Hf – Ta (Hafnium – Tantalum)

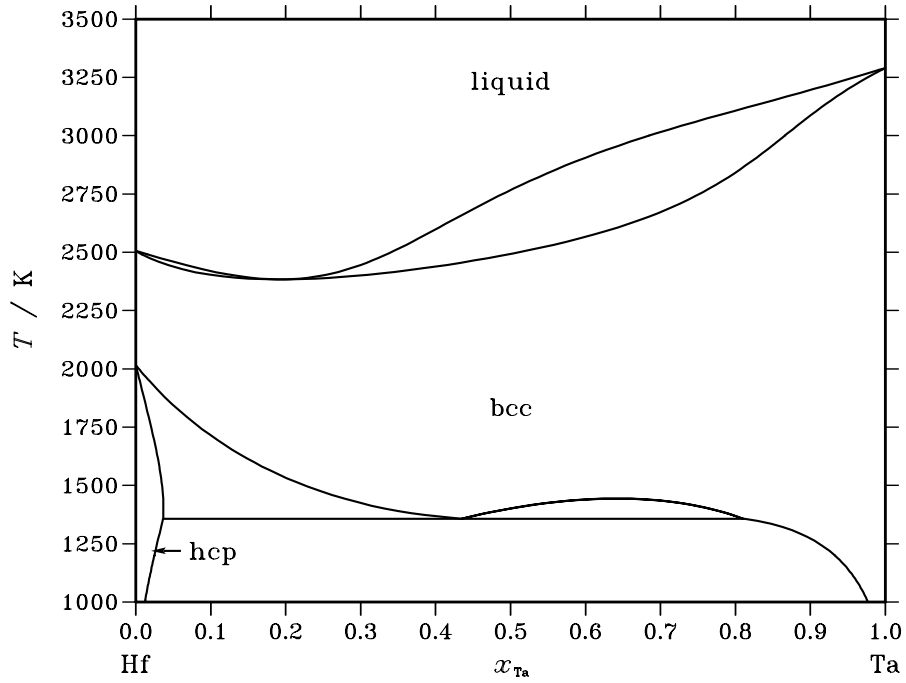

Fig. 1. Calculated phase diagram for the system Hf-Ta.

The Hf-Ta system has been critically assessed by A. Fernández Guillermet [95Fer]. The phase diagram exhibits at higher temperatures complete miscibility in the liquid and bcc phases. At lower temperatures, a miscibility gap occurs in the bcc phase with a monotectoid reaction involving hcp-Hf. Experimental phase diagram data have been reviewed repeatedly, the most recent being [89Kri], but no measurements of thermochemical properties have been reported. The calculated temperatures for the bcc/liquid equilibria are in a good agreement with the liquidus data from optical pyrometry [64Ode] and from incipient melting of various alloys and DTA measurements [69Rud]. Both [64Ode] and [69Rud] found a minimum in the solidus/liquidus lines at 2403 K and about 20 at.% Ta. The monotectoid reaction at 1356 K was determined by [75Kru] using DTA and microprobe analysis of high-purity alloys. Their results and the data from Oden [64Ode] were taken into account in the thermodynamic assessment. The experimentally determined phase boundaries between the bcc and hcp phases are represented well by the calculations.

Table I. Phases, structures and models.

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

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ta}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ bcc	congruent	2383.8	0.192	0.192		−24902
bcc $\rightleftharpoons$ bcc′ + bcc″	critical	1443.1	0.641	0.641	0.641	0
bcc′ $\rightleftharpoons$ hcp + bcc″	monotectoid	1357.5	0.435	0.036	0.810	−7454

Table IIIa. Integral quantities for the liquid phase at 3300 K.

