Mg – Sc (Magnesium – Scandium)

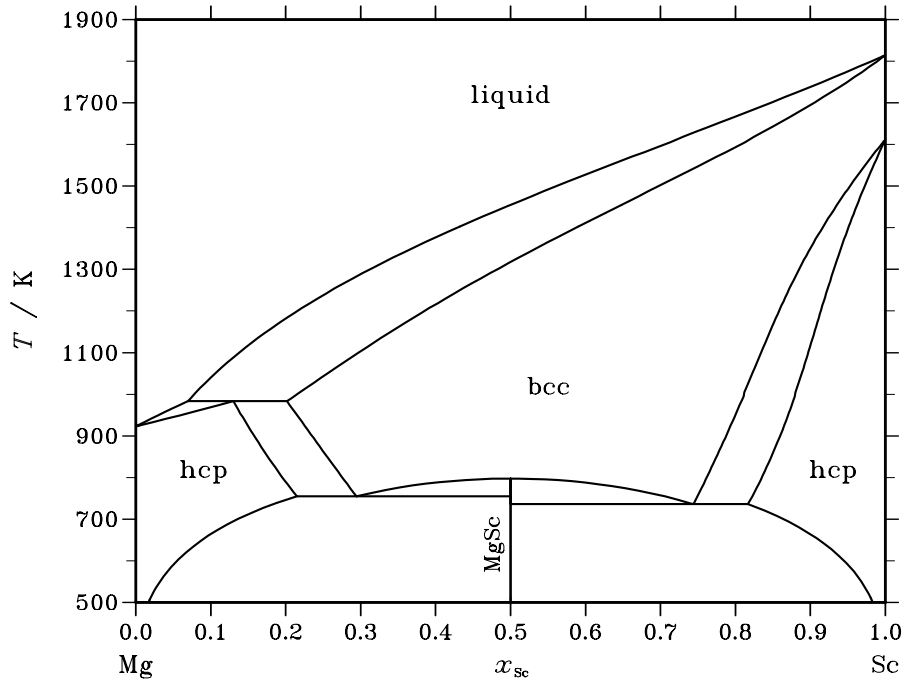

Fig. 1. Calculated phase diagram for the system Mg-Sc.

Scandium additions to Al and Mg light metal alloys improve considerably their mechanical properties and creep resistance. A thermodynamic assessment of the Mg-Sc system has been performed by Pisch *et al.* [98Pis] based on scarce literature information and own measurements using DTA and metallographic techniques. Mg-Sc is the only Mg-rare-earth system showing peritectic behaviour, while all others are eutectic. The system is further characterised by a large solid solubility of Mg in bcc-Sc (up to 80 at.% Mg at the peritectic point). The solid solubility of Sc in solid Mg increases with decreasing temperature to a maximum value of about 20 at.% Sc. There is one intermetallic phase, MgSc, which has an ordered $B2$ structure. This phase has been described stoichiometric in the present assessment due to missing experimental information. The solid-liquid equilibria are accepted from the work of Beaudy and Daane [69Bea] and the overall agreement between experimental and calculated values is good.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Mg,Sc)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Mg,Sc)_1$
MgSc	$B2$	CsCl	$cP2$	$Pm3m$	MGSC	Mg_1Sc_1
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Mg,Sc)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Sc}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid + bcc ⇌ hcp	peritectic	983.3	0.069	0.202	0.130	−5773
bcc ⇌ MgSc	congruent	797.6	0.500	0.500		−20566
bcc ⇌ hcp + MgSc	eutectoid	754.7	0.294	0.215	0.500	−6404
bcc ⇌ MgSc + hcp	eutectoid	736.0	0.744	0.500	0.817	−5025

Table IIIa. Integral quantities for the liquid phase at 1823 K.

x_{Sc}	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	−4572	−1080	1.915	356	−0.788	0.000
0.200	−6953	−1920	2.761	632	−1.400	0.000
0.300	−8429	−2520	3.242	830	−1.837	0.000
0.400	−9253	−2880	3.496	948	−2.100	0.000
0.500	−9518	−3000	3.576	988	−2.188	0.000
0.600	−9253	−2880	3.496	948	−2.100	0.000
0.700	−8429	−2520	3.242	830	−1.837	0.000
0.800	−6953	−1920	2.761	632	−1.400	0.000
0.900	−4572	−1080	1.915	356	−0.788	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Mg in the liquid phase at 1823 K.

