Re – Ta (Rhenium – Tantalum)

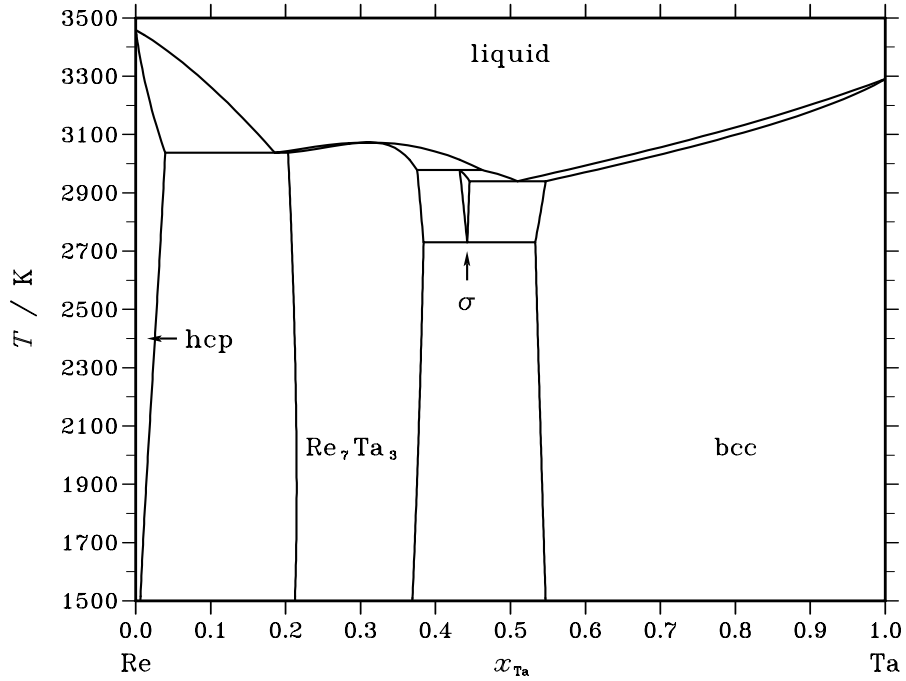

Fig. 1. Calculated phase diagram for the system Re-Ta.

Rhenium and tantalum are important additions to many alloys, such as superalloys and refractory alloys. The Re-Ta system consists of five condensed stable phases, liquid, bcc (Ta-rich terminal solid solution), hcp (Re-rich terminal solid solution) and two ordered intermediate phases, Re_7Ta_3 and σ. Two recent thermodynamic assessments exist, [99Cui] and [00Liu]. Each used a different number of excess terms for the description of the disordered solution phases and different model descriptions for the ordered phases but both assessments used a three sublattice model for the description of the Re_7Ta_3 phase; [99Cui] considered substitution to occur only on one of the sublattices while [00Liu] considered substitution on two of the sublattices. [99Cui] simplified the description of the small homogeneity range of the sigma phase by describing it to be stoichiometric whereas [00Liu] used a three-sublattice model description with substitution on one of these sublattices. Both assessments reproduce the experimental phase diagram and theoretical and derived enthalpy of formation data reasonably well. The description of [00Liu] is recommended since it uses less terms than that of [99Cui] to describe the excess Gibbs energies of the disordered solution phases and the models used for the ordered intermediate phases are in accord with the recommendations of [97Ans].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Re,Ta)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Re,Ta)_1$
Re_7Ta_3	$A12$	αMn	$cI58$	$I\bar{4}3m$	A12_CHI	$Re_{12}(Re,Ta)_5(Re,Ta)_{12}$
σ	$D8_b$	σCrFe	$tP30$	$P4_2/mnm$	D8B_SIGMA	$(Re,Ta)_{10}Ta_4(Re,Ta)_{16}$
bcc	$A2$	W	$cI2$	$Im\bar{3}m$	BCC_A2	$(Re,Ta)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ta}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons$ Re_7Ta_3	congruent	3024.8	0.083	0.083		−49112
liquid $\rightleftharpoons$ hcp + Re_7Ta_3	eutectic	3037.1	0.186	0.039	0.203	−50533
Re_7Ta_3 + liquid $\rightleftharpoons$ σ	peritectic	2977.7	0.375	0.462	0.432	−26850
liquid $\rightleftharpoons$ σ + bcc	eutectic	2940.1	0.509	0.445	0.547	−46475
σ $\rightleftharpoons$ Re_7Ta_3 + bcc	eutectoid	2730.2	0.442	0.384	0.533	−4920

