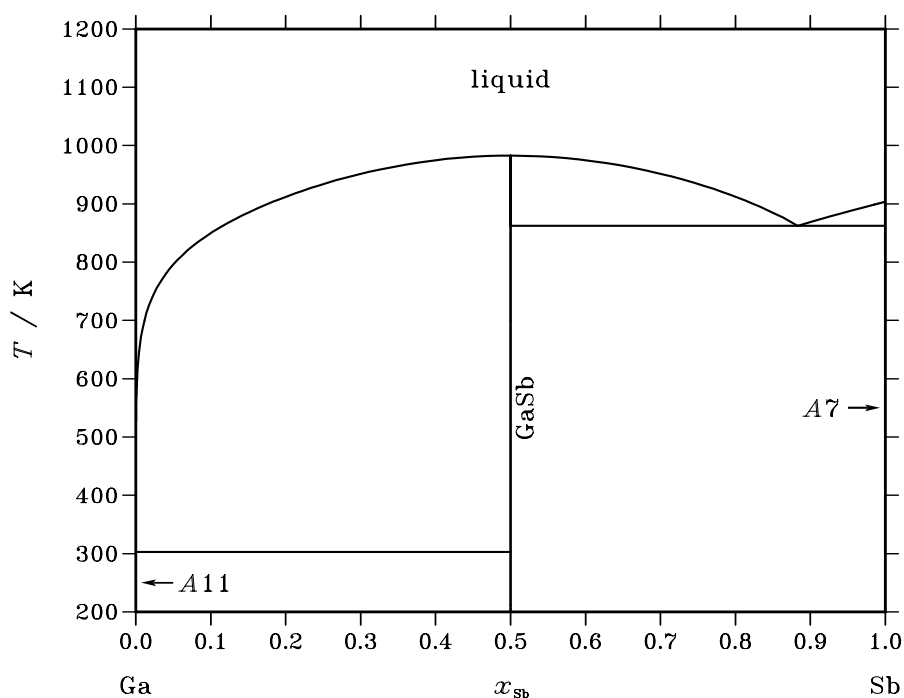


Ga – Sb (Gallium – Antimony)**Fig. 1.** Calculated phase diagram for the system Ga-Sb (constrained system).

The Ga-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 Ga-Sb system is very simple featuring a near stoichiometric compound GaSb which melts congruently at 982.6 K, a complete miscibility in the liquid phase and negligible mutual solubility of Ga and Sb in the crystalline phases. The assessed dataset reported in [94Ans] is based on a compilation of experimental data from the literature which has been reviewed in [85Ase]. The optimization takes account of data for the liquidus, enthalpies of mixing in the liquid and activities of Ga.

Table I. Phases, structures and models.

| Phase | Strukturbericht | Prototype | Pearson symbol | Space group | SGTE name | Model |
|--------|-----------------|-------------|----------------|----------------------|-------------------|---------------------------------|
| liquid | | | | | LIQUID | (Ga,Sb) ₁ |
| A11 | A11 | α Ga | <i>oC</i> 8 | <i>Cmca</i> | ORTHORHOMBIC_CMCA | Ga ₁ |
| GaSb | B3 | ZnS | <i>cF</i> 8 | <i>F</i> $\bar{4}3m$ | ZINCBLLENDE_B3 | Ga ₁ Sb ₁ |
| A7 | A7 | α As | <i>hR</i> 2 | <i>R</i> $\bar{3}m$ | RHOMBOHEDRAL_A7 | Sb ₁ |

Table II. Invariant reactions.

| Reaction | Type | T / K | Compositions / x_{Sb} | | | $\Delta_r H / (J/mol)$ |
|--|------------|---------|-------------------------|-------|-------|------------------------|
| liquid \rightleftharpoons GaSb | congruent | 982.6 | 0.500 | 0.500 | | –34710 |
| liquid \rightleftharpoons GaSb + A7 | eutectic | 862.1 | 0.883 | 0.500 | 1.000 | –22990 |
| liquid \rightleftharpoons A11 + GaSb | degenerate | 302.9 | 0.000 | 0.000 | 0.500 | –5590 |

