Au – Ti (Gold – Titanium)

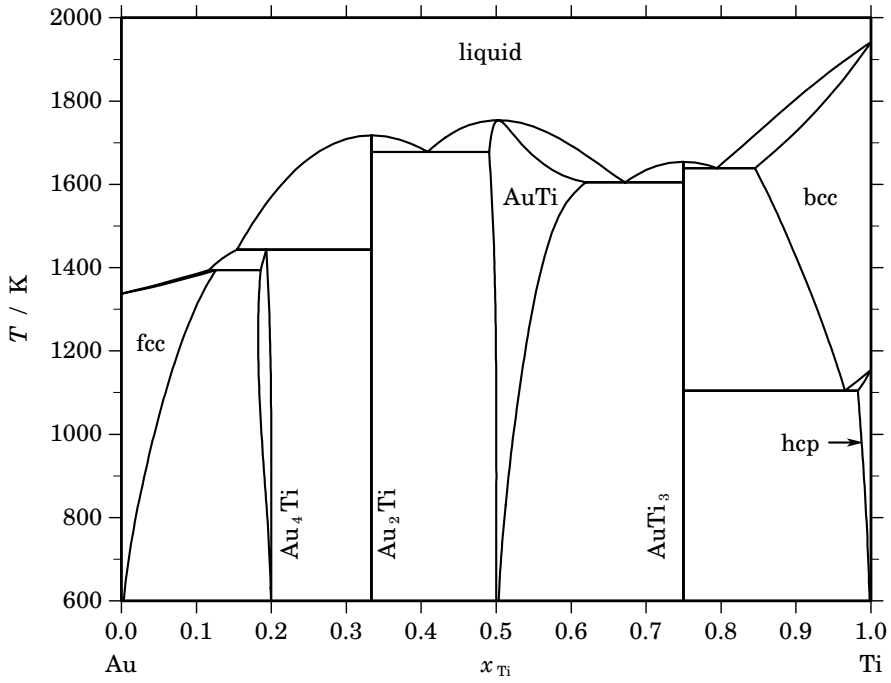

Fig. 1. Calculated phase diagram for the system Au-Ti.

Alloys of gold and titanium as well as gold platings on titanium are encountered in jewelry and also in dental applications. A thorough review of the literature on the thermodynamics of the Au-Ti system has been given in [1987Mur] and a thermodynamic optimised dataset has been reported by [2001Luo]. The optimisation takes into account 5 experimental datasets for the phase diagram from the literature, a calorimetric investigation of the mixing enthalpy in Au-rich melts and reported standard enthalpies of formation for three of the intermetallic compounds, $AuTi_3$, AuTi, and Au_2Ti which have been obtained from direct synthesis calorimetry. The low-temperature modifications of the AuTi compound have not been included in the optimisation due to a lack of data.

References

[1987Mur] J.L. Murray in: Phase Diagrams of Binary Titanium Alloys, J.L. Murray, Ed., ASM Intl., Metals Park, OH, 1987, pp. 27–32.

[2001Luo] W. Luo, Z. Jin, H. Liu, T. Wang: Calphad **25** (2001) 19–26.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Au,Ti)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Au,Ti)_1$
Au_4Ti	$D1_a$	$MoNi_4$	$tI10$	$I4/m$	AU4TI	$Au_4(Au,Ti)_1$
Au_2Ti	$C11_b$	$MoSi_2$	$tI6$	$I4/mmm$	AU2TI	Au_2Ti_1
αAuTi	$B11$	CuTi	$tP4$	$P4/nmm$	AUTI	$(Au,Ti)_1(Ti,\Box)_1$
βAuTi	$B19$	AuCd	$oP4$	$Pmma$	AUTI	$(Au,Ti)_1(Ti,\Box)_1$
γAuTi	$B2$	CsCl	$cP2$	$Pm\overline{3}m$	AUTI	$(Au,Ti)_1(Ti,\Box)_1$
$AuTi_3$	$A15$	Cr_3Si	$cP8$	$Pm3n$	AUTI3	Au_1Ti_3
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Au,Ti)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Au,Ti)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ti}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ AuTi	congruent	1754.6	0.503	0.503		−28799
liquid $\rightleftharpoons$ Au_2Ti	congruent	1717.9	0.333	0.333		−43289
liquid $\rightleftharpoons$ Au_2Ti + AuTi	eutectic	1678.0	0.409	0.333	0.490	−35388
liquid $\rightleftharpoons$ $AuTi_3$	congruent	1654.4	0.750	0.750		−23842
liquid $\rightleftharpoons$ $AuTi_3$ + bcc	eutectic	1639.3	0.794	0.750	0.845	−18241
liquid $\rightleftharpoons$ AuTi + $AuTi_3$	eutectic	1604.9	0.672	0.619	0.750	−21471
liquid + Au_2Ti $\rightleftharpoons$ Au_4Ti	peritectic	1443.7	0.154	0.333	0.193	−21679
liquid + Au_4Ti $\rightleftharpoons$ fcc	peritectic	1394.1	0.116	0.186	0.126	−8854
bcc $\rightleftharpoons$ $AuTi_3$ + hcp	eutectoid	1104.9	0.965	0.750	0.982	−5129