Table IIIa. Integral quantities for the liquid phase at 3500 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	−16706	−7246	2.703	−7246	0.000	0.000
0.200	−27285	−12723	4.161	−12723	0.000	0.000
0.300	−34268	−16491	5.079	−16491	0.000	0.000
0.400	−38195	−18610	5.596	−18610	0.000	0.000
0.500	−39308	−19137	5.763	−19137	0.000	0.000
0.600	−37719	−18134	5.596	−18134	0.000	0.000
0.700	−33436	−15659	5.079	−15659	0.000	0.000
0.800	−26335	−11772	4.161	−11772	0.000	0.000
0.900	−15993	−6533	2.703	−6533	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Re in the liquid phase at 3500 K.

x_{Re}	ΔG_{Re} [J/mol]	ΔH_{Re} [J/mol]	ΔS_{Re} [J/(mol·K)]	$G_{\mathrm{Re}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Re}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Re}	γ_{Re}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−3960	−894	0.876	−894	0.000	0.873	0.970
0.800	−9991	−3498	1.855	−3498	0.000	0.709	0.887
0.700	−18071	−7692	2.966	−7692	0.000	0.537	0.768
0.600	−28223	−13357	4.247	−13357	0.000	0.379	0.632
0.500	−40546	−20375	5.763	−20375	0.000	0.248	0.497
0.400	−55292	−28627	7.619	−28627	0.000	0.150	0.374
0.300	−73031	−37994	10.010	−37994	0.000	0.081	0.271
0.200	−95193	−48358	13.382	−48358	0.000	0.038	0.190
0.100	−126605	−59598	19.145	−59598	0.000	0.013	0.129
0.000	$-\infty$	−71597	∞	−71597	0.000	0.000	0.085

Reference state: Re(liquid)

Table IIIc. Partial quantities for Ta in the liquid phase at 3500 K.

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}
0.000	$-\infty$	−81501	∞	−81501	0.000	0.000	0.061
0.100	−131418	−64411	19.145	−64411	0.000	0.011	0.109
0.200	−96461	−49625	13.382	−49625	0.000	0.036	0.182
0.300	−72060	−37024	10.010	−37024	0.000	0.084	0.280
0.400	−53153	−26488	7.619	−26488	0.000	0.161	0.402
0.500	−38070	−17899	5.763	−17899	0.000	0.270	0.541
0.600	−26004	−11139	4.247	−11139	0.000	0.409	0.682
0.700	−16467	−6087	2.966	−6087	0.000	0.568	0.811
0.800	−9120	−2626	1.855	−2626	0.000	0.731	0.914
0.900	−3703	−637	0.876	−637	0.000	0.881	0.978
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ta(liquid)

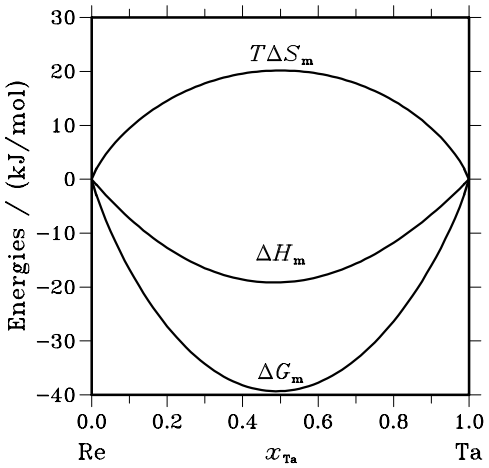

Fig. 2. Integral quantities of the liquid phase at T=3500 K.

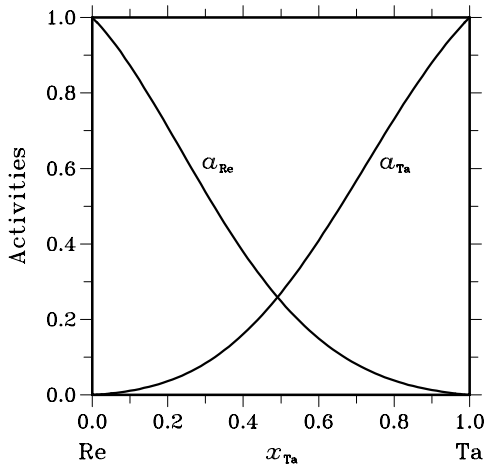

Fig. 3. Activities in the liquid phase at T=3500 K.

Table IVa. Integral quantities for the stable phases at 2000 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)]
hcp	0.000	0	0	0.000	0	0.000	0.000
	0.016	−1613	−306	0.654	−228	−0.039	0.000
Re_7Ta_3	0.215	−17799	−13876	1.961	−9152	−2.362	2.435
	0.300	−23726	−18855	2.436	−13568	−2.643	1.378
	0.377	−26104	−19801	3.152	−15091	−2.355	0.059
bcc	0.541	−27201	−21727	2.737	−15730	−2.998	0.000
	0.600	−27145	−22273	2.436	−15954	−3.160	0.000
	0.700	−24978	−20949	2.014	−14819	−3.065	0.000
	0.800	−20104	−16795	1.654	−11782	−2.506	0.000
	0.900	−12248	−9812	1.218	−6843	−1.485	0.000
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Re(hcp), Ta(bcc)

Table IVb. Partial quantities for Re in the stable phases at 2000 K.