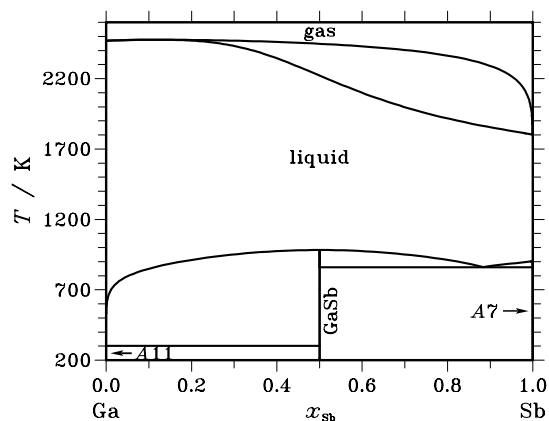


Fig. 2. Calculated phase diagram at 0.1 MPa.

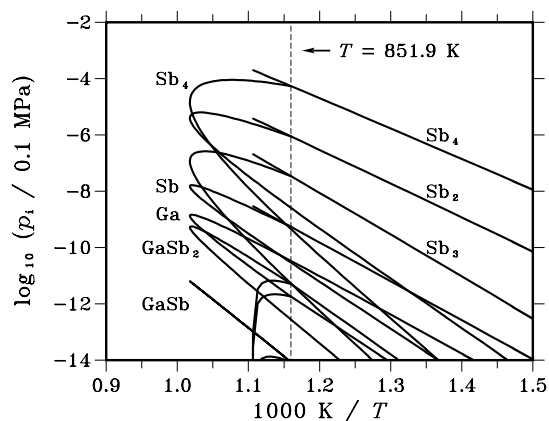


Fig. 3. Calculated partial pressures of gaseous species in the phase equilibria of the constrained system.

Table IIIa. Integral quantities for the liquid phase at 1023 K.

| x_{Sb} | ΔG_{m} [J/mol] | ΔH_{m} [J/mol] | ΔS_{m} [J/(mol·K)] | G_{m}^{E} [J/mol] | S_{m}^{E} [J/(mol·K)] | ΔC_P [J/(mol·K)] |
|-----------------|----------------------------------|----------------------------------|--------------------------------------|--------------------------------------|--|-----------------------------|
| 0.000 | 0 | 0 | 0.000 | 0 | 0.000 | 0.000 |
| 0.100 | −3512 | −123 | 3.313 | −747 | 0.610 | 0.866 |
| 0.200 | −5672 | −369 | 5.184 | −1416 | 1.023 | 1.540 |
| 0.300 | −7133 | −647 | 6.341 | −1938 | 1.262 | 2.021 |
| 0.400 | −7988 | −883 | 6.945 | −2264 | 1.350 | 2.310 |
| 0.500 | −8263 | −1027 | 7.073 | −2367 | 1.310 | 2.406 |
| 0.600 | −7964 | −1048 | 6.760 | −2240 | 1.165 | 2.310 |
| 0.700 | −7092 | −936 | 6.017 | −1896 | 0.938 | 2.021 |
| 0.800 | −5625 | −700 | 4.814 | −1369 | 0.653 | 1.540 |
| 0.900 | −3477 | −371 | 3.036 | −712 | 0.333 | 0.866 |
| 1.000 | 0 | 0 | 0.000 | 0 | 0.000 | 0.000 |

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

Table IIIb. Partial quantities for Ga in the liquid phase at 1023 K.

