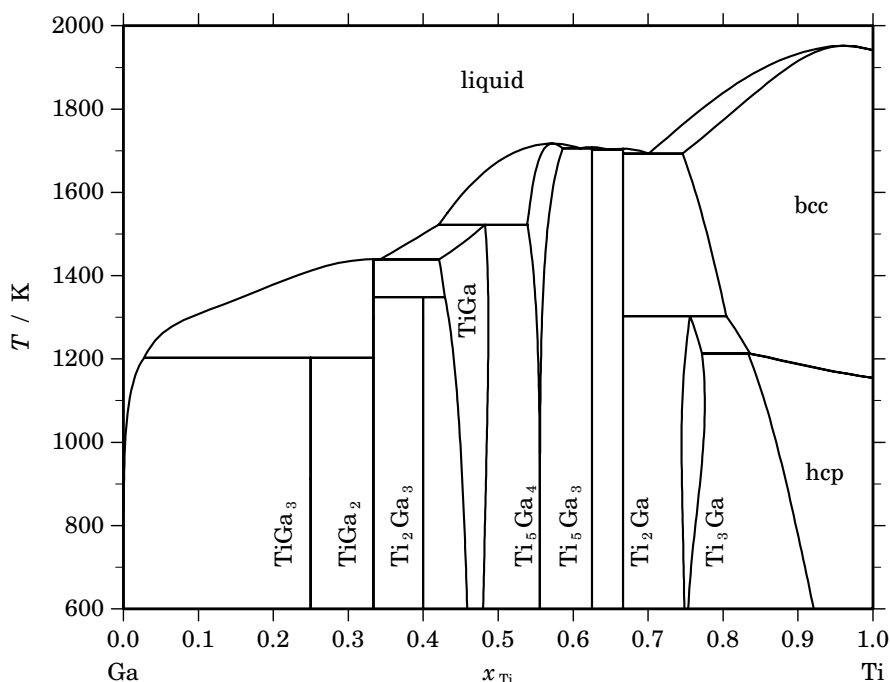


Ga – Ti (Gallium – Titanium)**Fig. 1.** Calculated phase diagram for the system Ga-Ti.

A review and a thermodynamically optimised dataset for the complete Ga-Ti system has been given by Li *et al.* [2003Li]. In a previous overview by Murray [1985Mur] a phase diagram has been assessed only for the Ti-rich part of the phase diagram because at that time only one experimental investigation [1962Pot] on almost the complete composition range of the phase diagram has been available but various questions remained open in that report. This investigation, a 2nd extended study of the phase diagram from the literature [2001Ant] and other partial evaluations of the phase diagram as well as additional own experiments have been used in [2003Li] to establish a complete phase diagram and an optimised thermodynamic dataset for the Ga-Ti system. The mixing enthalpy in the liquid has been measured by [1974Esi], however the calculated curve from the evaluated dataset shows significant deviations. The partial enthalpies of solution for Ti in Ga-rich melts [1985Nik] are in good agreement with the calculation within the experimental scatter. The experimental chemical potential differences between Ga and Ti in bcc alloys reported by [1973Geg] are in good agreement with the calculation. Except for the standard enthalpy of formation of GaTi_2 [1999Mes] no other thermodynamic data for the intermetallic compounds have been available. In order to estimate the respective values of the other compounds Li *et al.* [2003Li] used enthalpies of formation for Ti-Al alloys from the literature as a guide.

Table I. Phases, structures and models.

