In – P (Indium – Phosphorus)

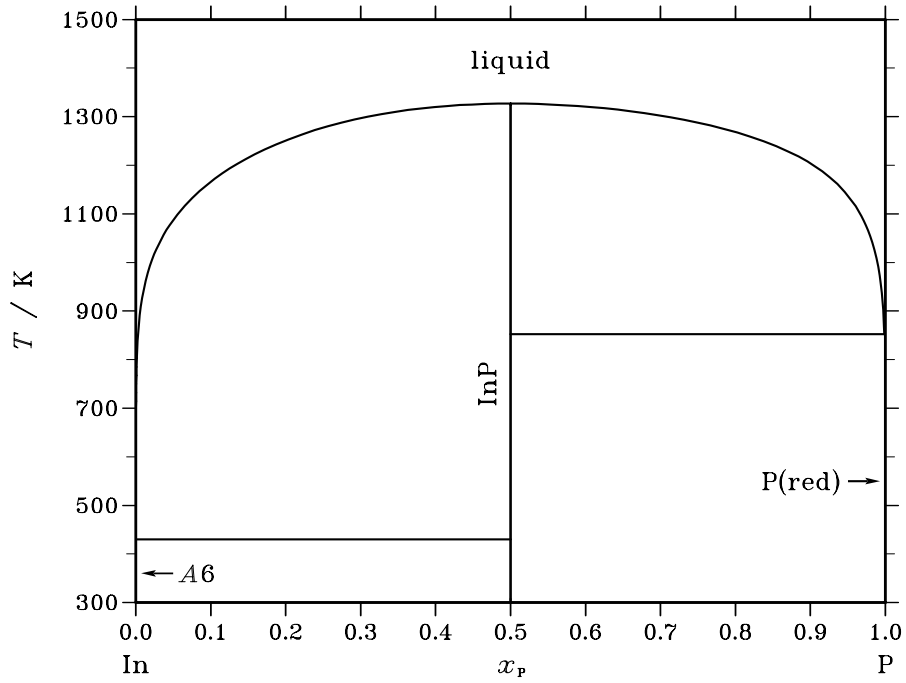

Fig. 1. Calculated phase diagram for the system In-P (constrained system).

The In-P 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-P system is very simple featuring a near stoichiometric compound InP which melts congruently at 1327 K, a complete miscibility in the liquid phase and negligible solubility of In in solid red P and of P in crystalline In. The eutectics on either side are both degenerate and close to the pure elements. The thermodynamic assessment by Ansara *et al.* [94Ans] is based on an extensive literature overview published by Tmar *et al.* [84Tma]. The calculated phase diagram is in good agreement with the experimental data.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(In,P)_1$
$A6$	$A6$	In	$tI2$	$I4/mmm$	BCT_A6	In_1
InP	$B3$	ZnS	$cF8$	$F\bar{4}3m$	FCC_B3	In_1P_1
P(red)	···	···	···	···	P_RED	P_1
αP	···	αP	$c*^*$	···	P_WHITE	P_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_P			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ InP	congruent	1327.0	0.500	0.500		−43751
liquid $\rightleftharpoons$ InP + P(red)	eutectic	852.4	0.999	0.500	1.000	−18627
liquid $\rightleftharpoons$ $A6$ + InP	degenerate	429.8	0.000	0.000	0.500	−3283

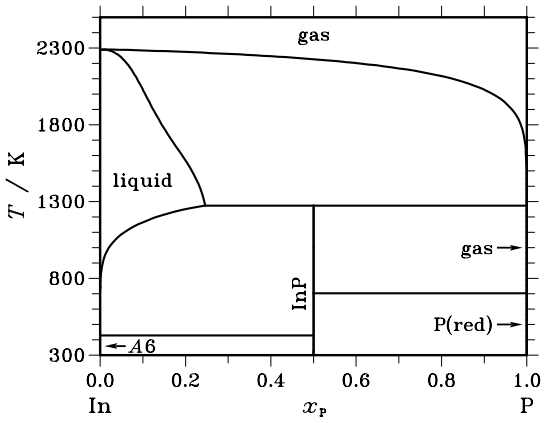

Fig. 2. Calculated phase diagram at 0.1 MPa.

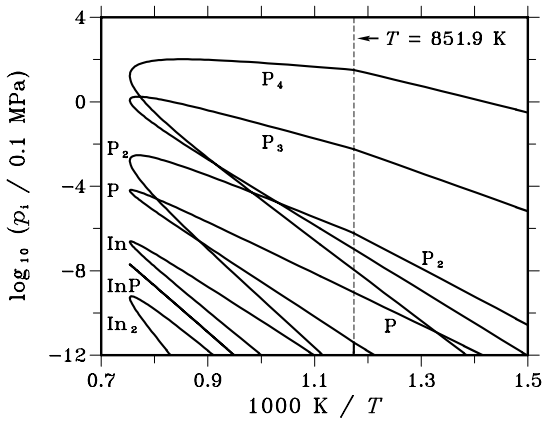

Fig. 3. Calculated partial pressures of gaseous species in the phase equilibria of the constrained system.