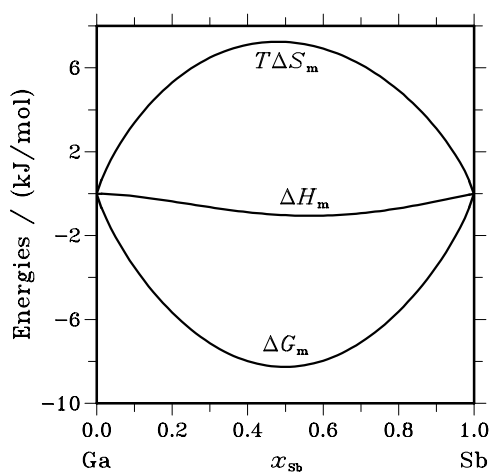
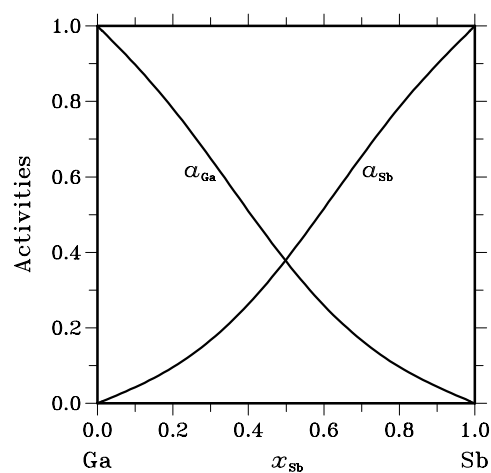
| x_{Ga} | ΔG_{Ga} [J/mol] | ΔH_{Ga} [J/mol] | ΔS_{Ga} [J/(mol·K)] | G_{Ga}^{E} [J/mol] | S_{Ga}^{E} [J/(mol·K)] | a_{Ga} | γ_{Ga} |
|-----------------|-----------------------------------|-----------------------------------|---------------------------------------|---------------------------------------|---|-----------------|----------------------|
| 1.000 | 0 | 0 | 0.000 | 0 | 0.000 | 1.000 | 1.000 |
| 0.900 | −922 | 79 | 0.978 | −26 | 0.102 | 0.897 | 0.997 |
| 0.800 | −2104 | 181 | 2.234 | −206 | 0.379 | 0.781 | 0.976 |
| 0.700 | −3681 | 154 | 3.749 | −647 | 0.783 | 0.649 | 0.927 |
| 0.600 | −5738 | −94 | 5.517 | −1393 | 1.269 | 0.509 | 0.849 |
| 0.500 | −8325 | −597 | 7.554 | −2429 | 1.791 | 0.376 | 0.752 |
| 0.400 | −11470 | −1322 | 9.920 | −3676 | 2.302 | 0.260 | 0.649 |
| 0.300 | −15238 | −2178 | 12.766 | −4997 | 2.755 | 0.167 | 0.556 |
| 0.200 | −19881 | −3014 | 16.487 | −6191 | 3.106 | 0.097 | 0.483 |
| 0.100 | −26582 | −3614 | 22.452 | −6997 | 3.307 | 0.044 | 0.439 |
| 0.000 | −∞ | −3704 | ∞ | −7092 | 3.312 | 0.000 | 0.434 |

Reference state: Ga(liquid)

Table IIIc. Partial quantities for Sb in the liquid phase at 1023 K.

| x_{Sb} | ΔG_{Sb} [J/mol] | ΔH_{Sb} [J/mol] | ΔS_{Sb} [J/(mol·K)] | G_{Sb}^{E} [J/mol] | S_{Sb}^{E} [J/(mol·K)] | a_{Sb} | γ_{Sb} |
|-----------------|-----------------------------------|-----------------------------------|---------------------------------------|---------------------------------------|---|-----------------|----------------------|
| 0.000 | $-\infty$ | –258 | ∞ | –7587 | 7.164 | 0.000 | 0.410 |
| 0.100 | –26823 | –1940 | 24.324 | –7237 | 5.179 | 0.043 | 0.427 |
| 0.200 | –19944 | –2573 | 16.981 | –6255 | 3.599 | 0.096 | 0.479 |
| 0.300 | –15189 | –2516 | 12.388 | –4949 | 2.378 | 0.168 | 0.559 |
| 0.400 | –11363 | –2066 | 9.088 | –3570 | 1.470 | 0.263 | 0.657 |
| 0.500 | –8201 | –1458 | 6.591 | –2305 | 0.828 | 0.381 | 0.763 |
| 0.600 | –5627 | –866 | 4.654 | –1282 | 0.407 | 0.516 | 0.860 |
| 0.700 | –3601 | –404 | 3.125 | –567 | 0.159 | 0.655 | 0.936 |
| 0.800 | –2061 | –122 | 1.895 | –163 | 0.040 | 0.785 | 0.981 |
| 0.900 | –910 | –11 | 0.878 | –13 | 0.002 | 0.899 | 0.998 |
| 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 $T=1023$ K.**Fig. 5.** Activities in the liquid phase at $T=1023$ 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)) |
|---------------------------------|-----------------|------------------------------|------------------------------|----------------------------------|------------------------------------|
| Ga ₁ Sb ₁ | 0.500 | –20428 | –22418 | –6.677 | –1.871 |

References

- [85Ase] T. Aselage, K.-M. Chang, T. Anderson: Calphad **9** (1985) 227–256.
 [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.