P – Sb (Phosphorus – Antimony)

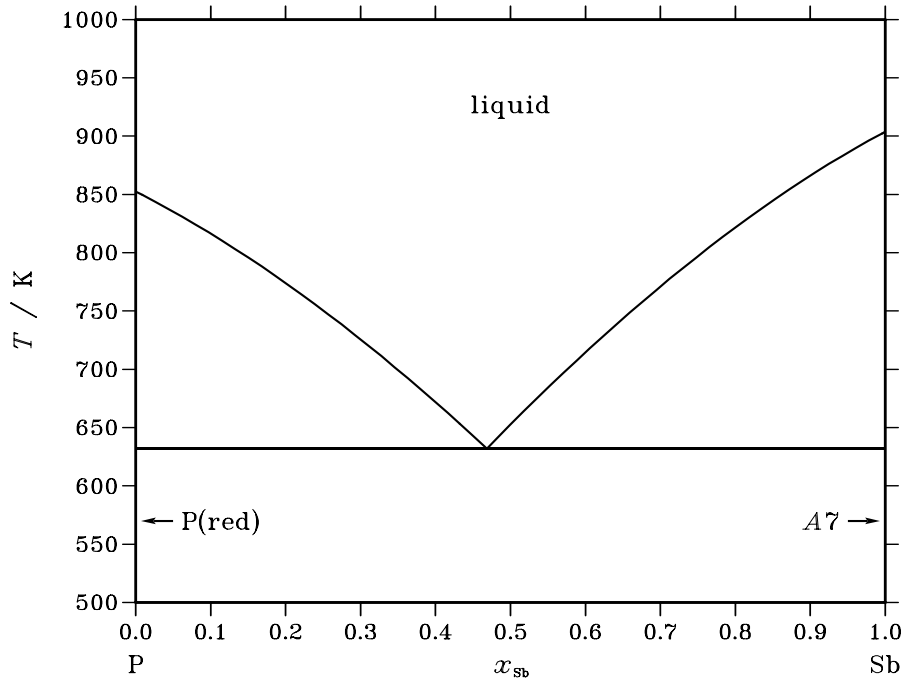

Fig. 1. Calculated phase diagram for the system P-Sb (constrained system).

The P-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 assessment of Ansara *et al.* [94Ans] has been accepted here. The phase diagram of the P-Sb system is simply eutectic with a liquid composition of 46.8 at.% Sb at 623 K. The only reported experimental data is the liquid=gas+$A7$ invariant reaction at 885 K [52Vog] which is in good agreement with the calculated temperature of 889 K in the present assessment.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(P,Sb)_1$
P(red)	···	···	···	···	P_RED	P_1
αP	···	αP	$c*$*	···	P_WHITE	P_1
$A7$	$A7$	αAs	$hR2$	$R\overline{3}m$	RHOMBO_A7	Sb_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Sb}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ P(red) + $A7$	eutectic	632.0	0.468	0.000	1.000	−17575

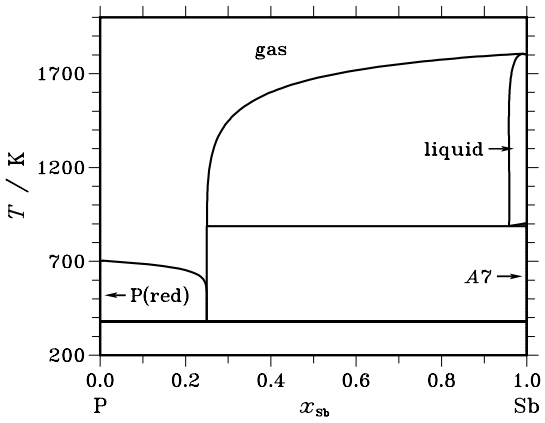

Fig. 2. Calculated phase diagram at 0.1 MPa.

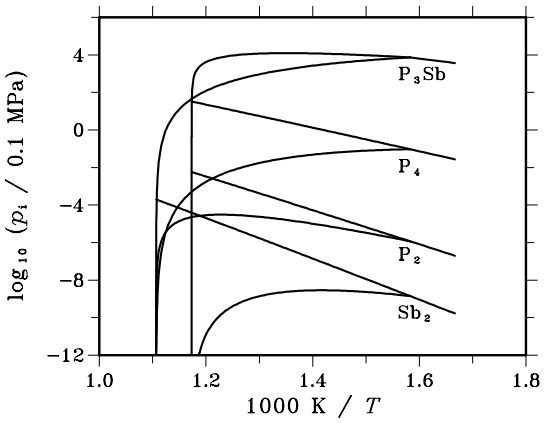

Fig. 3. Calculated partial pressures of gaseous species in the phase equilibria of the constrained system.

