta_f H°$ / (J/mol)	$\Delta_f S°$ / (J/(mol·K))	$\Delta_f C_P°$ / (J/(mol·K))
Al_3Sc_1	0.250	−39855	−42000	−7.193	0.000
Al_2Sc_1	0.333	−45764	−48000	−7.500	0.000
Al_1Sc_1	0.500	−43932	−46000	−6.937	0.000
Al_1Sc_2	0.667	−35887	−37000	−3.733	0.000

References

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[1998Mur] J.L. Murray: J. Phase Equilibria **19** (1998) 380–384.
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