Au – Hf (Gold – Hafnium)

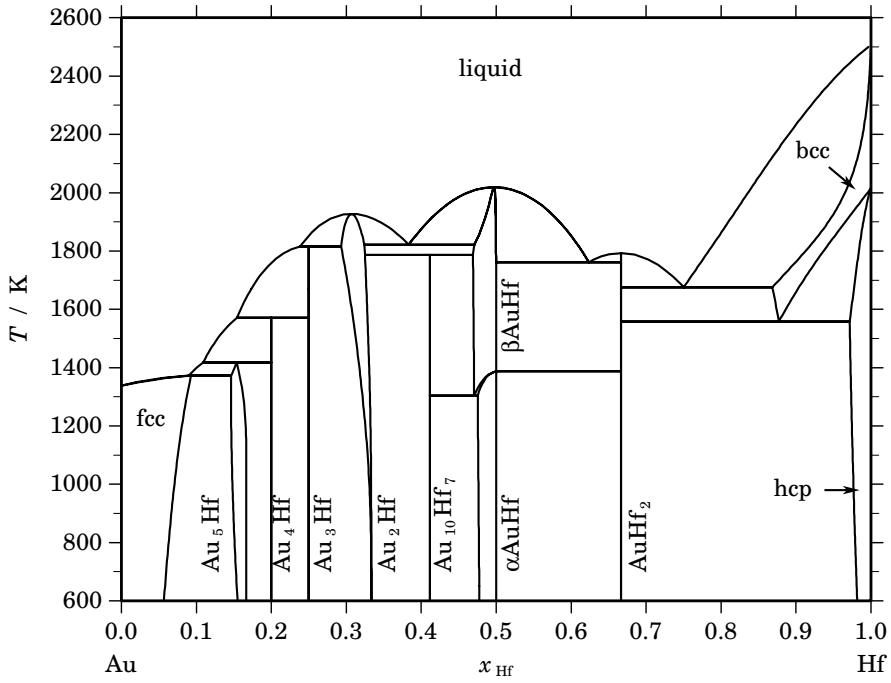

Fig. 1. Calculated phase diagram for the system Au-Hf.