Table IIIa. Integral quantities for the liquid phase at 1350 K.

x_P	ΔG_m [J/mol]	ΔH_m [J/mol]	ΔS_m [J/(mol·K)]	G^E_m [J/mol]	S^E_m [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−3823	1062	3.619	−174	0.916	0.000
0.200	−5834	1981	5.789	−217	1.629	0.000
0.300	−7020	2722	7.217	−163	2.138	0.000
0.400	−7602	3251	8.039	−48	2.443	0.000
0.500	−7685	3531	8.308	96	2.545	0.000
0.600	−7323	3529	8.039	231	2.443	0.000
0.700	−6533	3210	7.217	324	2.138	0.000
0.800	−5277	2538	5.789	340	1.629	0.000
0.900	−3406	1480	3.619	243	0.916	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for In in the liquid phase at 1350 K.

x_In	ΔG_In [J/mol]	ΔH_In [J/mol]	ΔS_In [J/(mol·K)]	G^E_In [J/mol]	S^E_In [J/(mol·K)]	a_In	γ_In
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1254	66	0.978	−72	0.102	0.894	0.994
0.800	−2745	310	2.263	−240	0.407	0.783	0.979
0.700	−4439	801	3.882	−435	0.916	0.673	0.962
0.600	−6322	1610	5.876	−588	1.629	0.569	0.949
0.500	−8410	2806	8.308	−629	2.545	0.473	0.945
0.400	−10774	4458	11.283	−489	3.665	0.383	0.957
0.300	−13611	6637	14.998	−97	4.988	0.297	0.991
0.200	−17450	9411	19.896	616	6.515	0.211	1.056
0.100	−24127	12850	27.390	1719	8.245	0.117	1.165
0.000	$-\infty$	17024	∞	3282	10.179	0.000	1.340

Reference state: In(liquid)

Table IIIc. Partial quantities for P in the liquid phase at 1350 K.

x_{P}	ΔG_{P} [J/mol]	ΔH_{P} [J/mol]	ΔS_{P} [J/(mol·K)]	$G_{\mathrm{P}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{P}}^{\mathrm{E}}$ [J/(mol·K)]	a_{P}	γ_{P}
0.000	$-\infty$	11224	∞	−2518	10.179	0.000	0.799
0.100	−26946	10031	27.390	−1100	8.245	0.091	0.907
0.200	−18192	8668	19.896	−127	6.515	0.198	0.989
0.300	−13043	7205	14.998	471	4.988	0.313	1.043
0.400	−9521	5711	11.283	764	3.665	0.428	1.070
0.500	−6960	4256	8.308	821	2.545	0.538	1.076
0.600	−5023	2909	5.876	711	1.629	0.639	1.065
0.700	−3499	1741	3.882	504	0.916	0.732	1.046
0.800	−2234	820	2.263	270	0.407	0.820	1.024
0.900	−1103	217	0.978	79	0.102	0.906	1.007
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: P(liquid)

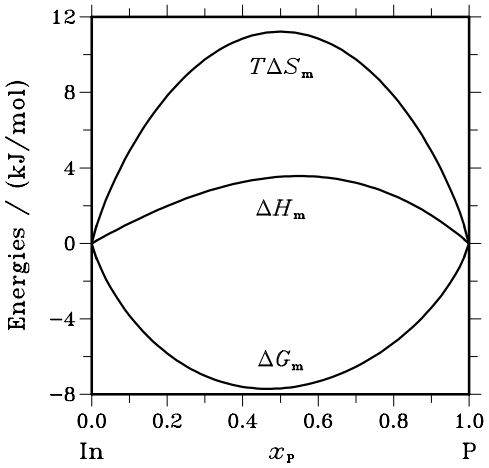

Fig. 4. Integral quantities of the liquid phase at T=1350 K.

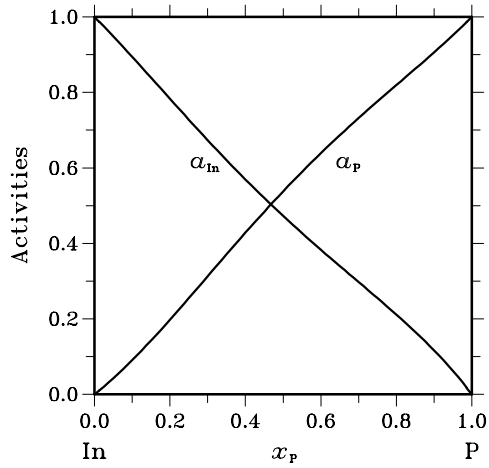

Fig. 5. Activities in the liquid phase at T=1350 K.

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

Compound	x_{P}	$\Delta_{\mathrm{f}}G^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}H^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}S^{\circ}$ / (J/(mol·K))	$\Delta_{\mathrm{f}}C_P^{\circ}$ / (J/(mol·K))
In_1P_1	0.500	−32053	−37244	−17.410	−2.269

References

[84Tma] M. Tmar, A. Gabriel, C. Chatillon, I. Ansara: J. Cryst. Growth **68** (1984) 557–580.

[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.