substance: Ti_nO_{2n-1} ($n \geq 3$)
property: crystal structure of low-temperature phase ($T < T_{tr}$) of Ti_3O_5

Structurally, Ti_3O_5 differs from the other Magnéli phases; disagreement exists on details of its structure. Two crystal structures have been reported [57A1, 57A2, 57A3, 59A, 69I].

crystal structure: Fig. 1b. Characteristic groups of six edge-sharing octahedra arranged in "steps"; some relationship to anatase (Fig. 2), to which it is converted on oxidation [69I], though reduction of anatase at 1250ºC for 3 h with H_2 gives a metastable form of the high-temperature phase [69I], which may be stabilized by quite small quantities of e.g. Fe^{3+} [59A]. Space group C_{2h}^3 – C2/m, $Z = 4$.

atomic position parameters

[59A]

In C2/m unit cell, all atoms occupy point position 4(i); (0, 0, 0; 1/2, 1/2, 0); *x*, 0, *z*; –*x*, 0, –*z*.

	x	*z*
Ti(1)	0.1280	0.0440
Ti(2)	0.7786	0.2669
Ti(3)	0.0538	0.3659
O(1)	0.676	0.060
O(2)	0.241	0.245
O(3)	0.588	0.345
O(4)	0.953	0.158
O(5)	0.866	0.441

lattice parameters

a	9.752 Å	*T* = 20ºC	59A
b	3.802 Å		
c	9.442 Å		
β	91.55º		
a	9.76 Å	RT	69I
b	3.80 Å		
c	9.43 Å		
β	91º35'		

density

d_{calc}	4.16 g cm^{-3}	RT	69I

interatomic distances

d(Ti(1) –	2	Ti(1))	3.174(10) Å	*T* = 20ºC	partial bond-strength analysis	59A
		Ti(1)	2.610(10) Å		suggests that Ti(1) is Ti^{3+} but	
	2	Ti(2)	3.168 (7) Å		the charges on Ti(2) and Ti(3)	
		Ti(2)	3.097(7) Å		are 10/3 and 11/3, respectively	
		Ti(3)	3.143(7) Å			
	2	O(1)	1.96(4) Å			
		O(1)	2.17(4) Å			
		O(2)	2.17(3) Å			
		O(4)	2.04(3) Å			
		O(4)	2.04(3) Å			

d(Ti(2) –	2	Ti (3))	3.067(7) Å
		Ti(3)	2.818(7) Å
		O(1)	2.18(4) Å
	2	O(2)	1.95(3) Å
		O(3)	2.01(3) Å
		O(4)	2.01(3) Å
		O(5)	1.83(2) Å
d(Ti(3) –		Ti(3))	2.767(10) Å
		O(2)	2.18(3) Å
	2	O(3)	1.94(3) Å
		O(4)	2.17(3) Å
		O(5)	1.99(2) Å
		O(5)	1.97(2) Å
d(O(1) –	2	O(1))	2.66(7) Å
	2	O(2)	2.65(5) Å
		O(2)	3.01(5) Å
		O(3)	2.84(4) Å
		O(4)	2.83(4) Å
	2	O(4)	3.05(4) Å
	2	O(4)	3.04(4) Å
d(O(2) –	2	O(3))	2.61(4) Å
	2	O(4)	2.94(4) Å
		O(4)	2.91(4) Å
	2	O(5)	2.90(4) Å
		O(5)	3.17(4) Å
d(O(3) –	2	O(4))	2.89(4) Å
		O(5)	2.83(4) Å
	2	O(5)	3.04(4) Å
	2	O(5)	2.81(4) Å
d(O(4) –		O(4))	3.14(5) Å
		O(5)	2.83(3) Å
d(O(5) –	2	O(5))	3.17(4) Å
		O(5)	2.82(4) Å

References:

57A1 Andersson, S., Collén, B., Kuylestrina, U., Magnéli, A.: Acta Chem. Scand. 11 (1957) 1641.

57A2 Andersson, S., Collén, B., Kruuse, G., Kuylestrina, U., Magnéli, A., Pestinalis, H., Asbrink, S.: Acta Chem. Scand. 11 (1957) 1653.

57A3 Asbrink, S., Magnéli, A.: Acta Chem. Scand. 11 (1957) 1606.

59A Asbrink, S., Magnéli, A.: Acta Crystallogr. 12 (1959) 575.

69I Iwasaki, H., Bright, N. F. H., Rowland, J. F.: J. Less-Common Met. 17 (1969) 99.

Fig. 1.

Ti_3O_5. Crystal structures of the high temperature (a) and low temperature (b) phases. Unit cells are indicated by dotted lines and primes refer to symmetry related atomic sites [59A].

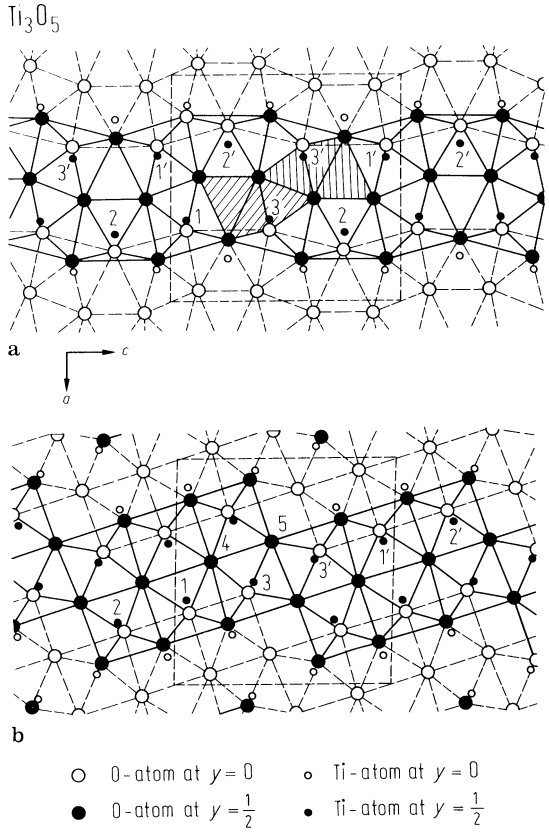

Fig. 2.

Ti_3O_5. Arrangements of TiO_6 octahedra in anatase (010) plane (a) and low-temperature M-type Ti_3O_5 (010) plane (b). (c) shows the common structural unit, present in (a) and (b) [69I].