Fe – Sb (Iron – Antimony)

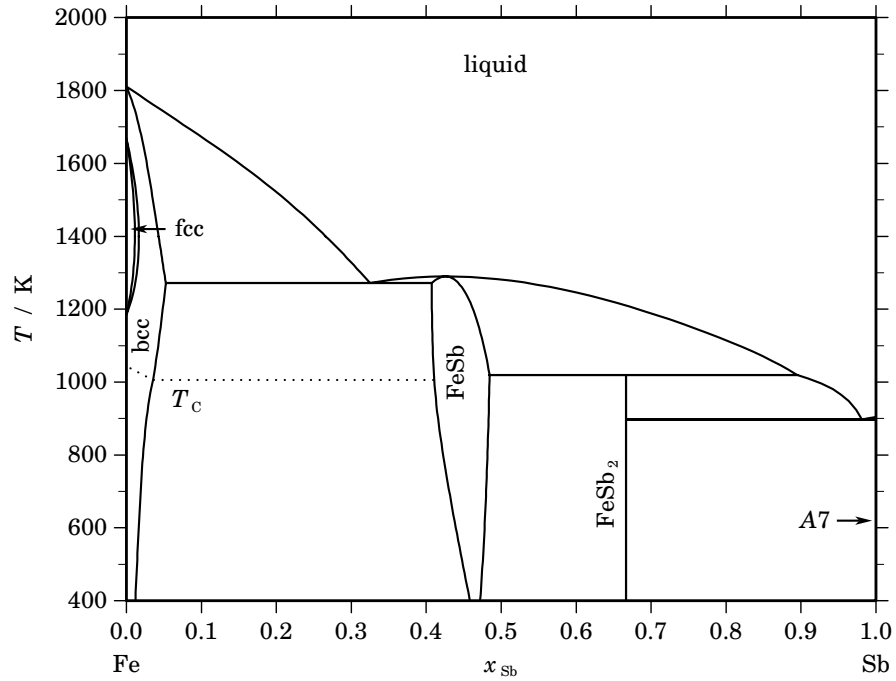

Fig. 1. Calculated phase diagram for the system Fe-Sb.

Iron and antimony are often found as substitutional elements in copper arsenide and sulfide minerals which are used in copper smelting processes. A thermodynamic optimisation of the Fe-Sb system has been reported by [1995Pei]. For the assessment a large number of reports has been evaluated which determine the phase diagram over the complete composition range and temperatures up to the liquidus. In addition, enthalpies of mixing and the activities of both elements have been available for Sb-rich melts as well as in the sub-solidus region across the whole composition range. In the assessment of the phases FeSb and $FeSb_2$ their magnetic properties have not been considered.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Fe,Sb)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Fe,Sb)_1$
$A2$	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Fe,Sb)_1$
FeSb	$B8_1$	NiAS	$hP4$	$P6_3/mmc$	FESB	$Fe_1(Fe,Sb)_1$
$FeSb_2$	$\cdots$	$\cdots$	$oP6$	$Pnn2$	FESB2	Fe_1Sb_2
$A7$	$A7$	αAs	$hR2$	$R\overline{3}m$	RHOMBOHEDRAL_A7	Sb_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Sb}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ $FeSb_2$	congruent	1038.3	0.155	0.155		−10899
liquid $\rightleftharpoons$ bcc + $FeSb_2$	eutectic	1271.5	0.325	0.053	0.407	−14416
$FeSb_2$ + liquid $\rightleftharpoons$ $FeSb_2$	peritectic	1018.9	0.485	0.895	0.667	−13680
liquid $\rightleftharpoons$ $FeSb_2$ + A7	eutectic	897.8	0.981	0.667	1.000	−20180

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

x_{Sb}	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	−3936	−3022	0.501	992	−2.202	0.000
0.200	−5949	−4989	0.526	1636	−3.634	0.000
0.300	−7240	−6007	0.676	2019	−4.403	0.000
0.400	−7995	−6202	0.983	2206	−4.612	0.000
0.500	−8267	−5723	1.396	2239	−4.367	0.000
0.600	−8063	−4741	1.822	2138	−3.773	0.000
0.700	−7359	−3450	2.145	1900	−2.935	0.000
0.800	−6085	−2067	2.204	1499	−1.956	0.000
0.900	−4038	−830	1.760	890	−0.943	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Fe(liquid), Sb(liquid)

