Hf – Ti (Hafnium – Titanium)

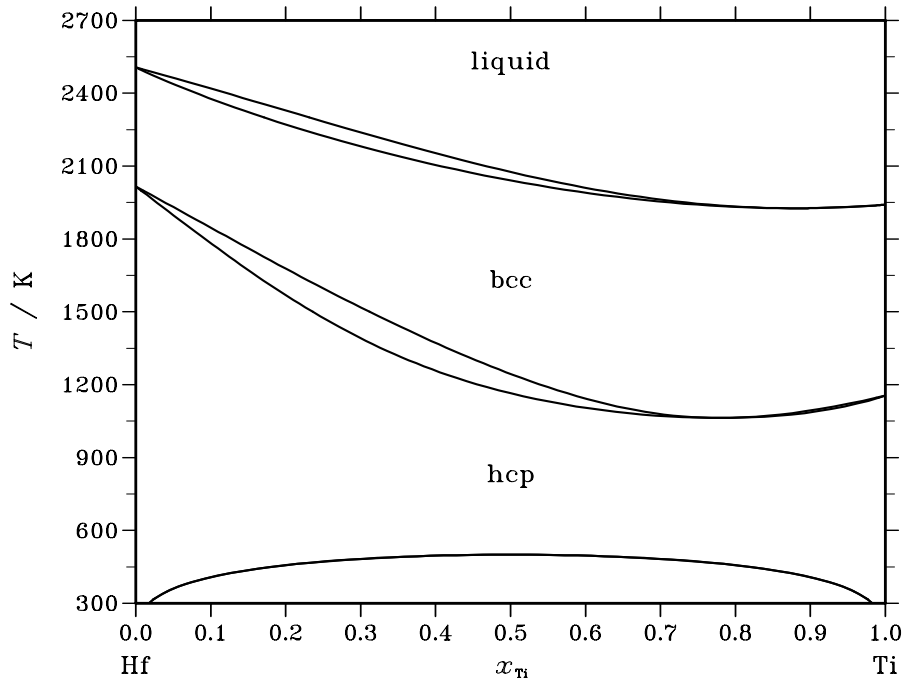

Fig. 1. Calculated phase diagram for the system Hf-Ti.

The thermodynamic description of Hf-Ti by Bittermann and Rogl [97Bit] is based on the critical assessment of all the available experimental data for this system. All solution phases have been described with a simple substitutional model. Both Hf and Ti have low-temperature (hcp) and high-temperature (bcc) modifications which form continuous solid solutions. The two phase field liquid/bcc is very narrow. It shows a minimum at about 15 at.% Hf and 1923 K [57Hay, 60Tho, 66Cha, 69Rud]. All experimental data on this congruent point are in reasonable agreement except for the measurements of Tylkina [59Tyl], who found a transition temperature of 1873 K. The hcp/bcc phase boundaries show the same trend as the liquid/bcc boundaries. Several experimental studies [57Hay, 59Tyl, 62Img, 66Cha, 75Rud] agree on a congruent transformation hcp/bcc at about 20 at.% Hf and 1073 K. The known phase boundaries are well reproduced by the calculations.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Hf,Ti)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Hf,Ti)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Hf,Ti)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ti}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ bcc	congruent	1926.3	0.880	0.880		−14183
bcc $\rightleftharpoons$ hcp	congruent	1063.3	0.780	0.780		−4210
hcp $\rightleftharpoons$ hcp′ + hcp″	critical	500.4	0.500	0.500	0.500	0

Table IIIa. Integral quantities for the liquid phase at 2600 K.

x_{Ti}	ΔG_{m} [J/mol]	ΔH_{m} [J/mol]	ΔS_{m} [J/(mol·K)]	$G_{\mathrm{m}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{m}}^{\mathrm{E}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−9139	−449	3.342	−2112	0.639	0.000
0.200	−14571	−799	5.297	−3754	1.137	0.000
0.300	−18133	−1049	6.571	−4927	1.492	0.000
0.400	−20180	−1198	7.301	−5631	1.705	0.000
0.500	−20850	−1248	7.539	−5865	1.776	0.000
0.600	−20180	−1198	7.301	−5631	1.705	0.000
0.700	−18133	−1049	6.571	−4927	1.492	0.000
0.800	−14571	−799	5.297	−3754	1.137	0.000
0.900	−9139	−449	3.342	−2112	0.639	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Hf in the liquid phase at 2600 K.