Phase	Struktur- bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	(Ga,Ti) ₁
A11	A11	α Ga	<i>oC8</i>	<i>Cmca</i>	ORTHORHOMBIC_CMCA	Ga ₁
TiGa ₃	<i>D0₂₂</i>	TiAl ₃	<i>tI8</i>	<i>I4/mmm</i>	TIGA3	Ti ₁ Ga ₃
TiGa ₂	...	HfGa ₂	<i>t*[*]</i>	...	TIGA2	Ti ₁ Ga ₂
Ti ₂ Ga ₃	...	Ti ₂ Ga ₃	<i>tP10</i>	<i>P4/m</i>	TI2GA3	Ti ₂ Ga ₃
TiGa	<i>L1₀</i>	AuCu	<i>tP4</i>	<i>P4/mmm</i>	TIGA	(Ga,Ti) ₁ (Ga,Ti) ₁
Ti ₅ Ga ₄	...	Ti ₅ Ga ₄	<i>hP18</i>	<i>P6₃/mcm</i>	TI5GA4	(Ga,Ti) ₅ (Ga,Ti) ₄
Ti ₅ Ga ₃	<i>D8_m</i>	W ₅ Si ₃	<i>tI32</i>	<i>I4/mcm</i>	TI5GA3	Ti ₅ Ga ₃
Ti ₂ Ga	<i>B8₂</i>	Ni ₂ In	<i>hP6</i>	<i>P6₃/mmc</i>	TI2GA	Ti ₂ Ga ₁
Ti ₃ Ga	<i>D0₁₉</i>	Ni ₃ Sn	<i>hP8</i>	<i>P6₃/mmc</i>	TI3GA	(Ga,Ti) ₃ (Ga,Ti) ₁
bcc	<i>A2</i>	W	<i>cI2</i>	<i>Im$\bar{3}m$</i>	BCC_A2	(Ga,Ti) ₁
hcp	<i>A3</i>	Ti	<i>hP2</i>	<i>P6₃/mmc</i>	HCP_A3	(Ga,Ti) ₁

Table II. Invariant reactions.

Reaction	Type	<i>T</i> / K	Compositions / <i>x</i> _{Ti}			$\Delta_r H$ / (J/mol)
liquid \rightleftharpoons bcc	congruent	1952.3	0.962	0.962		–13998
liquid \rightleftharpoons Ti ₅ Ga ₄	congruent	1401.2	0.794	0.794		–5211
liquid \rightleftharpoons Ti ₅ Ga ₃	congruent	1708.6	0.625	0.625		–16906
liquid \rightleftharpoons Ti ₅ Ga ₄ + Ti ₅ Ga ₃	eutectic	1706.1	0.609	0.586	0.625	–15396
liquid \rightleftharpoons Ti ₂ Ga	congruent	1704.8	0.667	0.667		–17888
liquid \rightleftharpoons Ti ₅ Ga ₃ + Ti ₂ Ga	eutectic	1702.0	0.650	0.625	0.667	–17414
liquid \rightleftharpoons Ti ₂ Ga + bcc	eutectic	1693.2	0.701	0.667	0.746	–14630
liquid + Ti ₅ Ga ₄ \rightleftharpoons TiGa	peritectic	1522.2	0.421	0.539	0.482	–9722
liquid \rightleftharpoons TiGa ₂	congruent	1439.7	0.333	0.333		–22280
liquid \rightleftharpoons TiGa ₂ + TiGa	eutectic	1439.3	0.343	0.333	0.421	–21733
TiGa ₂ + TiGa \rightleftharpoons Ti ₂ Ga ₃	peritectoid	1348.0	0.333	0.429	0.400	–408
Ti ₂ Ga + bcc \rightleftharpoons Ti ₃ Ga	peritectoid	1303.1	0.667	0.804	0.756	–4499
Ti ₃ Ga + bcc \rightleftharpoons hcp	peritectoid	1213.2	0.772	0.836	0.833	–1823
liquid + TiGa ₂ \rightleftharpoons TiGa ₃	peritectic	1203.1	0.028	0.333	0.250	–7164
liquid \rightleftharpoons A11 + TiGa ₃	eutectic	302.9	0.000	0.000	0.250	–5590

Table IIIa. Integral quantities for the liquid phase at 2000 K.

x_{Ti}	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	–6656	–7793	–0.569	–1250	–3.271	0.000
0.200	–11774	–15923	–2.074	–3453	–6.235	0.000
0.300	–16000	–23309	–3.655	–5842	–8.734	0.000
0.400	–19017	–29045	–5.014	–7826	–10.610	0.000
0.500	–20513	–32400	–5.944	–8986	–11.707	0.000
0.600	–20272	–32815	–6.271	–9080	–11.867	0.000
0.700	–18195	–29905	–5.855	–8037	–10.934	0.000
0.800	–14283	–23461	–4.589	–5962	–8.750	0.000
0.900	–8538	–13447	–2.455	–3132	–5.157	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Ga in the liquid phase at 2000 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	–1134	363	0.748	618	–0.128	0.934	1.038
0.800	–2346	–76	1.135	1365	–0.721	0.868	1.086
0.700	–4961	–3216	0.873	970	–2.093	0.742	1.060
0.600	–9811	–10433	–0.311	–1316	–4.559	0.554	0.924
0.500	–17246	–22585	–2.669	–5719	–8.433	0.354	0.709
0.400	–27182	–40003	–6.410	–11945	–14.029	0.195	0.488
0.300	–39195	–62498	–11.651	–19175	–21.662	0.095	0.316
0.200	–52833	–89362	–18.264	–26070	–31.646	0.042	0.209
0.100	–69058	–119359	–25.151	–30768	–44.295	0.016	0.157
0.000	–∞	–150737	∞	–30888	–59.925	0.000	0.156

