Cu – Ti (Copper – Titanium)

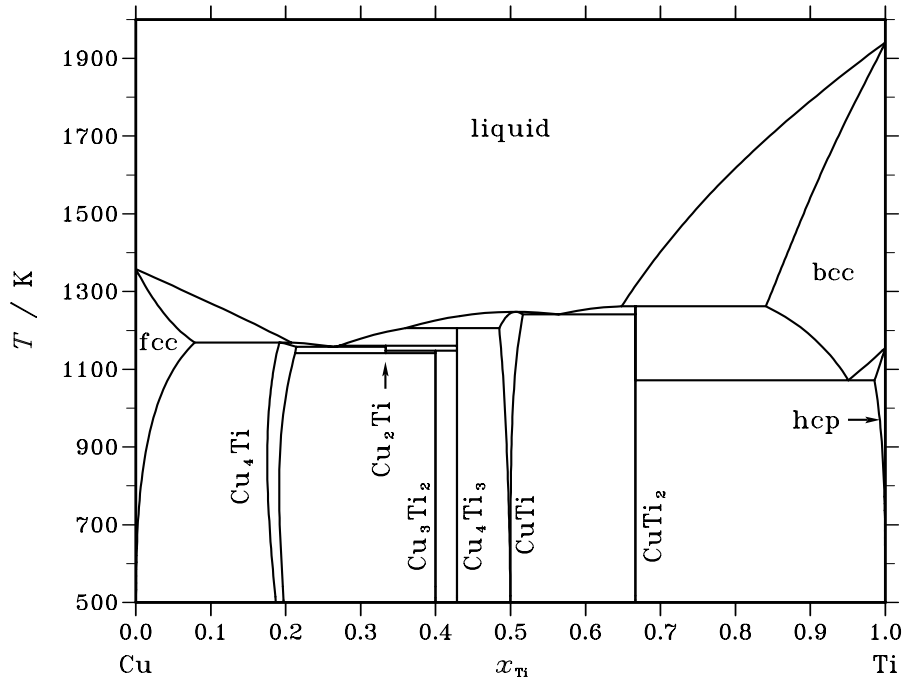

Fig. 1. Calculated phase diagram for the system Cu-Ti.

The Cu-Ti system is characterised by fairly extensive primary solid solution phases and 5 intermetallic phases with compositions lying between approximately 20 and 66.67 at.% Ti [86Mas, 94Oka]. The phases with compositions denoted as CuTi and Cu_4Ti display narrow ranges of stoichiometry. The thermodynamic assessment of the system by Hari Kumar *et al.* [96Har] provides a good representation of the published experimental thermodynamic and phase diagram information. There is a general small negative departure of thermodynamic values from ideal behaviour in the solution phases and enthalpies of formation of the intermetallic compound phases have small negative values.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Cu,Ti)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Cu,Ti)_1$
βCu_4Ti	$\cdots$	Au_4Zr	$oP20$	$Pnma$	CU4TI	$(Cu,Ti)_4(Cu,Ti)_1$
αCu_4Ti	$D1_a$	$MoNi_4$	$tI10$	$I4/m$	CU4TI	$(Cu,Ti)_4(Cu,Ti)_1$
Cu_2Ti	$\cdots$	Au_2V	$oC12$	$Amm2$	CU2TI	Cu_2Ti_1
Cu_3Ti_2	$\cdots$	Ti_2Cu_3	$tP10$	$P4/nmm$	CU3TI2	Cu_3Ti_2
Cu_4Ti_3	$\cdots$	Ti_3Cu_4	$tI14$	$I4/mmm$	CU4TI3	Cu_4Ti_3
CuTi	$B11$	γCuTi	$tP4$	$P4/nmm$	B11_CUTI	$(Cu,Ti)_1(Cu,Ti)_1$
$CuTi_2$	$C11_b$	$MoSi_2$	$tI6$	$I4/mmm$	C11B_CUTI2	Cu_1Ti_2
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Cu,Ti)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Cu,Ti)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ti}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid + bcc $\rightleftharpoons$ $CuTi_2$	peritectic	1262.2	0.648	0.841	0.667	−20039
liquid $\rightleftharpoons$ CuTi	congruent	1247.8	0.507	0.507		−17903
liquid $\rightleftharpoons$ CuTi + $CuTi_2$	eutectic	1241.4	0.564	0.517	0.667	−18488
liquid + CuTi $\rightleftharpoons$ Cu_4Ti_3	peritectic	1205.6	0.360	0.485	0.429	−8040
fcc + liquid $\rightleftharpoons$ Cu_4Ti	peritectic	1168.9	0.079	0.208	0.192	−12937
liquid + Cu_4Ti_3 $\rightleftharpoons$ Cu_2Ti	peritectic	1160.3	0.272	0.429	0.333	−7761
liquid $\rightleftharpoons$ Cu_4Ti + Cu_2Ti	eutectic	1157.8	0.265	0.214	0.333	−14288
Cu_2Ti + Cu_4Ti_3 $\rightleftharpoons$ Cu_3Ti_2	peritectoid	1147.6	0.333	0.429	0.400	−663
Cu_2Ti $\rightleftharpoons$ Cu_4Ti + Cu_3Ti_2	eutectoid	1141.6	0.333	0.213	0.400	−1539
bcc $\rightleftharpoons$ $CuTi_2$ + hcp	eutectoid	1071.5	0.951	0.667	0.986	−5818

