Hf – W (Hafnium – Tungsten)

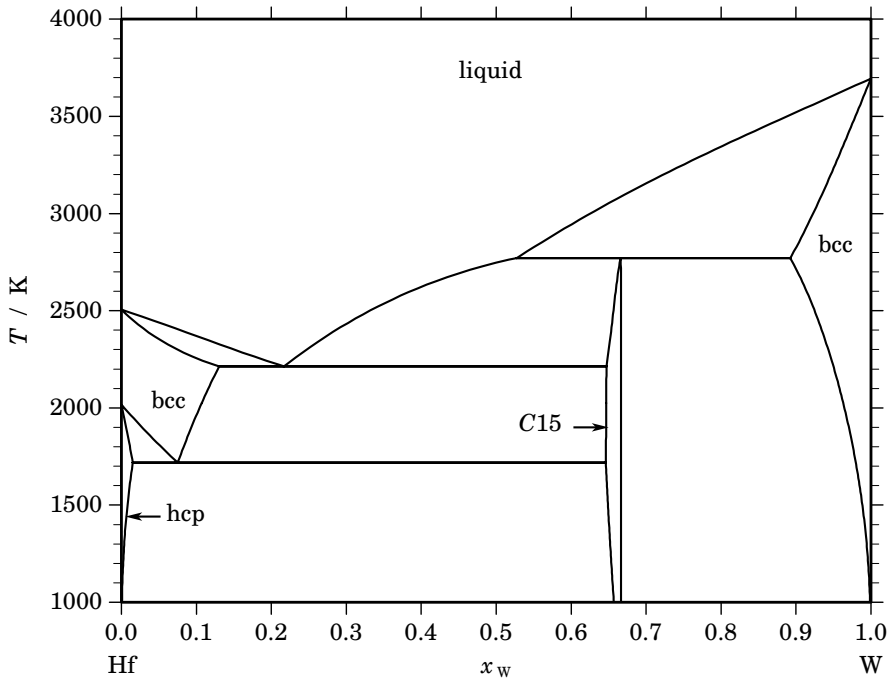

Fig. 1. Calculated phase diagram for the system Hf-W.

Hafnium and carbon are typically added in small amounts to tungsten alloys in order to improve their high-temperature creep strength. The literature on the Hf-W system has been reviewed in [1981Spe, 1991Nag] and thermodynamic optimised datasets have been reported by [1986Lee, 2002Sha]. The phase diagram is based mostly on the results of Rudy and co-workers [1960Bra, 1969Rud]. The eutectic reaction and part of the liquidus curve have been investigated by Ackermann and Rauh [1972Ack] using samples of high purity. No experimental investigations of thermodynamic mixing properties have been reported. The assessed dataset of Shao [2002Sha] is preferred over that of Lee and Lee [1986Lee] because it is based on the SGTE recommended element data. However, the calculated invariant points differ to some extent from the values which have been recommended in previous reviews [1981Spe, 1991Nag].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Hf,W)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Hf,W)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Hf,W)_1$
$C15$	$C15$	$MgCu_2$	$cF24$	$Fd\overline{3}m$	LAVES_C15	$(Hf,W)_2(Hf,W)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_W			$\Delta_r H$ / (J/mol)
liquid + bcc $\rightleftharpoons$ $C15$	peritectic	2771.0	0.527	0.892	0.666	−36470
liquid $\rightleftharpoons$ bcc + $C15$	eutectic	2213.7	0.217	0.130	0.647	−28411
bcc $\rightleftharpoons$ hcp + $C15$	eutectoid	1718.0	0.075	0.015	0.646	−8302

Table IIIa. Integral quantities for the liquid phase at 3700 K.

x_{W}	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	−11013	−2344	2.343	−1012	−0.360	0.000
0.200	−17002	−3976	3.521	−1608	−0.640	0.000
0.300	−20650	−4966	4.239	−1858	−0.840	0.000
0.400	−22540	−5387	4.636	−1835	−0.960	0.000
0.500	−22936	−5312	4.763	−1612	−1.000	0.000
0.600	−21964	−4811	4.636	−1259	−0.960	0.000
0.700	−19642	−3958	4.239	−850	−0.840	0.000
0.800	−15850	−2824	3.521	−456	−0.640	0.000
0.900	−10149	−1480	2.343	−148	−0.360	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Hf in the liquid phase at 3700 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	−3462	−368	0.836	−220	−0.040	0.894	0.993
0.800	−7651	−1378	1.695	−786	−0.160	0.780	0.975
0.700	−12525	−2884	2.606	−1552	−0.360	0.666	0.951
0.600	−18090	−4744	3.607	−2376	−0.640	0.555	0.926
0.500	−24436	−6812	4.763	−3112	−1.000	0.452	0.904
0.400	−31805	−8945	6.179	−3617	−1.440	0.356	0.889
0.300	−40786	−10999	8.050	−3747	−1.960	0.266	0.885
0.200	−52870	−12830	10.822	−3358	−2.560	0.179	0.897
0.100	−73142	−14294	15.905	−2306	−3.240	0.093	0.928
0.000	$-\infty$	−15247	∞	−447	−4.000	0.000	0.986