x_{Ta}	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	−8988	−68	2.703	−68	0.000	0.000
0.200	−13427	303	4.161	303	0.000	0.000
0.300	−15807	954	5.079	954	0.000	0.000
0.400	−16740	1726	5.596	1726	0.000	0.000
0.500	−16558	2461	5.763	2461	0.000	0.000
0.600	−15467	2999	5.596	2999	0.000	0.000
0.700	−13580	3181	5.079	3181	0.000	0.000
0.800	−10883	2847	4.161	2847	0.000	0.000
0.900	−7079	1840	2.703	1840	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Hf in the liquid phase at 3300 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	−3137	−246	0.876	−246	0.000	0.892	0.991
0.800	−6895	−773	1.855	−773	0.000	0.778	0.972
0.700	−11048	−1261	2.966	−1261	0.000	0.669	0.955
0.600	−15410	−1394	4.247	−1394	0.000	0.570	0.950
0.500	−19871	−853	5.763	−853	0.000	0.485	0.969
0.400	−24460	681	7.619	681	0.000	0.410	1.025
0.300	−29510	3525	10.010	3525	0.000	0.341	1.137
0.200	−36163	7997	13.382	7997	0.000	0.268	1.338
0.100	−48763	14415	19.145	14415	0.000	0.169	1.691
0.000	$-\infty$	23098	∞	23098	0.000	0.000	2.321

Reference state: Hf(liquid)

Table IIIc. Partial quantities for Ta in the liquid phase at 3300 K.

x_{Ta}	ΔG_{Ta} [J/mol]	ΔH_{Ta} [J/mol]	ΔS_{Ta} [J/(mol·K)]	$G_{\mathrm{Ta}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Ta}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Ta}	γ_{Ta}
0.000	$-\infty$	−3410	∞	−3410	0.000	0.000	0.883
0.100	−61646	1532	19.145	1532	0.000	0.106	1.057
0.200	−39556	4604	13.382	4604	0.000	0.237	1.183
0.300	−26912	6122	10.010	6122	0.000	0.375	1.250
0.400	−18734	6407	7.619	6407	0.000	0.505	1.263
0.500	−13244	5775	5.763	5775	0.000	0.617	1.234
0.600	−9472	4544	4.247	4544	0.000	0.708	1.180
0.700	−6753	3033	2.966	3033	0.000	0.782	1.117
0.800	−4562	1560	1.855	1560	0.000	0.847	1.059
0.900	−2448	443	0.876	443	0.000	0.915	1.016
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ta(liquid)

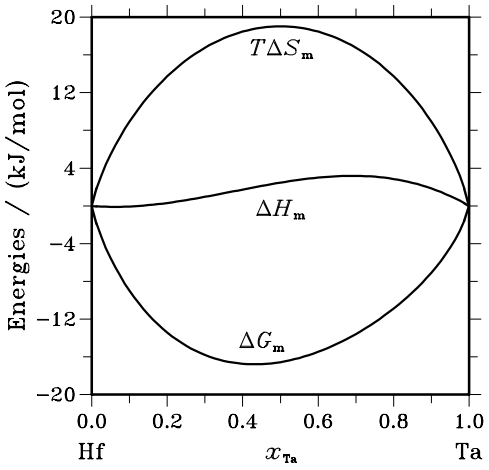

Fig. 2. Integral quantities of the liquid phase at T=3300 K.

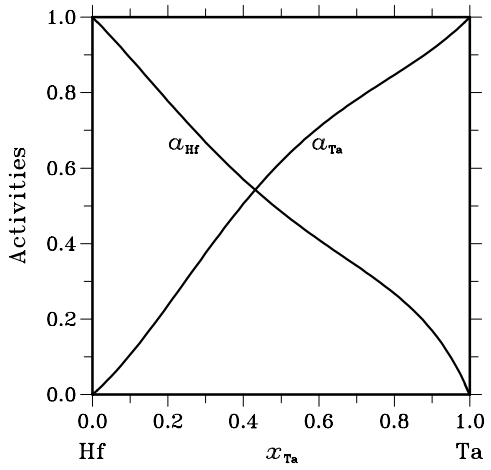

Fig. 3. Activities in the liquid phase at T=3300 K.

Table IVa. Integral quantities for the stable phases at 2200 K.