x_{Mg}	ΔG_{Mg} [J/mol]	ΔH_{Mg} [J/mol]	ΔS_{Mg} [J/(mol·K)]	$G_{\mathrm{Mg}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Mg}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Mg}	γ_{Mg}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1557	−120	0.789	40	−0.087	0.902	1.003
0.800	−3224	−480	1.505	158	−0.350	0.808	1.010
0.700	−5051	−1080	2.178	356	−0.788	0.717	1.024
0.600	−7111	−1920	2.847	632	−1.400	0.626	1.043
0.500	−9518	−3000	3.576	988	−2.188	0.534	1.067
0.400	−12466	−4320	4.469	1422	−3.150	0.439	1.098
0.300	−16313	−5880	5.723	1936	−4.287	0.341	1.136
0.200	−21866	−7680	7.782	2529	−5.600	0.236	1.182
0.100	−31701	−9720	12.057	3201	−7.088	0.124	1.235
0.000	$-\infty$	−12000	∞	3951	−8.750	0.000	1.298

Reference state: Mg(liquid)

Table IIIc. Partial quantities for Sc in the liquid phase at 1823 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	$-\infty$	−12000	∞	3951	−8.750	0.000	1.298
0.100	−31701	−9720	12.057	3201	−7.088	0.124	1.235
0.200	−21866	−7680	7.782	2529	−5.600	0.236	1.182
0.300	−16313	−5880	5.723	1936	−4.287	0.341	1.136
0.400	−12466	−4320	4.469	1422	−3.150	0.439	1.098
0.500	−9518	−3000	3.576	988	−2.188	0.534	1.067
0.600	−7111	−1920	2.847	632	−1.400	0.626	1.043
0.700	−5051	−1080	2.178	356	−0.788	0.717	1.024
0.800	−3224	−480	1.505	158	−0.350	0.808	1.010
0.900	−1557	−120	0.789	40	−0.087	0.902	1.003
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Sc(liquid)

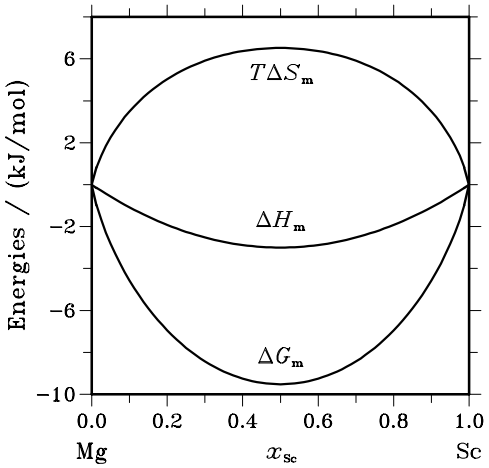

Fig. 2. Integral quantities of the liquid phase at T=1823 K.

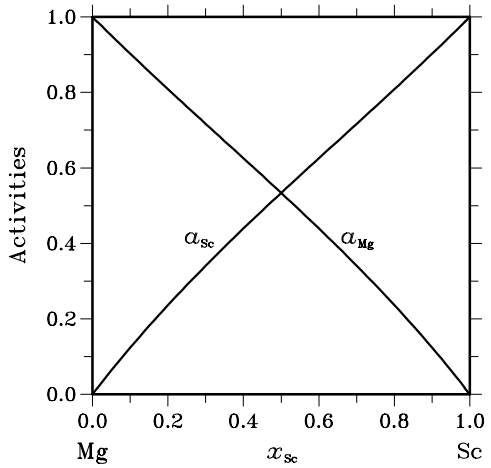

Fig. 3. Activities in the liquid phase at T=1823 K.

Table IVa. Integral quantities for the stable phases at 850 K.

Phase	x_{Sc}	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)]
hcp	0.000	0	0	0.000	0	0.000	0.000
	0.100	−2599	−1450	1.351	−301	−1.352	0.000
	0.176	−3776	−2339	1.691	−486	−2.180	0.000
bcc	0.255	−4810	−1758	3.590	−795	−1.133	0.000
	0.300	−5337	−2287	3.589	−1020	−1.490	0.000
	0.400	−6122	−3120	3.531	−1365	−2.065	0.000
	0.500	−6393	−3473	3.435	−1494	−2.328	0.000
	0.600	−6163	−3344	3.316	−1406	−2.280	0.000
	0.700	−5419	−2735	3.158	−1102	−1.921	0.000
	0.775	−4503	−1965	2.987	−733	−1.449	0.000
hcp	0.848	−3445	−2078	1.608	−432	−1.937	0.000
	0.900	−2599	−1450	1.351	−301	−1.352	0.000
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Mg(hcp), Sc(hcp)

Table IVb. Partial quantities for Mg in the stable phases at 850 K.