Reference state: Hf(liquid)

Table IIIc. Partial quantities for W in the liquid phase at 3700 K.

x_{W}	ΔG_{W} [J/mol]	ΔH_{W} [J/mol]	ΔS_{W} [J/(mol·K)]	$G_{\mathrm{W}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{W}}^{\mathrm{E}}$ [J/(mol·K)]	a_{W}	γ_{W}
0.000	$-\infty$	−27247	∞	−12447	−4.000	0.000	0.667
0.100	−78974	−20126	15.905	−8138	−3.240	0.077	0.768
0.200	−54406	−14366	10.822	−4894	−2.560	0.171	0.853
0.300	−39610	−9823	8.050	−2571	−1.960	0.276	0.920
0.400	−29213	−6353	6.179	−1025	−1.440	0.387	0.967
0.500	−21436	−3812	4.763	−112	−1.000	0.498	0.996
0.600	−15402	−2056	3.607	312	−0.640	0.606	1.010
0.700	−10581	−940	2.606	392	−0.360	0.709	1.013
0.800	−6595	−322	1.695	270	−0.160	0.807	1.009
0.900	−3150	−56	0.836	92	−0.040	0.903	1.003
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: W(liquid)

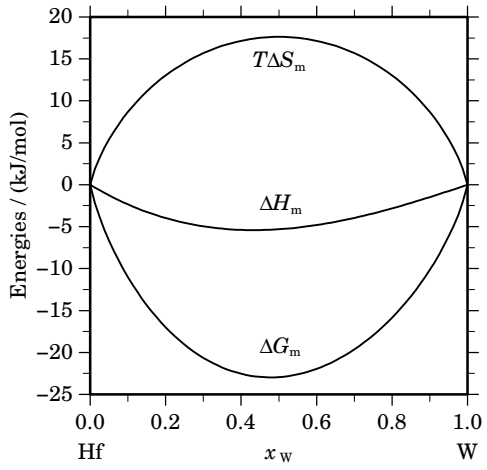

Fig. 2. Integral quantities of the liquid phase at T=3700 K.

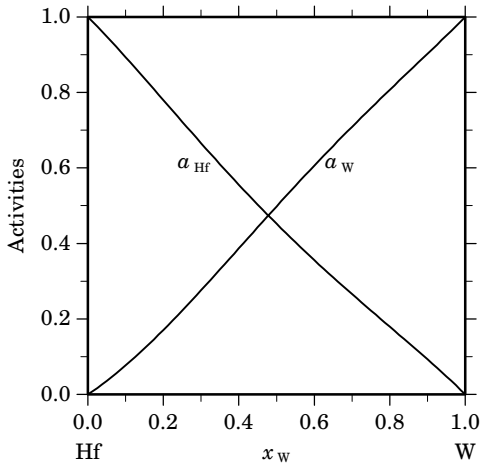

Fig. 3. Activities in the liquid phase at T=3700 K.

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

Compound	x_W	$\Delta_f G^\circ$ / (J/mol)	$\Delta_f H^\circ$ / (J/mol)	$\Delta_f S^\circ$ / (J/(mol·K))	$\Delta_f C_P^\circ$ / (J/(mol·K))
$C15$	0.667	−13677	−14109	1.450	0.000

References

[1960Bra] H. Braun, E. Rudy: Z. Metallkd. **51** (1960) 360–363.

[1962Gie] B.C. Giessen, I. Rump, N.J. Grant: Trans. AIME **224** (1962) 60–64.

[1969Rud] E. Rudy: Compendium of Phase Diagram Data, AFML, Wright-Patterson AFB, Ohio, Rep. No. AFML-TR-65-2, Part 5, 1969.

[1972Ack] R.J. Ackermann, E.G. Rauh: High Temp. Sci. **4** (1972) 272–282.

[1981Spe] P.J. Spencer in: "Hafnium: Physico-Chemical Properties of its Compounds and Alloys", K.L. Komarek (ed.), Atomic Energy Rev. Spec. Issue 8, IAEA, Vienna, 1981, pp. 108–110.

[1986Lee] S.K. Lee, D.N. Lee: Calphad **10** (1986) 61–76.

[1991Nag] S.V. Nagender Naidu, P. Rama Rao in: "Phase Diagrams of Binary Tungsten Alloys", S.V. Nagender Naidu, P. Rama Rao, Eds., The Indian Institute of Metals, Calcutta, 1991, pp. 114–121.

[2002Sha] G. Shao: Intermetallics **10** (2002) 429–434.