Table IIIa. Integral quantities for the liquid phase at 950 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	−3198	−630	2.703	−630	0.000	0.000
0.200	−5073	−1120	4.161	−1120	0.000	0.000
0.300	−6295	−1470	5.079	−1470	0.000	0.000
0.400	−6996	−1680	5.596	−1680	0.000	0.000
0.500	−7225	−1750	5.763	−1750	0.000	0.000
0.600	−6996	−1680	5.596	−1680	0.000	0.000
0.700	−6295	−1470	5.079	−1470	0.000	0.000
0.800	−5073	−1120	4.161	−1120	0.000	0.000
0.900	−3198	−630	2.703	−630	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for P in the liquid phase at 950 K.

x_{P}	ΔG_{P} [J/mol]	ΔH_{P} [J/mol]	ΔS_{P} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{P}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{P}}$ [J/(mol·K)]	a_{P}	γ_{P}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−902	−70	0.876	−70	0.000	0.892	0.991
0.800	−2043	−280	1.855	−280	0.000	0.772	0.965
0.700	−3447	−630	2.966	−630	0.000	0.646	0.923
0.600	−5155	−1120	4.247	−1120	0.000	0.521	0.868
0.500	−7225	−1750	5.763	−1750	0.000	0.401	0.801
0.400	−9758	−2520	7.619	−2520	0.000	0.291	0.727
0.300	−12940	−3430	10.010	−3430	0.000	0.194	0.648
0.200	−17193	−4480	13.382	−4480	0.000	0.113	0.567
0.100	−23858	−5670	19.145	−5670	0.000	0.049	0.488
0.000	$-\infty$	−7000	∞	−7000	0.000	0.000	0.412

Reference state: P(liquid)

Table IIIc. Partial quantities for Sb in the liquid phase at 950 K.

x_{Sb}	ΔG_{Sb} [J/mol]	ΔH_{Sb} [J/mol]	ΔS_{Sb} [J/(mol·K)]	G^E_{Sb} [J/mol]	S^E_{Sb} [J/(mol·K)]	a_{Sb}	γ_{Sb}
0.000	$-\infty$	−7000	∞	−7000	0.000	0.000	0.412
0.100	−23858	−5670	19.145	−5670	0.000	0.049	0.488
0.200	−17193	−4480	13.382	−4480	0.000	0.113	0.567
0.300	−12940	−3430	10.010	−3430	0.000	0.194	0.648
0.400	−9758	−2520	7.619	−2520	0.000	0.291	0.727
0.500	−7225	−1750	5.763	−1750	0.000	0.401	0.801
0.600	−5155	−1120	4.247	−1120	0.000	0.521	0.868
0.700	−3447	−630	2.966	−630	0.000	0.646	0.923
0.800	−2043	−280	1.855	−280	0.000	0.772	0.965
0.900	−902	−70	0.876	−70	0.000	0.892	0.991
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Sb(liquid)

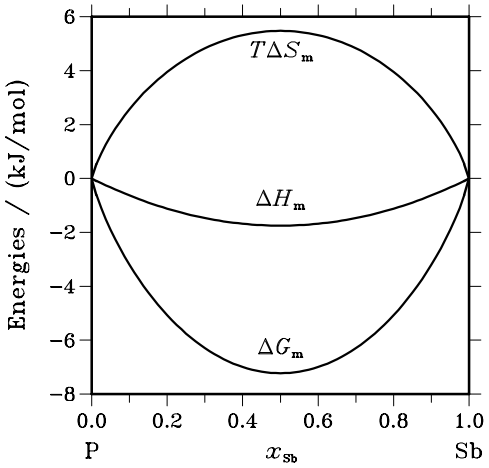

Fig. 4. Integral quantities of the liquid phase at T=950 K.

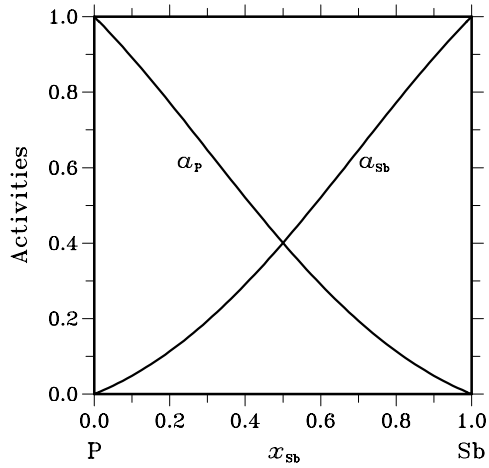

Fig. 5. Activities in the liquid phase at T=950 K.

References

[52Vog] R. Vogel, D. Horstmann: Arch. Eisenhüttenwes. **23** (1952) 127–128.

[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.