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)]	$G^{\mathrm{E}}_{\mathrm{m}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{m}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−5856	−1199	2.328	−450	−0.375	0.000
0.200	−9053	−2552	3.250	−732	−0.910	0.000
0.300	−11055	−3744	3.655	−897	−1.424	0.000
0.400	−12173	−4549	3.812	−981	−1.784	0.000
0.500	−12533	−4833	3.850	−1007	−1.913	0.000
0.600	−12173	−4549	3.812	−981	−1.784	0.000
0.700	−11055	−3744	3.655	−897	−1.424	0.000
0.800	−9053	−2552	3.250	−732	−0.910	0.000
0.900	−5856	−1199	2.328	−450	−0.375	0.000
1.000	0	0	0.000	0	0.000	0.000

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

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

x_{Cu}	ΔG_{Cu} [J/mol]	ΔH_{Cu} [J/mol]	ΔS_{Cu} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Cu}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Cu}}$ [J/(mol·K)]	a_{Cu}	γ_{Cu}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−1846	137	0.991	−94	0.115	0.895	0.994
0.800	−4010	82	2.046	−299	0.191	0.786	0.982
0.700	−6468	−659	2.905	−537	−0.061	0.678	0.968
0.600	−9265	−2312	3.476	−770	−0.771	0.573	0.955
0.500	−12533	−4833	3.850	−1007	−1.913	0.471	0.941
0.400	−16535	−7905	4.315	−1297	−3.304	0.370	0.925
0.300	−21757	−10943	5.407	−1736	−4.603	0.270	0.901
0.200	−29225	−13092	8.067	−2462	−5.315	0.172	0.862
0.100	−41945	−13226	14.360	−3655	−4.785	0.080	0.803
0.000	$-\infty$	−9948	∞	−5542	−2.203	0.000	0.717

Reference state: Cu(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	$-\infty$	−9948	∞	−5542	−2.203	0.000	0.717
0.100	−41945	−13226	14.360	−3655	−4.785	0.080	0.803
0.200	−29225	−13092	8.067	−2462	−5.315	0.172	0.862
0.300	−21757	−10943	5.407	−1736	−4.603	0.270	0.901
0.400	−16535	−7905	4.315	−1297	−3.304	0.370	0.925
0.500	−12533	−4833	3.850	−1007	−1.913	0.471	0.941
0.600	−9265	−2312	3.476	−770	−0.771	0.573	0.955
0.700	−6468	−659	2.905	−537	−0.061	0.678	0.968
0.800	−4010	82	2.046	−299	0.191	0.786	0.982
0.900	−1846	137	0.991	−94	0.115	0.895	0.994
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(liquid)

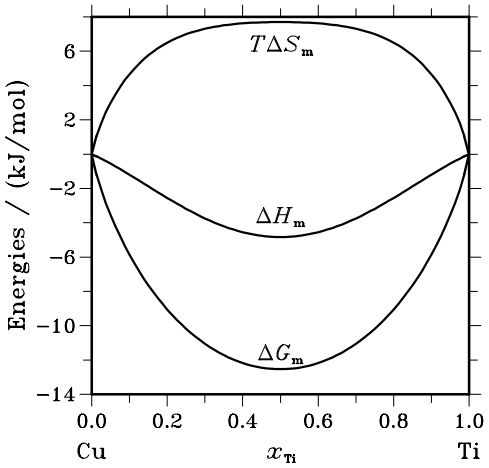

Fig. 2. Integral quantities of the liquid phase at T=2000 K.

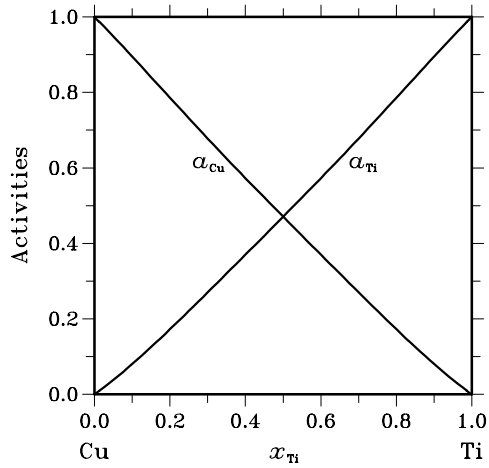

Fig. 3. Activities in the liquid phase at T=2000 K.

Table IVa. Integral quantities for the stable phases at 1373 K.