x_{Hf}	ΔG_{Hf} [J/mol]	ΔH_{Hf} [J/mol]	ΔS_{Hf} [J/(mol·K)]	$G_{\mathrm{Hf}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Hf}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Hf}	γ_{Hf}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2512	−50	0.947	−235	0.071	0.890	0.989
0.800	−5762	−200	2.139	−938	0.284	0.766	0.958
0.700	−9822	−449	3.605	−2112	0.639	0.635	0.907
0.600	−14797	−799	5.384	−3754	1.137	0.504	0.841
0.500	−20850	−1248	7.539	−5865	1.776	0.381	0.762
0.400	−28254	−1798	10.176	−8446	2.557	0.271	0.677
0.300	−37523	−2447	13.491	−11496	3.481	0.176	0.588
0.200	−49808	−3196	17.928	−15016	4.546	0.100	0.499
0.100	−68781	−4045	24.898	−19004	5.754	0.042	0.415
0.000	$-\infty$	−4994	∞	−23462	7.103	0.000	0.338

Reference state: Hf(liquid)

Table IIIc. Partial quantities for Ti in the liquid phase at 2600 K.

x_{Ti}	ΔG_{Ti} [J/mol]	ΔH_{Ti} [J/mol]	ΔS_{Ti} [J/(mol·K)]	$G_{\mathrm{Ti}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Ti}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Ti}	γ_{Ti}
0.000	$-\infty$	−4994	∞	−23462	7.103	0.000	0.338
0.100	−68781	−4045	24.898	−19004	5.754	0.042	0.415
0.200	−49808	−3196	17.928	−15016	4.546	0.100	0.499
0.300	−37523	−2447	13.491	−11496	3.481	0.176	0.588
0.400	−28254	−1798	10.176	−8446	2.557	0.271	0.677
0.500	−20850	−1248	7.539	−5865	1.776	0.381	0.762
0.600	−14797	−799	5.384	−3754	1.137	0.504	0.841
0.700	−9822	−449	3.605	−2112	0.639	0.635	0.907
0.800	−5762	−200	2.139	−938	0.284	0.766	0.958
0.900	−2512	−50	0.947	−235	0.071	0.890	0.989
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(liquid)

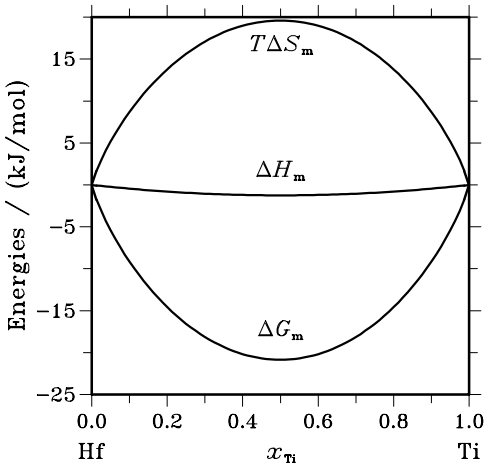

Fig. 2. Integral quantities of the liquid phase at T=2600 K.

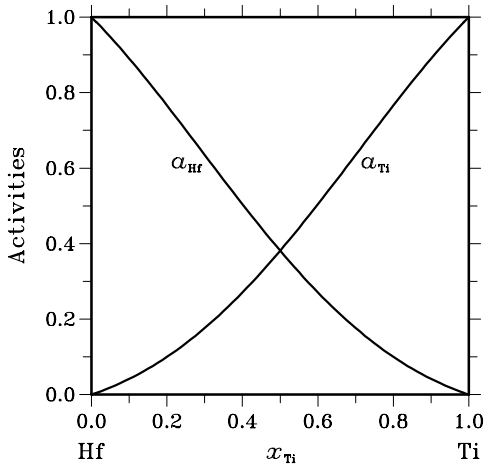

Fig. 3. Activities in the liquid phase at T=2600 K.

Table IVa. Integral quantities for the stable phases at 1000 K.

Phase	x_{Ti}	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)]
hcp	0.000	0	0	0.000	0	0.000	0.000
	0.100	−2432	1228	3.660	271	0.957	0.000
	0.200	−3680	2183	5.863	481	1.702	0.000
	0.300	−4448	2865	7.313	631	2.234	0.000
	0.400	−4874	3275	8.149	721	2.553	0.000
	0.500	−5012	3411	8.423	751	2.660	0.000
	0.600	−4874	3275	8.149	721	2.553	0.000
	0.700	−4448	2865	7.313	631	2.234	0.000
	0.800	−3680	2183	5.863	481	1.702	0.000
	0.900	−2432	1228	3.660	271	0.957	0.000
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Hf(hcp), Ti(hcp)

Table IVb. Partial quantities for Hf in the stable phases at 1000 K.