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

x_{Fe}	ΔG_{Fe} [J/mol]	ΔH_{Fe} [J/mol]	ΔS_{Fe} [J/(mol·K)]	$G_{\mathrm{Fe}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Fe}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Fe}	γ_{Fe}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1407	−542	0.474	190	−0.402	0.911	1.013
0.800	−2748	−2042	0.387	634	−1.468	0.834	1.043
0.700	−4216	−4257	−0.023	1190	−2.988	0.757	1.082
0.600	−5956	−6878	−0.506	1787	−4.753	0.675	1.125
0.500	−8090	−9528	−0.789	2417	−6.552	0.586	1.173
0.400	−10746	−11764	−0.559	3142	−8.177	0.492	1.230
0.300	−14157	−13075	0.594	4092	−9.417	0.393	1.310
0.200	−18933	−12881	3.320	5462	−10.062	0.287	1.434
0.100	−27386	−10538	9.242	7515	−9.903	0.164	1.642
0.000	$-\infty$	−5332	∞	10583	−8.730	0.000	2.010

Reference state: Fe(liquid)

Table IIIc. Partial quantities for Sb in the liquid phase at 1823 K.

x_{Sb}	ΔG_{Sb} [J/mol]	ΔH_{Sb} [J/mol]	ΔS_{Sb} [J/(mol·K)]	$G_{\mathrm{Sb}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Sb}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Sb}	γ_{Sb}
0.000	$-\infty$	−35777	∞	12004	−26.210	0.000	2.208
0.100	−26695	−25334	0.747	8206	−18.398	0.172	1.718
0.200	−18751	−16778	1.082	5644	−12.300	0.290	1.451
0.300	−14296	−10091	2.307	3953	−7.704	0.389	1.298
0.400	−11053	−5188	3.217	2835	−4.401	0.482	1.206
0.500	−8445	−1917	3.581	2062	−2.182	0.573	1.146
0.600	−6274	−58	3.410	1468	−0.837	0.661	1.102
0.700	−4446	675	2.809	960	−0.156	0.746	1.065
0.800	−2873	637	1.926	509	0.070	0.827	1.034
0.900	−1444	249	0.929	153	0.053	0.909	1.010
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Sb(liquid)

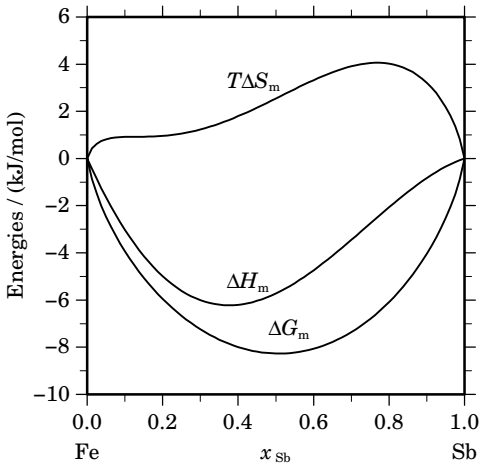

Fig. 2. Integral quantities of the liquid phase at T=1823 K.

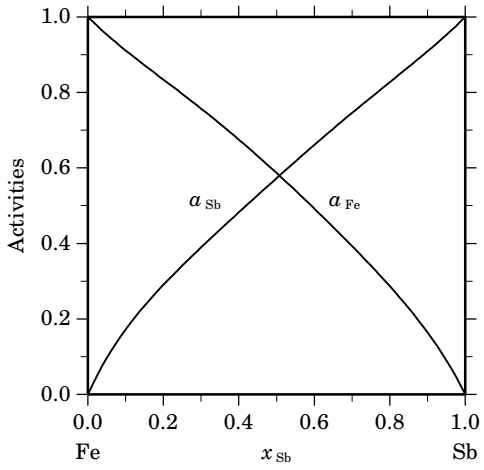

Fig. 3. Activities in the liquid phase at T=1823 K.

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

Compound	x_{Sb}	$\Delta_f G^\circ$ / (J/mol)	$\Delta_f H^\circ$ / (J/mol)	$\Delta_f S^\circ$ / (J/(mol·K))	$\Delta_f C_P^\circ$ / (J/(mol·K))
Fe_1Sb_2	0.667	−7055	−7012	0.145	−0.139

References

[1995Pei] B. Pei, B. Björkman, B. Sundman, B. Jansson: Calphad **19** (1995) 1–15.