The Au-Hf system has been reviewed in [1984Oka, 2000Oka, 2003Du] and a thermodynamic dataset has been optimised in [2003Du]. The assessment is based mainly on investigations of the phase diagram by [2000Lom] using differential thermal analysis, x-ray diffraction, and electron microprobe analysis. Seven intermetallic compounds have been identified in agreement with previous studies of the phase diagram by [1962Sto]. The enthalpies of formation of the compounds Au_3Hf, Au_2Hf, AuHf and $AuHf_2$ have been determined by [1992Fit]. The terminal solid solutions bcc, hcp, fcc and the liquid phase were described by substitutional solution models using Redlich-Kister polynomials. The three intermetallic compounds Au_5Hf, Au_2Hf, αAuHf and βAuHf with certain homogeneity ranges were treated by two-sublattice models with Au and Hf in one sublattice and the other filled with Au only. The four other compounds Au_4Hf, Au_3Hf, $Au_{10}Hf_7$, $AuHf_2$ were considered as stoichiometric. Satisfactory agreement is obtained between the calculated and experimental data.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Au,Hf)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Au,Hf)_1$
Au_5Hf	$D1_a$	$MoNi_4$	$tI10$	$I4/m$	AU5HF	$Au_5(Au,Hf)_1$
Au_4Hf	⋯	Au_4Zr	$oP20$	$Pnma$	AU4HF	Au_4Hf_1
Au_3Hf	$D0_a$	βCu_3Ti	$oP8$	$Pmmn$	AU3HF	Au_3Hf_1
Au_2Hf	$C11_b$	$MoSi_2$	$tI6$	$I4/mmm$	AU2HF	$Au_2(Au,Hf)_1$
$Au_{10}Hf_7$	⋯	$Ni_{10}Zr_7$	$oC68$	$C2ca$	AU10HF7	$Au_{10}Hf_7$
αAuHf	$B11$	γCuTi	$tP4$	$P4/nmm$	AUHF_ALPHA	$Au_1(Au,Hf)_1$
βAuHf	⋯	⋯	⋯	⋯	AUHF_BETA	$Au_1(Au,Hf)_1$
$AuHf_2$	$C11_b$	$MoSi_2$	$tI6$	$I4/mmm$	AUHF2	Au_1Hf_2
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Au,Hf)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Au,Hf)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Hf}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ βAuHf	congruent	2019.4	0.497	0.497		−19153
liquid $\rightleftharpoons$ Au_2Hf	congruent	1927.4	0.307	0.307		−13252
liquid $\rightleftharpoons$ Au_2Hf + βAuHf	eutectic	1821.8	0.383	0.324	0.471	−14870
liquid + Au_2Hf $\rightleftharpoons$ Au_3Hf	peritectic	1815.4	0.238	0.293	0.250	−13909
liquid $\rightleftharpoons$ $AuHf_2$	congruent	1793.0	0.667	0.667		−15652
Au_2Hf + βAuHf $\rightleftharpoons$ $Au_{10}Hf_7$	peritectoid	1786.0	0.325	0.469	0.412	−3431
liquid $\rightleftharpoons$ βAuHf + $AuHf_2$	eutectic	1761.3	0.624	0.500	0.667	−15378
liquid $\rightleftharpoons$ $AuHf_2$ + bcc	eutectic	1675.8	0.750	0.667	0.868	−14897
liquid + Au_3Hf $\rightleftharpoons$ Au_4Hf	peritectic	1570.9	0.154	0.250	0.200	−11984
bcc $\rightleftharpoons$ $AuHf_2$ + hcp	eutectoid	1558.3	0.877	0.667	0.971	−5377
liquid + Au_4Hf $\rightleftharpoons$ Au_5Hf	peritectic	1418.1	0.109	0.200	0.154	−11632
βAuHf + $AuHf_2$ $\rightleftharpoons$ αAuHf	peritectoid	1386.9	0.500	0.667	0.500	−1117
liquid + Au_5Hf $\rightleftharpoons$ fcc	peritectic	1373.1	0.090	0.146	0.093	−12475
βAuHf $\rightleftharpoons$ $Au_{10}Hf_7$ + αAuHf	eutectoid	1304.0	0.471	0.412	0.475	−651

Table IIIa. Integral quantities for the liquid phase at 2573 K.

x_{Hf}	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	−13352	−28636	−5.940	−6397	−8.643	0.000
0.200	−22532	−48065	−9.923	−11826	−14.084	0.000
0.300	−29186	−59351	−11.724	−16118	−16.803	0.000
0.400	−33498	−63563	−11.685	−19101	−17.281	0.000
0.500	−35434	−61767	−10.234	−20605	−15.998	0.000
0.600	−34859	−55030	−7.839	−20461	−13.435	0.000
0.700	−31568	−44418	−4.994	−18499	−10.073	0.000
0.800	−25254	−30998	−2.232	−14548	−6.393	0.000
0.900	−15393	−15836	−0.172	−8439	−2.875	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Au in the liquid phase at 2573 K.

x_{Au}	ΔG_{Au} [J/mol]	ΔH_{Au} [J/mol]	ΔS_{Au} [J/(mol·K)]	$G_{\mathrm{Au}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Au}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Au}	γ_{Au}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2710	−4782	−0.805	−456	−1.681	0.881	0.979
0.800	−6823	−17705	−4.229	−2049	−6.085	0.727	0.909
0.700	−12752	−36636	−9.283	−5121	−12.248	0.551	0.787
0.600	−20940	−59442	−14.964	−10012	−19.211	0.376	0.626
0.500	−31890	−83990	−20.249	−17061	−26.012	0.225	0.450
0.400	−46212	−108145	−24.070	−26609	−31.689	0.115	0.288
0.300	−64754	−129775	−25.271	−38997	−35.281	0.048	0.162
0.200	−88995	−146746	−22.445	−54564	−35.827	0.016	0.078
0.100	−122910	−156925	−13.220	−73650	−32.365	0.003	0.032
0.000	$-\infty$	−158179	∞	−96597	−23.934	0.000	0.011