Phase	x_{Ta}	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)]
bcc	0.000	0	0	0.000	0	0.000	0.000
	0.100	−4136	1810	2.703	1810	0.000	0.000
	0.200	−5840	3314	4.161	3314	0.000	0.000
	0.300	−6684	4490	5.079	4490	0.000	0.000
	0.400	−7001	5310	5.596	5310	0.000	0.000
	0.500	−6943	5736	5.763	5736	0.000	0.000
	0.600	−6588	5722	5.596	5722	0.000	0.000
	0.700	−5963	5211	5.079	5211	0.000	0.000
	0.800	−5015	4138	4.161	4138	0.000	0.000
	0.900	−3517	2429	2.703	2429	0.000	0.000
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Hf(bcc), Ta(bcc)

Table IVb. Partial quantities for Hf in the stable phases at 2200 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}
bcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1776	151	0.876	151	0.000	0.907	1.008
	0.800	−3455	626	1.855	626	0.000	0.828	1.035
	0.700	−5046	1478	2.966	1478	0.000	0.759	1.084
	0.600	−6556	2788	4.247	2788	0.000	0.699	1.165
	0.500	−8016	4663	5.763	4663	0.000	0.645	1.290
	0.400	−9524	7237	7.619	7237	0.000	0.594	1.485
	0.300	−11349	10674	10.010	10674	0.000	0.538	1.792
	0.200	−14277	15162	13.382	15162	0.000	0.458	2.291
	0.100	−21199	20919	19.145	20919	0.000	0.314	3.138
	0.000	$-\infty$	28189	∞	28189	0.000	0.000	4.670

Reference state: Hf(bcc)

Table IVc. Partial quantities for Ta in the stable phases at 2200 K.

Phase	x_{Ta}	ΔG_{Ta} [J/mol]	ΔH_{Ta} [J/mol]	ΔS_{Ta} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ta}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ta}}$ [J/(mol·K)]	a_{Ta}	γ_{Ta}
bcc	0.000	$-\infty$	19598	∞	19598	0.000	0.000	2.920
	0.100	−25374	16744	19.145	16744	0.000	0.250	2.498
	0.200	−15377	14063	13.382	14063	0.000	0.431	2.157
	0.300	−10507	11516	10.010	11516	0.000	0.563	1.877
	0.400	−7668	9093	7.619	9093	0.000	0.658	1.644
	0.500	−5869	6810	5.763	6810	0.000	0.726	1.451
	0.600	−4632	4712	4.247	4712	0.000	0.776	1.294
	0.700	−3654	2870	2.966	2870	0.000	0.819	1.170
	0.800	−2699	1382	1.855	1382	0.000	0.863	1.078
	0.900	−1553	374	0.876	374	0.000	0.919	1.021
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ta(bcc)

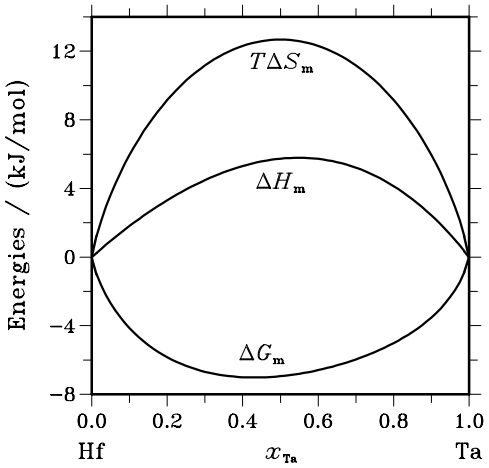

Fig. 4. Integral quantities of the stable phases at T=2200 K.

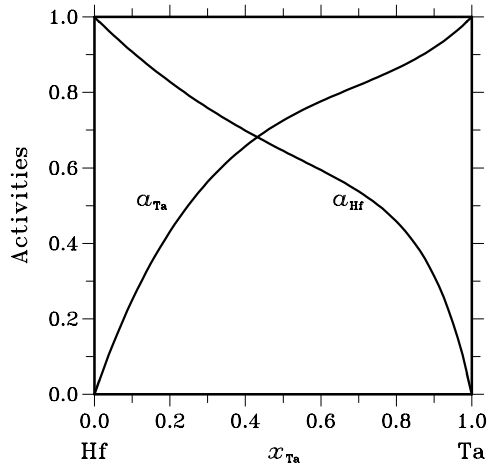

Fig. 5. Activities in the stable phases at T=2200 K.

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