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O-Ti (Oxygen-Titanium)

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The Ti-O phase diagram in [Massalski2] was adopted from [1987Mur]. [2001Oka] introduced two versions of the Ti-O phase diagram calculated by [1997Fis] and by [1999Wal].

A new thermodynamic assessment was carried out on this system by [2007Can] to refine the phase diagram of [1999Wal], as shown in Fig. 1 and 2.

The lack of reliable experimental phase boundary data caused difficulty in confirming the validity of each phase diagram in [2001Oka]. This problem still persists because few experimental data have been added since then. Therefore, as stated in [2001Oka], the differences among the phase diagrams of [1987Mur], [1997Fis], [1999Wal], and [2007Can] can only suggest the areas where further experimental work is needed. Furthermore, [2007Vil] lists quite a few Ti-O compounds not shown in Fig. 1. Some of these may be equilibrium phases. It is also needed to examine the stability of phases expressed by Ti_nO_{2n-1} $(n = 2, 3, 4\ldots)$ in Fig. 2 because these phases are so closely neighbored that their stability over a wide temperature range is questionable [1993Oka]. Experimental confirmation is needed in this regard also.

Table 1 shows Ti-O crystal structure data adopted from [1987Mur] with modifications for consistency with Fig. 1 and additional information from [2007Vil].

References

1987Mur: J.L. Murray and H.A. Wriedt, The O-Ti (Oxygen-Titanium) System, *Bull. Alloy Phase Diagr.*, 1987, **8**(2), p 148-165

1993Oka: H. Okamoto and T.B. Massalski, Guidelines for Binary Phase Diagram Assessment, *J. Phase Equilb.*, 1993, **14**(3), p 316-335

1997Fis: E. Fischer, Thermodynamic Calculation of the O-Ti System, *J. Phase Equilb.*, 1997, **18**(4), p 338-343

1999Wal: P. Waldner and G. Eriksson, Thermodynamic Modeling of the System Titanium-Oxygen, *Calphad*, 1999, **23**(2), p 189-218

2001Oka: H. Okamoto, O-Ti (Oxygen-Titanium), *J. Phase Equilb.*, 2001, **22**(4), p 515-517

2007Can: M. Cancarevic, M. Zinkevich, and F. Aldinger, Thermodynamic Description of the Ti-O System Using the Associate Model for the Liquid Phase, *Calphad*, 2007, **31**, p 330-342 (2007)

2007Vil: P. Villars and K. Cenzual, *Pearson's Crystal Data CD-ROM*, ASM International, Materials Park, OH, Release 2007/8

Table 1 Ti-O crystal structure data

Phase	Composition, at.% O	Pearson symbol	Space group	Strukturbericht designation	Prototype
(βTi)	0-8	*cI*2	$Im\bar{3}m$	*A*2	W
(αTi)	0-33.3	*hP*2	$P6_3/mmc$	*A*3	Mg
Ti_3O(a)	20-30	*hP*16	$P\bar{3}1c$	…	…
Ti_2O(a)	25-33.4	*hP*16	$P\bar{3}m1$	…	…
Ti_3O_2	40	*hP*5	*P*6/*mmm*	…	…
γTiO	40-55.3	*cF*8	$Fm\bar{3}m$	*B*1	NaCl
βTiO(a)	?	*c***	…	…	…
αTiO	50	*mC*16	…	…	…
$\beta Ti_{1-x}O$(a)	55.5	*oI*12	*I*222	…	…
$\alpha Ti_{1-x}O$(a)	55.5	*tI*18	*I*4/*m*	…	…
Ti_2O_3	60	*hR*10	$R\bar{3}c$	$D5_1$	αAl_2O_3
Ti_3O_5	62.5	*mC*32	*C*12/*m*1	…	…
Ti_4O_7	63.64	*aP*22	$P\bar{1}$	…	…
Ti_5O_9	64.39	*aP*28	$P\bar{1}$	…	…
Ti_6O_{11}	64.71	*aP*34	$P\bar{1}$	…	…
Ti_7O_{13}	65.00	*aP*40	$P\bar{1}$	…	…
Ti_8O_{15}	65.22	*aP*46	$P\bar{1}$	…	…
Ti_9O_{17}	65.38	*aP*52	$P\bar{1}$	…	…
$Ti_{10}O_{19}$	65.52	…	…	…	…
$Ti_{20}O_{39}$	66.11	*aP**	$P\bar{1}$	…	…
TiO_2	66.5-66.7	*tP*6	$P4_2/mnm$	*C*4	TiO_2 (rutile)

