In – Sb (Indium – Antimony)

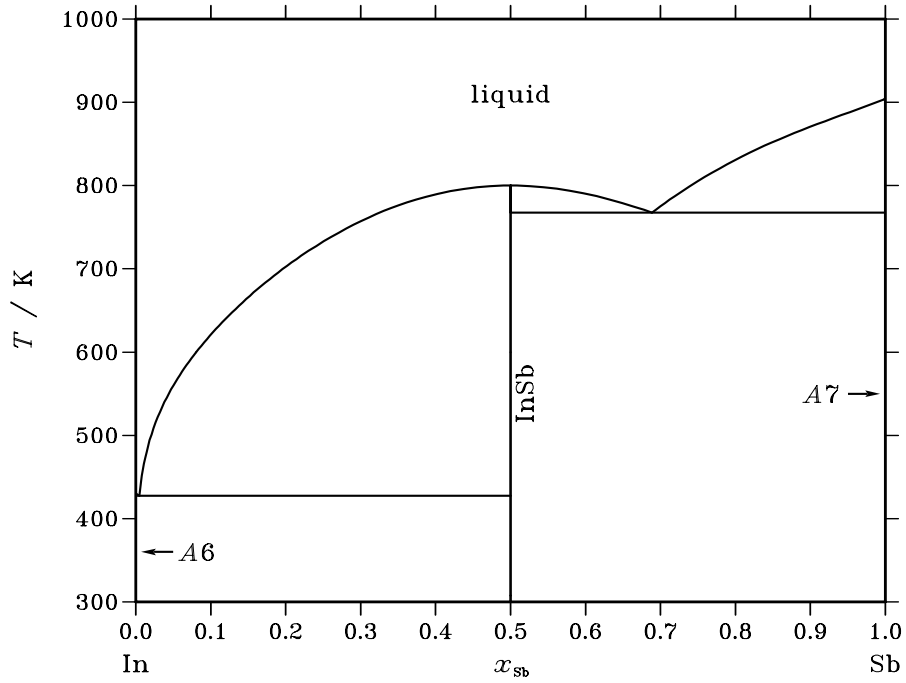

Fig. 1. Calculated phase diagram for the system In-Sb (constrained system).

The In-Sb system is part of the III-V semiconductor systems used in optoelectronic and high speed device applications. An understanding of the phase diagram and the thermochemistry of the system is essential to model the process conditions for device fabrication. The phase diagram of the In-Sb system is very simple featuring a near stoichiometric compound InSb which melts congruently at 800 K, a complete miscibility in the liquid phase and negligible solubility of In in solid Sb and Sb in solid In. The eutectic on the Sb rich side is given at 767.3 K and a composition of 68.8 at.% In. The eutectic on the In rich side is close to the pure element. The thermodynamic assessment by Anderson which is cited in [94Ans] is in good agreement with the experimental data given in a review by Sharma *et al.* [89Sha].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(In,Sb)_1$
$A6$	$A6$	In	$tI2$	$I4/mmm$	TETRAGONAL_A6	In_1
InSb	$B3$	ZnS	$cF8$	$F\overline{4}3m$	ZINCBLENDE_B3	In_1Sb_1
$A7$	$A7$	αAs	$hR2$	$R\overline{3}m$	RHOMBOHEDRAL_A7	$(In,Sb)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Sb}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ InSb	congruent	799.9	0.500	0.500		−24732
liquid $\rightleftharpoons$ InSb + $A7$	eutectic	767.3	0.688	0.500	1.000	−22153
liquid $\rightleftharpoons$ $A6$ + InSb	eutectic	427.5	0.005	0.000	0.500	−3426

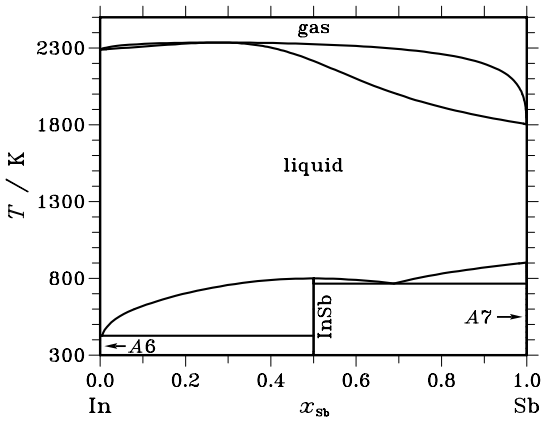

Fig. 2. Calculated phase diagram at 0.1 MPa.

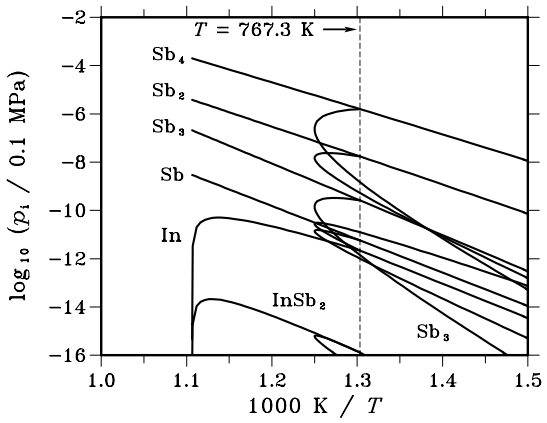

Fig. 3. Calculated partial pressures of gaseous species in the phase equilibria of the constrained system.