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	−19206	−12370	3.418	−13800	0.715	0.000
0.200	−31822	−20984	5.419	−23501	1.258	0.000
0.300	−39648	−26222	6.713	−29490	1.634	0.000
0.400	−43347	−28459	7.444	−32155	1.848	0.000
0.500	−43409	−28074	7.668	−31883	1.904	0.000
0.600	−40251	−25442	7.404	−29059	1.809	0.000
0.700	−34231	−20942	6.644	−24073	1.565	0.000
0.800	−25630	−14950	5.340	−17309	1.179	0.000
0.900	−14562	−7844	3.359	−9156	0.656	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Au in the liquid phase at 2000 K.

x_{Au}	ΔG_{Au} [J/mol]	ΔH_{Au} [J/mol]	ΔS_{Au} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Au}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Au}}$ [J/(mol·K)]	a_{Au}	γ_{Au}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−3866	−1940	0.963	−2114	0.087	0.793	0.881
0.800	−11650	−7258	2.196	−7939	0.341	0.496	0.620
0.700	−22633	−15198	3.718	−16702	0.752	0.256	0.366
0.600	−36123	−25007	5.558	−27629	1.311	0.114	0.190
0.500	−51471	−35931	7.770	−39945	2.007	0.045	0.091
0.400	−68114	−47215	10.449	−52877	2.831	0.017	0.042
0.300	−85671	−58105	13.783	−65650	3.773	0.006	0.019
0.200	−104255	−67846	18.205	−77492	4.823	0.002	0.009
0.100	−125916	−75684	25.116	−87627	5.971	0.001	0.005
0.000	−∞	−80866	∞	−95281	7.208	0.000	0.003

Reference state: Au(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)]	$G^{\mathrm{E}}_{\mathrm{Ti}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ti}}$ [J/(mol·K)]	a_{Ti}	γ_{Ti}
0.000	−∞	−143724	∞	−159779	8.028	0.000	0.000
0.100	−157262	−106234	25.514	−118973	6.370	0.000	0.001
0.200	−112511	−75892	18.309	−85747	4.928	0.001	0.006
0.300	−79350	−51944	13.703	−59330	3.693	0.008	0.028
0.400	−54182	−33637	10.272	−38945	2.654	0.038	0.096
0.500	−35347	−20216	7.565	−23820	1.802	0.119	0.239
0.600	−21676	−10927	5.374	−13181	1.127	0.272	0.453
0.700	−12185	−5015	3.585	−6253	0.619	0.481	0.687
0.800	−5974	−1726	2.124	−2263	0.269	0.698	0.873
0.900	−2189	−306	0.942	−437	0.066	0.877	0.974
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(liquid)

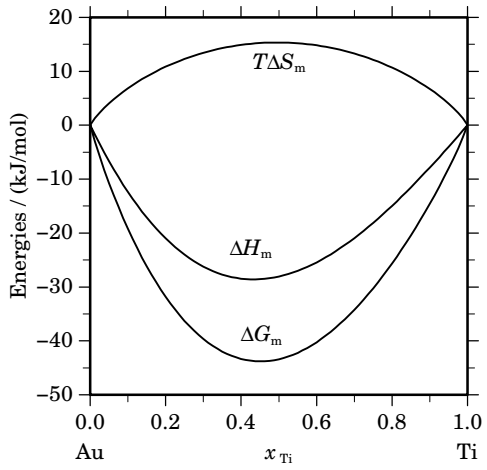

Fig. 2. Integral quantities of the liquid phase at T=2000 K.

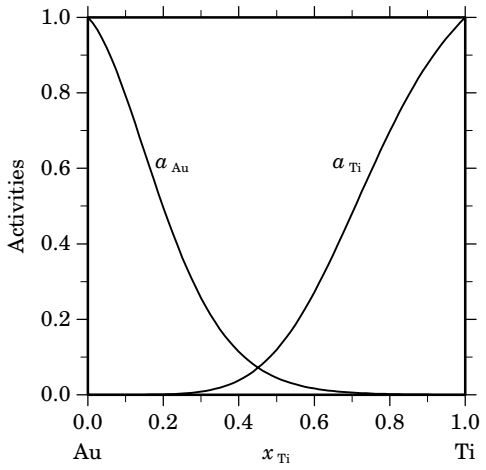

Fig. 3. Activities in the liquid phase at T=2000 K.

Table IVa. Integral quantities for the stable phases at 1300 K.