Phase	x_{Hf}	ΔG_{Hf} [J/mol]	ΔH_{Hf} [J/mol]	ΔS_{Hf} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Hf}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Hf}}$ [J/(mol·K)]	a_{Hf}	γ_{Hf}
hcp	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−846	136	0.982	30	0.106	0.903	1.004
	0.800	−1735	546	2.281	120	0.426	0.812	1.015
	0.700	−2695	1228	3.923	271	0.957	0.723	1.033
	0.600	−3766	2183	5.949	481	1.702	0.636	1.060
	0.500	−5012	3411	8.423	751	2.660	0.547	1.095
	0.400	−6536	4912	11.448	1082	3.830	0.456	1.139
	0.300	−8538	6686	15.223	1473	5.213	0.358	1.194
	0.200	−11458	8732	20.190	1924	6.809	0.252	1.260
	0.100	−16710	11052	27.762	2435	8.617	0.134	1.340
	0.000	$-\infty$	13644	∞	3006	10.638	0.000	1.435

Reference state: Hf(hcp)

Table IVc. Partial quantities for Ti in the stable phases at 1000 K.

Phase	x_{Ti}	ΔG_{Ti} [J/mol]	ΔH_{Ti} [J/mol]	ΔS_{Ti} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ti}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ti}}$ [J/(mol·K)]	a_{Ti}	γ_{Ti}
hcp	0.000	$-\infty$	13644	∞	3006	10.638	0.000	1.435
	0.100	−16710	11052	27.762	2435	8.617	0.134	1.340
	0.200	−11458	8732	20.190	1924	6.809	0.252	1.260
	0.300	−8538	6686	15.223	1473	5.213	0.358	1.194
	0.400	−6536	4912	11.448	1082	3.830	0.456	1.139
	0.500	−5012	3411	8.423	751	2.660	0.547	1.095
	0.600	−3766	2183	5.949	481	1.702	0.636	1.060
	0.700	−2695	1228	3.923	271	0.957	0.723	1.033
	0.800	−1735	546	2.281	120	0.426	0.812	1.015
	0.900	−846	136	0.982	30	0.106	0.903	1.004
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(hcp)

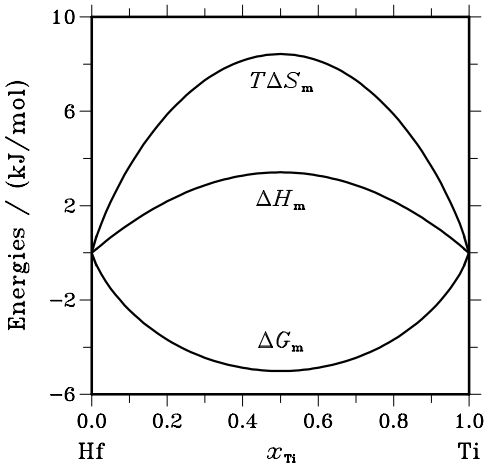

Fig. 4. Integral quantities of the stable phases at T=1000 K.

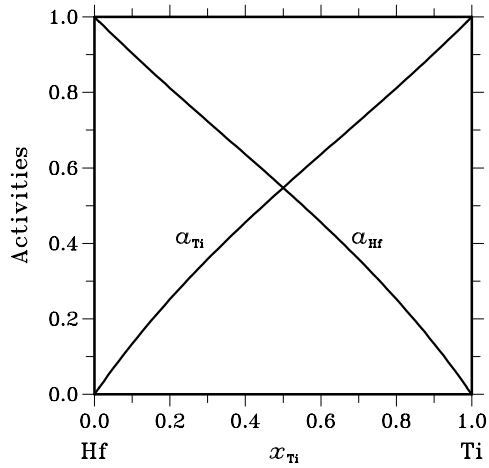

Fig. 5. Activities in the stable phases at T=1000 K.

References

[57Hay] E.T. Hayes, D.K. Deardorff: US At. Energy Comm. USBM-V-345, 1957.
[59Tyl] M.A. Tylkina, A.I. Pekarev E.M. Savitskii: Zh. Neorg. Khim. **4** (1959) 2320–2322.
[60Tho] D.E. Thomas, E.T. Hayes: US At. Energy Comm. Tech. Rept., (1960) 205–206.
[62Img] A.G. Imgram, D.N. Williams, H.R. Ogden: J. Less-Common Met. **4** (1962) 217–225.
[66Cha] Y.A. Chang: USAF Tech. Rept. AFML-TR-65-2, Part II, Vol. V (1966).
[69Rud] E. Rudy: USAF Tech. Rep. AFML-TR-65-2, Part V (1969).
[75Rud] G.I. Ruda, I.I. Kornilov, V.V. Vavilova: Izv. Akad. Nauk SSSR Met. **5** (1975) 203–205.
[97Bit] H. Bittermann, P. Rogl: J. Phase Equilibria **18** (1997) 24–47.