Phase	x_{Ti}	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)]
liquid	0.000	0	0	0.000	0	0.000	0.000
	0.100	−4067	−276	2.761	−355	0.058	0.616
	0.200	−6356	−706	4.115	−644	−0.045	1.232
	0.300	−7775	−974	4.953	−802	−0.126	1.848
	0.400	−8466	−856	5.542	−783	−0.054	2.464
	0.500	−8473	−216	6.013	−560	0.250	3.081
	0.600	−7807	990	6.407	−124	0.812	3.697
	0.688	−6650	2496	6.661	432	1.503	4.242
bcc	0.864	−3811	−863	2.147	731	−1.161	−0.187
	0.900	−3162	−622	1.850	549	−0.853	−0.138
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Cu(liquid), Ti(bcc)

Table IVb. Partial quantities for Cu in the stable phases at 1373 K.

Phase	x_{Cu}	ΔG_{Cu} [J/mol]	ΔH_{Cu} [J/mol]	ΔS_{Cu} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Cu}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Cu}}$ [J/(mol·K)]	a_{Cu}	γ_{Cu}
liquid	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1224	137	0.991	−21	0.115	0.898	0.998
	0.800	−2727	82	2.046	−180	0.191	0.788	0.984
	0.700	−4647	−659	2.905	−575	−0.061	0.666	0.951
	0.600	−7085	−2312	3.476	−1254	−0.771	0.538	0.896
	0.500	−10119	−4833	3.850	−2206	−1.913	0.412	0.824
	0.400	−13829	−7905	4.315	−3369	−3.304	0.298	0.744
	0.312	−17791	−10618	5.224	−4478	−4.472	0.210	0.676
bcc	0.136	−17791	−6740	8.049	4972	−8.530	0.210	1.546
	0.100	−21098	−6523	10.615	5188	−8.530	0.158	1.575
	0.000	$-\infty$	−5879	∞	5832	−8.530	0.000	1.667

Reference state: Cu(liquid)

Table IVc. Partial quantities for Ti in the stable phases at 1373 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}
liquid	0.000	$-\infty$	−716	∞	−3631	2.123	0.000	0.728
	0.100	−29649	−3993	18.686	−3363	−0.459	0.074	0.745
	0.200	−20875	−3859	12.393	−2502	−0.989	0.161	0.803
	0.300	−15074	−1711	9.733	−1330	−0.277	0.267	0.890
	0.400	−10536	1328	8.641	−76	1.022	0.397	0.993
	0.500	−6826	4400	8.176	1086	2.413	0.550	1.100
	0.600	−3793	6920	7.802	2039	3.555	0.717	1.196
	0.688	−1608	8430	7.311	2654	4.207	0.869	1.262
bcc	0.864	−1608	63	1.217	63	0.000	0.869	1.006
	0.900	−1169	34	0.876	34	0.000	0.903	1.003
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ti(bcc)

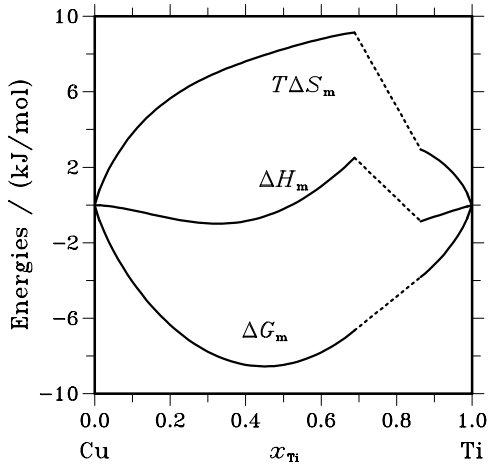

Fig. 4. Integral quantities of the stable phases at T=1373 K.

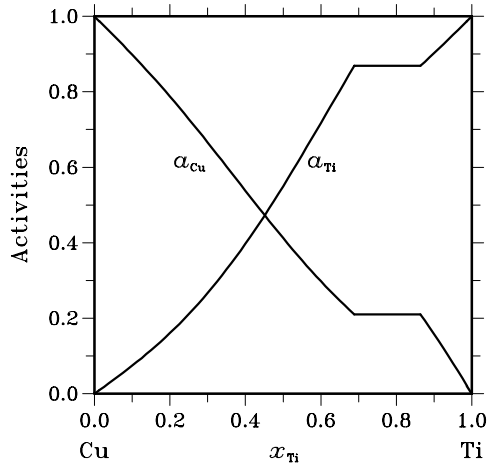

Fig. 5. Activities in the stable phases at T=1373 K.

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))	$\Delta_{\mathrm{f}}C_P^{\circ}$ / (J/(mol·K))
Cu_4Ti_1	0.200	−5314	−6010	−2.337	0.020
Cu_2Ti_1	0.333	−5876	−5876	0.000	0.000
Cu_3Ti_2	0.400	−8601	−9249	−2.172	0.000
Cu_4Ti_3	0.429	−9069	−9748	−2.278	0.000
Cu_1Ti_1	0.500	−10230	−11206	−3.272	0.000
Cu_1Ti_2	0.667	−10733	−12131	−4.688	0.000

References

[86Mas] T.B. Massalski (ed.): Binary Alloy Phase Diagrams, ASM, Metals Park, Ohio, 1986.
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[96Har] K.C. Hari Kumar, I. Ansara, P. Wollants, L. Delaey: Z. Metallkd. **87** (1996) 666–672.