Phase	x_{Mg}	ΔG_{Mg} [J/mol]	ΔH_{Mg} [J/mol]	ΔS_{Mg} [J/(mol·K)]	$G_{\mathrm{Mg}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Mg}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Mg}	γ_{Mg}
hcp	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−778	−161	0.726	−33	−0.150	0.896	0.995
	0.824	−1473	−500	1.145	−104	−0.466	0.812	0.985
bcc	0.745	−1473	1533	3.537	610	1.086	0.812	1.090
	0.700	−2180	935	3.665	341	0.700	0.735	1.049
	0.600	−4027	−748	3.858	−417	−0.390	0.566	0.943
	0.500	−6290	−2913	3.973	−1391	−1.790	0.411	0.821
	0.400	−9058	−5558	4.117	−2582	−3.502	0.278	0.694
	0.300	−12498	−8685	4.486	−3989	−5.524	0.171	0.569
	0.225	−15718	−11337	5.154	−5183	−7.240	0.108	0.480
hcp	0.152	−15718	−11587	4.860	−2408	−10.799	0.108	0.711
	0.100	−18986	−13054	6.979	−2713	−12.166	0.068	0.681
	0.000	$-\infty$	−16116	∞	−3349	−15.020	0.000	0.623

Reference state: Mg(hcp)

Table IVc. Partial quantities for Sc in the stable phases at 850 K.

Phase	x_{Sc}	ΔG_{Sc} [J/mol]	ΔH_{Sc} [J/mol]	ΔS_{Sc} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Sc}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Sc}}$ [J/(mol·K)]	a_{Sc}	γ_{Sc}
hcp	0.000	$-\infty$	−16116	∞	−3349	−15.020	0.000	0.623
	0.100	−18986	−13054	6.979	−2713	−12.166	0.068	0.681
	0.176	−14545	−10938	4.243	−2273	−10.194	0.128	0.725
bcc	0.255	−14545	−11360	3.747	−4895	−7.606	0.128	0.500
	0.300	−12704	−9805	3.410	−4195	−6.600	0.166	0.552
	0.400	−9264	−6679	3.041	−2788	−4.577	0.270	0.674
	0.500	−6496	−4033	2.897	−1597	−2.866	0.399	0.798
	0.600	−4233	−1868	2.782	−623	−1.465	0.549	0.916
	0.700	−2386	−185	2.589	135	−0.376	0.713	1.019
	0.775	−1243	760	2.357	560	0.235	0.839	1.082
hcp	0.848	−1243	−373	1.024	−77	−0.347	0.839	0.989
	0.900	−778	−161	0.726	−33	−0.150	0.896	0.995
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Sc(hcp)

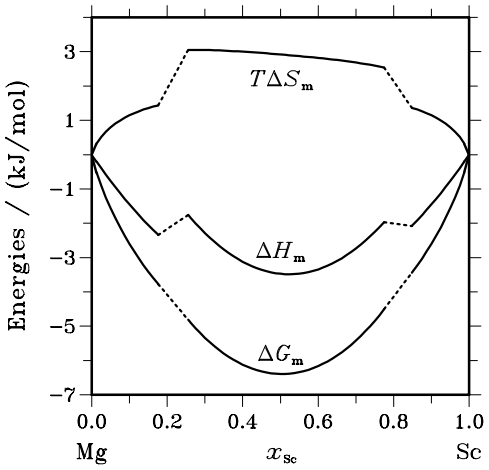

Fig. 4. Integral quantities of the stable phases at T=850 K.

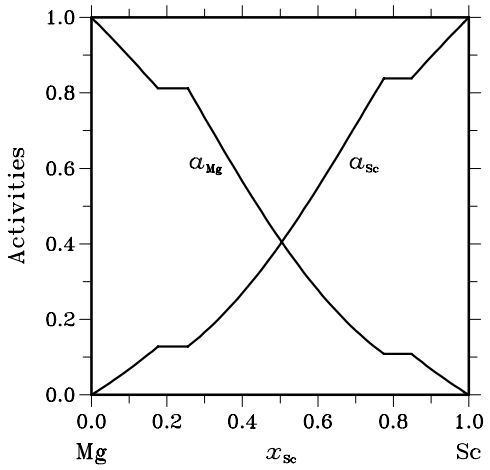

Fig. 5. Activities in the stable phases at T=850 K.

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

Compound	x_{Sc}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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))
Mg_1Sc_1	0.500	−16830	−22716	−19.742	−2.649

References

[69Bea] B.J. Beaudy, A.H. Daane: J. Less-Common Met. **18** (1969) 305–308.
[98Pis] A. Pisch, R. Schmid-Fetzer, G. Cacciamani, P. Riani, A. Saccone, R. Ferro: Z. Metallkd. **89** (1998) 474–477.