Reference state: Au(liquid)

Table IIIc. Partial quantities for Hf in the liquid phase at 2573 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}
0.000	$-\infty$	−335959	∞	−68244	−104.048	0.000	0.041
0.100	−109131	−243326	−52.155	−59871	−71.300	0.006	0.061
0.200	−85366	−169502	−32.700	−50935	−46.082	0.018	0.092
0.300	−67532	−112353	−17.420	−41775	−27.430	0.043	0.142
0.400	−52336	−69745	−6.766	−32734	−14.384	0.087	0.217
0.500	−38978	−39545	−0.220	−24149	−5.984	0.162	0.323
0.600	−27291	−19620	2.981	−16363	−1.266	0.279	0.465
0.700	−17345	−7836	3.696	−9714	0.730	0.445	0.635
0.800	−9318	−2060	2.821	−4544	0.965	0.647	0.809
0.900	−3447	−160	1.278	−1193	0.402	0.851	0.946
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Hf(liquid)

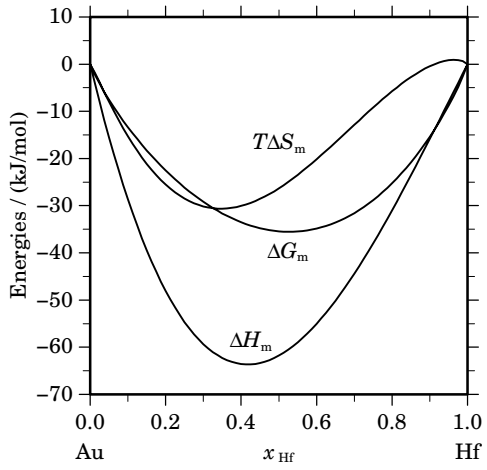

Fig. 2. Integral quantities of the liquid phase at T=2573 K.

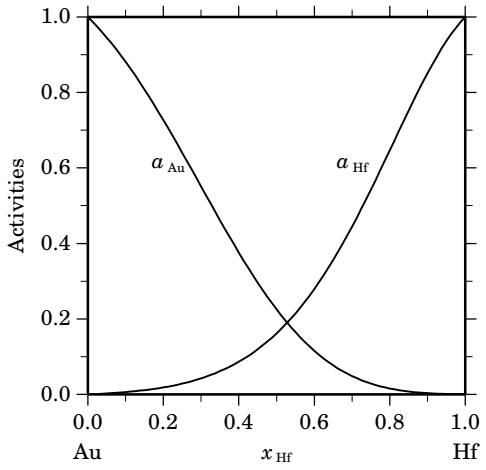

Fig. 3. Activities in the liquid phase at T=2573 K.

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

Compound	x_{Hf}	$\Delta_f G^\circ$ / (J/mol)	$\Delta_f H^\circ$ / (J/mol)	$\Delta_f S^\circ$ / (J/(mol·K))	$\Delta_f C_P^\circ$ / (J/(mol·K))
Au_5Hf	0.167	−44927	−49061	−13.867	0.000
Au_4Hf_1	0.200	−47656	−51155	−11.738	0.000
Au_3Hf_1	0.250	−51314	−54301	−10.020	0.000
Au_2Hf	0.333	−56382	−59453	−10.299	0.000
$Au_{10}Hf_7$	0.412	−60171	−63666	−11.719	0.000
αAuHf	0.500	−58264	−61203	−9.858	0.000
βAuHf	0.500	−57386	−60085	−9.052	0.000
Au_1Hf_2	0.667	−39665	−40794	−3.784	0.000

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