Phase	x_{Re}	ΔG_{Re} [J/mol]	ΔH_{Re} [J/mol]	ΔS_{Re} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Re}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Re}}$ [J/(mol·K)]	a_{Re}	γ_{Re}
hcp	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.984	−282	−8	0.137	−8	0.000	0.983	1.000
Re_7Ta_3	0.785	−282	1062	0.672	3735	−1.336	0.983	1.252
	0.700	−7645	−7626	0.010	−1714	−2.956	0.631	0.902
	0.623	−23595	−21784	0.906	−15739	−3.022	0.242	0.388
bcc	0.459	−23595	−12206	5.695	−10646	−0.780	0.242	0.527
	0.400	−32287	−21729	5.279	−17050	−2.339	0.143	0.359
	0.300	−49440	−40120	4.660	−29419	−5.351	0.051	0.170
	0.200	−70453	−61341	4.556	−43690	−8.826	0.014	0.072
	0.100	−98153	−85391	6.381	−59863	−12.764	0.003	0.027
	0.000	$-\infty$	−112270	∞	−77940	−17.165	0.000	0.009

Reference state: Re(hcp)

Table IVc. Partial quantities for Ta in the stable phases at 2000 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}
hcp	0.000	$-\infty$	−19286	∞	−14486	−2.400	0.000	0.418
	0.016	−81917	−18274	31.822	−13474	−2.400	0.007	0.445
Re_7Ta_3	0.215	−81917	−68557	6.680	−56323	−6.117	0.007	0.034
	0.300	−61250	−45058	8.096	−41229	−1.914	0.025	0.084
	0.377	−30260	−16517	6.871	−14016	−1.250	0.162	0.430
bcc	0.541	−30260	−29805	0.227	−20044	−4.880	0.162	0.300
	0.600	−23717	−22635	0.541	−15222	−3.706	0.240	0.400
	0.700	−14494	−12732	0.881	−8563	−2.085	0.418	0.598
	0.800	−7516	−5659	0.929	−3806	−0.927	0.636	0.795
	0.900	−2703	−1415	0.644	−951	−0.232	0.850	0.944
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ta(bcc)

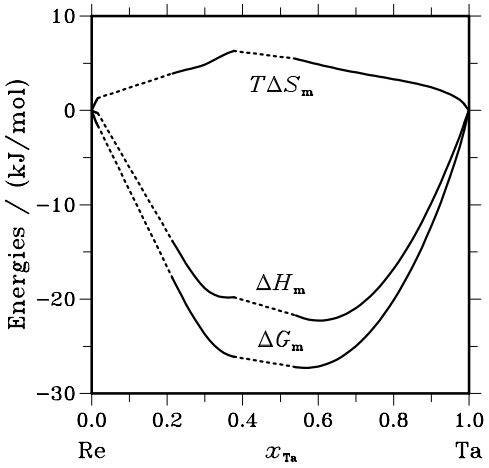

Fig. 4. Integral quantities of the stable phases at T=2000 K.

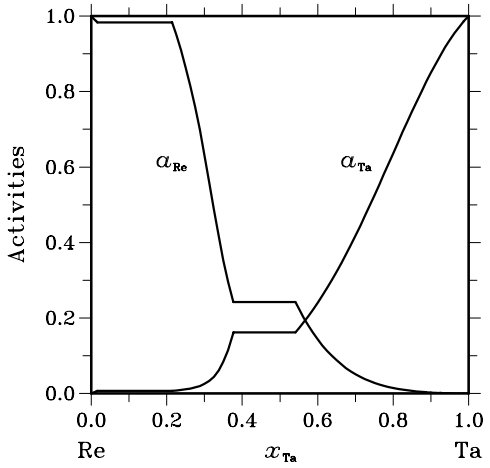

Fig. 5. Activities in the stable phases at T=2000 K.

References

[97Ans] I. Ansara, T.G. Chart, A. Fernández Guillermet, F.H. Hayes, U.R. Kattner, D.G. Pettifor, N. Saunders, K. Zeng: Calphad **21** (1997) 171–218.
[99Cui] Y. Cui, Z. Jin: J. Alloys Comp. **285** (1999) 150–155.
[00Liu] Z.-K. Liu, Y.A. Chang: J. Alloys Comp. **299** (2000) 153–162.