Reference state: Ga(liquid)

Table IIIc. Partial quantities for Ti in the liquid phase at 2000 K.

x_{Ti}	ΔG_{Ti} [J/mol]	ΔH_{Ti} [J/mol]	ΔS_{Ti} [J/(mol·K)]	G_{Ti}^{E} [J/mol]	S_{Ti}^{E} [J/(mol·K)]	a_{Ti}	γ_{Ti}
0.000	–∞	–72213	∞	–4753	–33.730	0.000	0.751
0.100	–56357	–81197	–12.420	–18067	–31.565	0.034	0.337
0.200	–49488	–79311	–14.911	–22724	–28.293	0.051	0.255
0.300	–41757	–70194	–14.219	–21736	–24.229	0.081	0.271
0.400	–32827	–56964	–12.068	–17590	–19.687	0.139	0.347
0.500	–23780	–42215	–9.218	–12253	–14.981	0.239	0.479
0.600	–15665	–28023	–6.179	–7170	–10.426	0.390	0.650
0.700	–9195	–15936	–3.371	–3264	–6.336	0.575	0.822
0.800	–4645	–6986	–1.170	–935	–3.026	0.756	0.945
0.900	–1813	–1679	0.067	–61	–0.809	0.897	0.996
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(liquid)

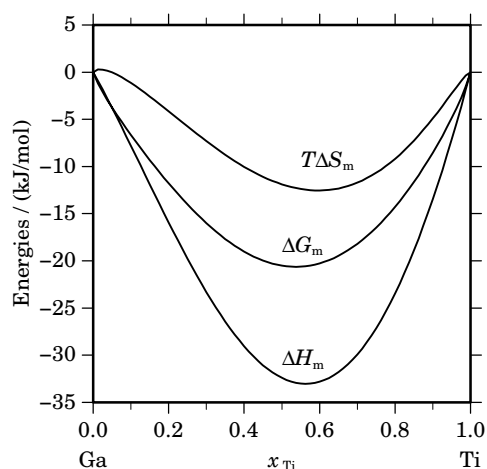


Fig. 2. Integral quantities of the liquid phase at $T=2000$ K.

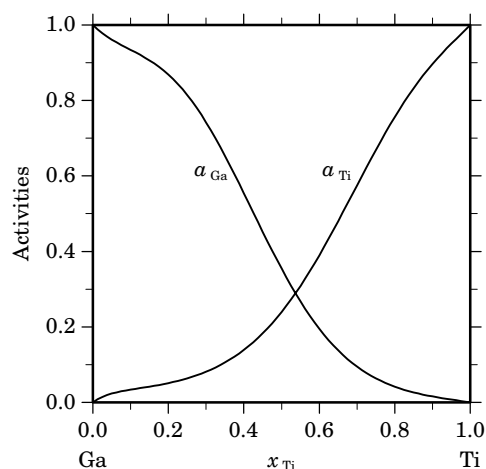


Fig. 3. Activities in the liquid phase at $T=2000$ K.

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

Compound	x_{Ti}	$\Delta_f G^\circ$ / (J/mol)	$\Delta_f H^\circ$ / (J/mol)	$\Delta_f S^\circ$ / (J/(mol·K))	$\Delta_f C_P^\circ$ / (J/(mol·K))
Ti ₁ Ga ₃	0.250	−33809	−35130	−4.429	0.000
Ti ₁ Ga ₂	0.333	−38427	−39867	−4.827	0.000
Ti ₂ Ga ₃	0.400	−38795	−40064	−4.257	0.000
Ti ₅ Ga ₄	0.556	−38491	−39500	−3.384	0.000
Ti ₅ Ga ₃	0.625	−37787	−39125	−4.487	0.000
Ti ₂ Ga ₁	0.667	−37056	−38667	−5.403	0.000
Ti ₃ Ga	0.750	−32028	−34127	−7.040	0.000

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