(a) In [1987Mur], but not shown in Fig. 1 and 2

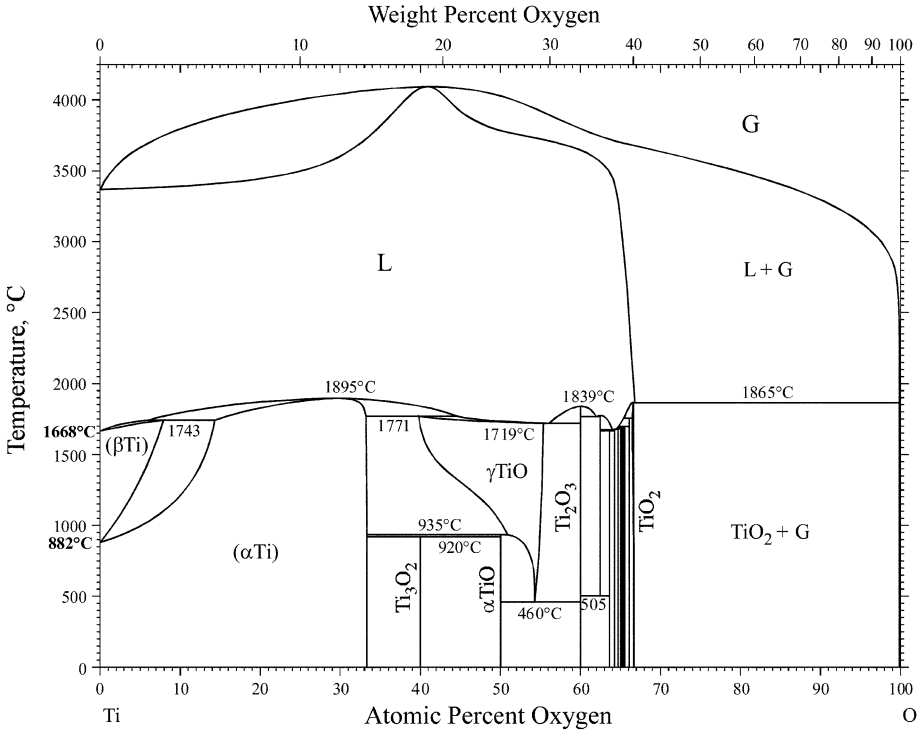

Fig. 1 Ti-O phase diagram

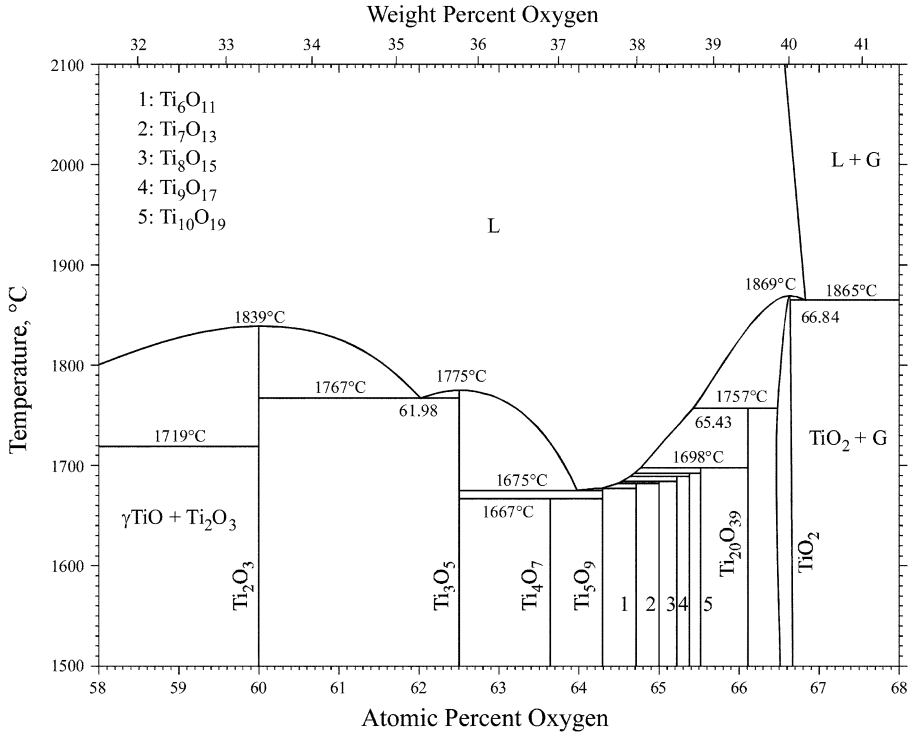

Fig. 2 Enlargement of Fig. 1 from 58 to 68 at.% O