Al – Sr (Aluminium – Strontium)

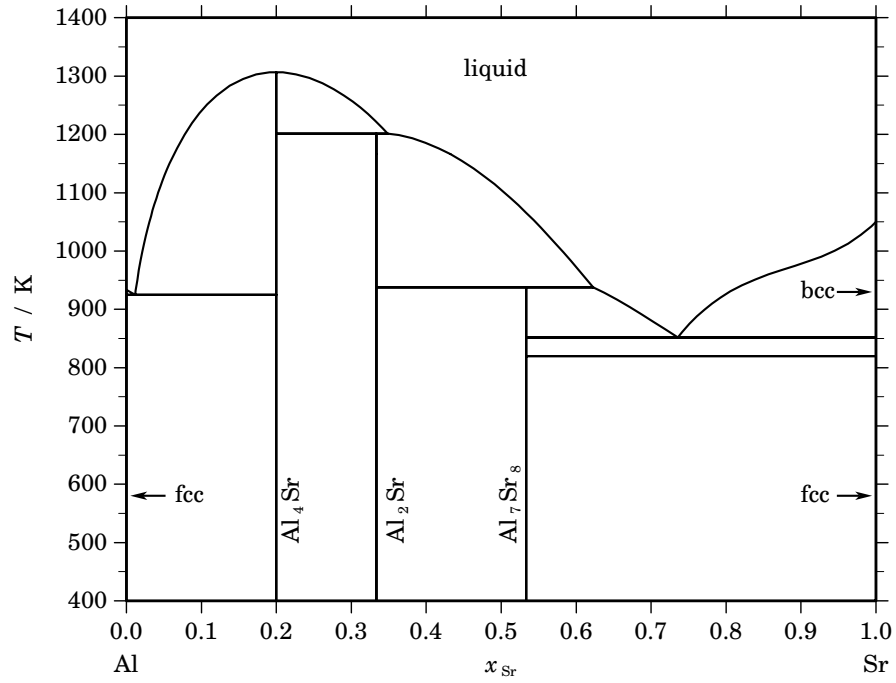

Fig. 1. Calculated phase diagram for the system Al-Sr.

Small amounts of strontium are added to Al-Si alloys in order to improve their eutectic microstructure. For this purpose, aluminium-strontium master alloys are used with Sr-concentrations up to 90%. Reviews and thermodynamical assessments for the Al-Sr system have been prepared by [1989Gsc, 2003Wan] the latter dataset being selected here. The optimisation is based on investigations of the phase diagram from the literature which are well reproduced within the scatter of data between the various literature sources. The thermodynamics of the liquid has been evaluated throughout the whole composition range using data for the mixing enthalpy and the activity of Sr at several temperatures. In lack of experimental data for the thermodynamics of the three intermetallic compounds, results for the enthalpy of formation from first-principle calculations have been used in the optimisation. The dataset should not be used at too high temperatures because an artificial inverse miscibility gap opens in the liquid above 3100 K.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Al,Sr)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Al,Sr)_1$
Al_4Sr	$D1_3$	Al_4Ba	$tI10$	$I4/mmm$	D13_AL4SR	Al_4Sr_1
Al_2Sr	···	$CeCu_2$	$oI12$	$Imma$	AL2SR	Al_2Sr_1
Al_7Sr_8	···	Al_7Sr_8	$cP60$	$P2_13$	AL7SR8	Al_7Sr_8
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Al,Sr)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Sr}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons$ Al_4Sr	congruent	1306.7	0.200	0.200		−20921
Al_4Sr + liquid $\rightleftharpoons$ Al_2Sr	peritectic	1201.3	0.200	0.349	0.333	−19401
Al_2Sr + liquid $\rightleftharpoons$ Al_7Sr_8	peritectic	937.6	0.333	0.623	0.533	−7067
liquid $\rightleftharpoons$ fcc + Al_4Sr	eutectic	924.7	0.012	0.000	0.200	−10987
liquid $\rightleftharpoons$ Al_7Sr_8 + bcc	eutectic	851.9	0.736	0.533	1.000	−8737
bcc $\rightleftharpoons$ Al_7Sr_8 + fcc	eutectoid	820.0	1.000	0.533	1.000	−837

Table IIIa. Integral quantities for the liquid phase at 1400 K.