Phase	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)]
fcc	0.000	0	0	0.000	0	0.000	0.000
	0.098	−16627	−12738	2.992	−13162	0.326	0.555
Au_4Ti	0.183	−28381	−36195	−6.011	−23239	−9.966	1.036
	0.197	−30204	−39797	−7.379	−24840	−11.505	1.117
Au_2Ti	0.333	−45454	−59020	−10.435			1.889
AuTi	0.499	−43625	−46728	−2.387	−36133	−8.150	3.677
	0.500	−43609	−46730	−2.401	−36117	−8.164	3.820
	0.549	−41077	−42600	−1.171	−33636	−6.895	3.931
$AuTi_3$	0.750	−28254	−31825	−2.746			4.250
bcc	0.928	−8823	−5846	2.290	−6027	0.139	0.000
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Au(fcc), Ti(bcc)

Table IVb. Partial quantities for Au in the stable phases at 1300 K.

Phase	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}
fcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.902	−3051	−1910	0.878	−1936	0.020	0.754	0.836
Au_4Ti	0.817	−3051	10000	10.039	−869	8.360	0.754	0.923
	0.803	−8140	10000	13.954	−5767	12.128	0.471	0.587
Au_2Ti	0.667	−8140	−11983	−2.957			0.471	
	0.667	−49135	−83749	−26.627			0.011	
AuTi	0.501	−49135	−31745	13.377	−41665	7.631	0.011	0.021
	0.500	−53273	−58340	−3.897	−45781	−9.660	0.007	0.014
	0.451	−75984	−92162	−12.445	−67389	−19.056	0.001	0.002
$AuTi_3$	0.250	−75984	−71932	3.117			0.001	
	0.250	−110118	−141273	−23.965			0.000	
bcc	0.072	−110118	−81613	21.927	−81676	0.049	0.000	0.001
	0.000	$-\infty$	−80242	∞	−85583	4.108	0.000	0.000

Reference state: Au(fcc)

Table IVc. Partial quantities for Ti in the stable phases at 1300 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}
fcc	0.000	$-\infty$	−150030	∞	−154550	3.477	0.000	0.000
	0.098	−141592	−112406	22.450	−116485	3.137	0.000	0.000
Au_4Ti	0.183	−141592	−242664	−77.748	−123225	−91.876	0.000	0.000
	0.197	−120094	−242664	−94.284	−102540	−107.788	0.000	0.000
Au_2Ti	0.333	−120094	−153107	−25.394			0.000	
	0.333	−38092	−9553	21.953			0.029	
AuTi	0.499	−38092	−61773	−18.216	−30577	−23.997	0.029	0.059
	0.500	−33945	−35121	−0.905	−26452	−6.668	0.043	0.087
	0.549	−12344	−1803	8.109	−5853	3.115	0.319	0.582
$AuTi_3$	0.750	−12344	−18456	−4.701			0.319	
	0.750	−966	4658	4.327			0.914	
bcc	0.928	−966	31	0.767			0.914	0.985
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(bcc)

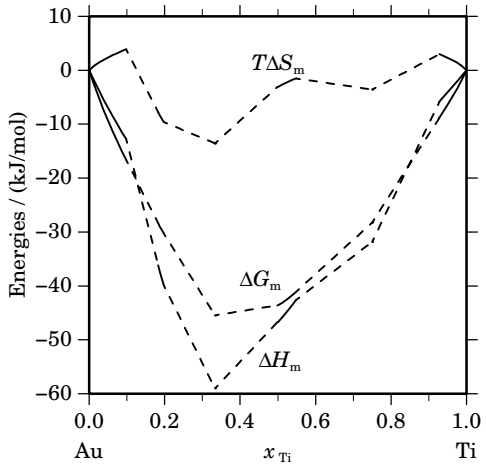

Fig. 4. Integral quantities of the stable phases at T=1300 K.

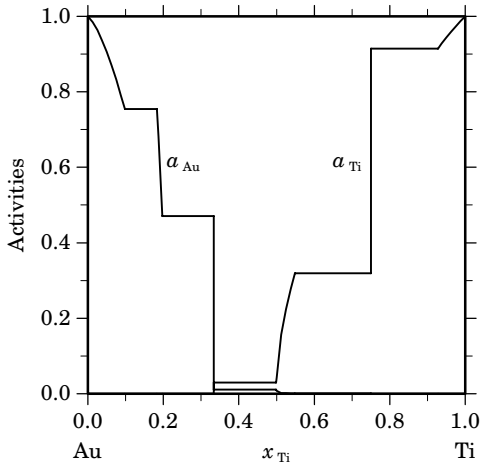

Fig. 5. Activities in the stable phases at T=1300 K.

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

Compound	x_{Ti}	$\Delta_{\mathrm{f}}G^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}H^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}S^{\circ}$ / (J/(mol·K))	$\Delta_{\mathrm{f}}C^{\circ}_{P}$ / (J/(mol·K))
Au_4Ti	0.200	−37730	−39855	−7.125	0.000
Au_2Ti_1	0.333	−55074	−57889	−9.443	0.000
AuTi	0.500	−44914	−45242	−1.098	0.013
Au_1Ti_3	0.750	−29128	−29281	−0.514	0.000