Table IIIa. Integral quantities for the liquid phase at 973 K.

x_{Sb}	ΔG_{m} [J/mol]	ΔH_{m} [J/mol]	ΔS_{m} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{m}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{m}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−4109	−1113	3.079	−1479	0.376	1.211
0.200	−6699	−2041	4.787	−2651	0.626	2.153
0.300	−8400	−2713	5.846	−3459	0.767	2.826
0.400	−9318	−3082	6.409	−3873	0.813	3.230
0.500	−9501	−3134	6.544	−3894	0.781	3.365
0.600	−8992	−2879	6.282	−3547	0.686	3.230
0.700	−7829	−2357	5.624	−2888	0.545	2.826
0.800	−6046	−1635	4.534	−1998	0.373	2.153
0.900	−3619	−808	2.889	−989	0.186	1.211
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for In in the liquid phase at 973 K.

x_{In}	ΔG_{In} [J/mol]	ΔH_{In} [J/mol]	ΔS_{In} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{In}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{In}}$ [J/(mol·K)]	a_{In}	γ_{In}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−994	−78	0.942	−142	0.066	0.884	0.983
0.800	−2462	−422	2.096	−657	0.241	0.738	0.922
0.700	−4503	−1136	3.460	−1617	0.495	0.573	0.819
0.600	−7144	−2238	5.042	−3011	0.795	0.414	0.689
0.500	−10351	−3663	6.874	−4744	1.111	0.278	0.556
0.400	−14047	−5263	9.028	−6634	1.409	0.176	0.440
0.300	−18161	−6806	11.670	−8421	1.660	0.106	0.353
0.200	−22777	−7976	15.212	−9756	1.830	0.060	0.299
0.100	−28838	−8372	21.034	−10210	1.889	0.028	0.283
0.000	$-\infty$	−7512	∞	−9267	1.804	0.000	0.318

Reference state: In(liquid)

Table IIIc. Partial quantities for Sb in the liquid phase at 973 K.

x_{Sb}	ΔG_{Sb} [J/mol]	ΔH_{Sb} [J/mol]	ΔS_{Sb} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Sb}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Sb}}$ [J/(mol·K)]	a_{Sb}	γ_{Sb}
0.000	$-\infty$	−11743	∞	−16065	4.442	0.000	0.137
0.100	−32142	−10429	22.316	−13514	3.171	0.019	0.188
0.200	−23647	−8517	15.549	−10627	2.168	0.054	0.269
0.300	−17495	−6392	11.411	−7755	1.401	0.115	0.383
0.400	−12579	−4349	8.458	−5166	0.839	0.211	0.528
0.500	−8652	−2605	6.214	−3044	0.451	0.343	0.686
0.600	−5621	−1290	4.451	−1489	0.204	0.499	0.832
0.700	−3402	−450	3.033	−516	0.067	0.657	0.938
0.800	−1864	−50	1.864	−59	0.009	0.794	0.993
0.900	−817	32	0.873	35	−0.003	0.904	1.004
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Sb(liquid)

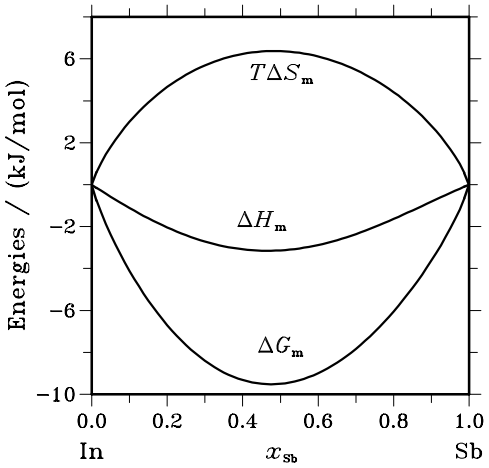

Fig. 4. Integral quantities of the liquid phase at T=973 K.

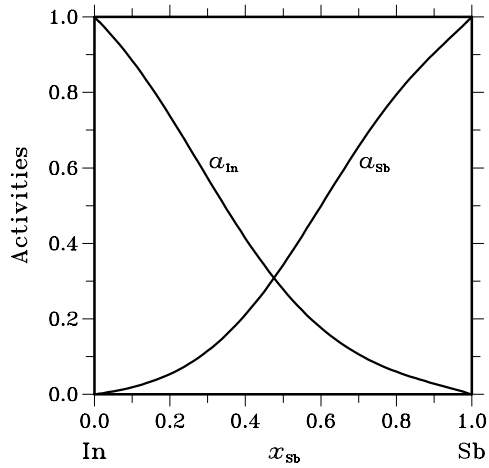

Fig. 5. Activities in the liquid phase at T=973 K.

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

Compound	x_{Sb}	$\Delta_{\mathrm{f}}G^{\circ}$ / (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))
$\mathrm{In_1Sb_1}$	0.500	−13564	−16235	−8.957	−1.294

References

[89Sha] R.C. Sharma, T.L. Ngai, Y.A. Chang: Bull. Alloy Phase Diagrams **10** (1989) 657–664.

[94Ans] I. Ansara, C. Chatillon, H.L. Lukas, T. Nishizawa, H. Ohtani, K. Ishida, M. Hillert, B. Sundman, B.B. Argent, A. Watson, T.G. Chart, T. Anderson: Calphad **18** (1994) 177–222.