x_{Sr}	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	−6688	−9102	−1.724	−2904	−4.427	0.000
0.200	−10614	−15292	−3.341	−4789	−7.502	0.000
0.300	−12857	−18767	−4.221	−5747	−9.300	0.000
0.400	−13732	−19805	−4.338	−5897	−9.934	0.000
0.500	−13457	−18758	−3.787	−5388	−9.550	0.000
0.600	−12227	−16056	−2.735	−4393	−8.331	0.000
0.700	−10224	−12206	−1.416	−3114	−6.495	0.000
0.800	−7604	−7793	−0.135	−1779	−4.296	0.000
0.900	−4431	−3478	0.680	−647	−2.022	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Al in the liquid phase at 1400 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	−1749	−1483	0.190	−523	−0.686	0.860	0.956
0.800	−4579	−5705	−0.805	−1981	−2.660	0.675	0.843
0.700	−8302	−12154	−2.752	−4150	−5.717	0.490	0.700
0.600	−12668	−20085	−5.298	−6722	−9.545	0.337	0.561
0.500	−17375	−28521	−7.962	−9306	−13.725	0.225	0.450
0.400	−22098	−36257	−10.114	−11432	−17.732	0.150	0.375
0.300	−26558	−41852	−10.924	−12544	−20.935	0.102	0.340
0.200	−30741	−43639	−9.213	−12006	−22.595	0.071	0.356
0.100	−35904	−39714	−2.722	−9101	−21.867	0.046	0.458
0.000	$-\infty$	−27947	∞	−3027	−17.800	0.000	0.771

Reference state: Al(liquid)

Table IIIc. Partial quantities for Sr in the liquid phase at 1400 K.

x_{Sr}	ΔG_{Sr} [J/mol]	ΔH_{Sr} [J/mol]	ΔS_{Sr} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Sr}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Sr}}$ [J/(mol·K)]	a_{Sr}	γ_{Sr}
0.000	$-\infty$	−106053	∞	−34373	−51.200	0.000	0.052
0.100	−51138	−77674	−18.954	−24335	−38.099	0.012	0.124
0.200	−34753	−53636	−13.488	−16019	−26.870	0.051	0.253
0.300	−23486	−34198	−7.651	−9472	−17.662	0.133	0.443
0.400	−15327	−19386	−2.899	−4661	−10.518	0.268	0.670
0.500	−9538	−8995	0.388	−1470	−5.375	0.441	0.881
0.600	−5646	−2589	2.184	300	−2.063	0.616	1.026
0.700	−3224	499	2.659	928	−0.306	0.758	1.083
0.800	−1820	1168	2.134	777	0.279	0.855	1.069
0.900	−934	548	1.058	292	0.182	0.923	1.025
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Sr(liquid)

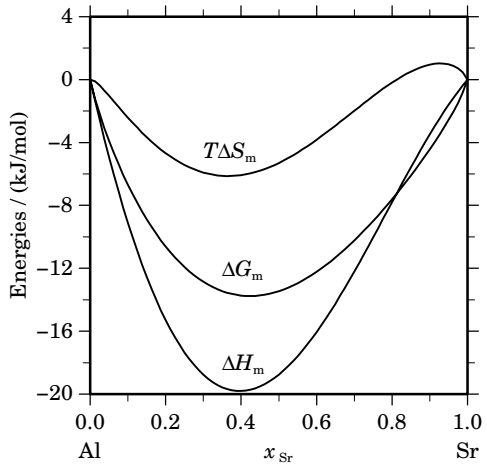

Fig. 2. Integral quantities of the liquid phase at T=1400 K.

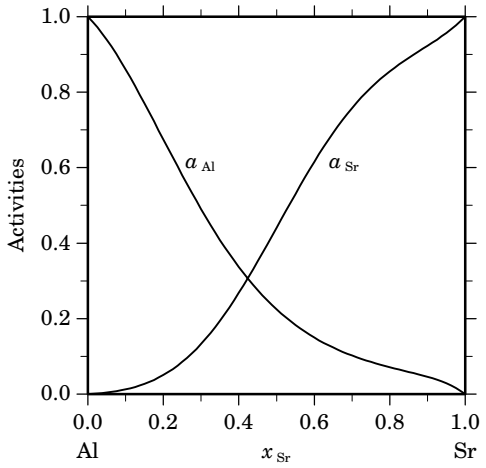

Fig. 3. Activities in the liquid phase at T=1400 K.

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

Compound	x_{Sr}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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_4Sr_1	0.200	−23484	−26069	−8.670	0.000
Al_2Sr_1	0.333	−27361	−30903	−11.880	0.000
Al_7Sr_8	0.533	−19291	−21385	−7.020	0.000

References

[1989Gsc] K.A. Gschneidner Jr., F.W. Calderwood: Bull. Alloy Phase Diagrams **10** (1989) 34–36.
[2003Wan] C. Wang, Z. Jin, Y. Du: J. Alloys Comp. **358** (2003) 288–293.