substance: titanium oxide (TiO_2)
property: crystal structure, lattice parameters and related parameters of rutile

crystal structure: tetragonal, space group D_{4h}^{14} – $P4_2/mnm$, $Z = 2$ [79M]. The structure may be derived from the hexagonal B8 structure of NiAs by ordering Ti^{4+} ions into alternate sites of the *c*-axis chains of face-shared octahedra. Within a hexagonal plane, the Ti^{4+} ions are ordered into alternate [100] strings. Reduction of the bridging O – O band produces, in this case with $c_{hex} = 3^{1/2}a$, a tetragonal unit cell having as *c* the Ti – Ti distance in the strings of edge-shared TiO_6 octahedra (Fig. 2). Each oxygen is coplanar with three nearest-neighbour Ti^{4+} ions and has a p_π orbital directed perpendicular to this plane toward a cation vacancy on one side, a pair of cation vacancies on the other.

lattice parameters

a	4.5941 Å	*T* = 30ºC	70R
c	2.9589 Å		
a	4.5963 Å	*T* = 84ºC	
c	2.9601 Å		
a	4.5981 Å	*T* = 161ºC	
c	2.9619 Å		
a	4.6007 Å	*T* = 210ºC	
c	2.9639 Å		
a	4.6025 Å	*T* = 258ºC	
c	2.9654 Å		
a	4.6035 Å	*T* = 306ºC	
c	2.9668 Å		
a	4.6059 Å	*T* = 354ºC	
c	2.9684 Å		
a	4.6074 Å	*T* = 401ºC	
c	2.9699 Å		
a	4.6091 Å	*T* = 449ºC	
c	2.9710 Å		
a	4.6105 Å	*T* = 497ºC	
c	2.9726 Å		
a	4.6123 Å	*T* = 534ºC	
c	2.9741 Å		
a	4.6141 Å	*T* = 571ºC	
c	2.9757 Å		
a	4.6163 Å	*T* = 608ºC	
c	2.9772 Å		
a	4.6176 Å	*T* = 645ºC	
c	2.9788 Å		

density

d_{calc}	4.250 g cm^{-3}	*T* = 298 K	70R

interatomic distances and angles

(distances in Å, angles in °) (from [79M])

	T = 25°C	T = 300°C	T = 600°C	T = 900°C	
d(Ti–O_{Ia}) (4)	1.947(2)	1.954(2)	1.961(2)	1.962(2)	Number behind d in
d(Ti–O_{Ib}) (2)	1.982(3)	1.983(3)	1.988(3)	1.995(3)	parentheses: multiplicity
d(Ti–O)$_{av}$	1.959	1.964	1.970	1.973	of interatomic distance
d(O_{Ia}–O_{Ia}) (s) (2)	2.532(5)	2.544(6)	2.552 (6)	2.547 (5)	(s) shared edge,
d(O_{Ib}–O_{Ia}) (8)	2.778(2)	2.784(2)	2.792(2)	2.799(2)	(u) unshared edge
d(O_{Ia}–O_{Ia}) (u) (2)	2.959 (2)	2.966(2)	2.977(2)	2.986(2)	
d(O–O)$_{av}$	2.767	2.774	2.783	2.788	
d(Ti–Ti)	2.959 (2)	2.966(2)	2.977 (2)	2.986 (2)	
angle (O_{Ia}–Ti–O_{Ia})(5)	81.12(12)	81.23(14)	81.22(14)	80.93(12)	
angle (Ti–O_{Ia}–Ti)	130.56(6)	130.62(7)	130.61(7)	130.47(6)	

coefficient of linear thermal expansion

$\alpha_{\parallel}$	$8.816\cdot10^{-6} + 3.653\cdot10^{-9}(T–273) + 6.329\cdot10^{-12}(T–273)^2$	see Fig. 1	70R
$\alpha_{\perp}$	$7.249\cdot10^{-6} + 2.198\cdot10^{-9}(T–273) + 1.298\cdot10^{-12}(T–273)^2$		

References:

70R Rao, K. V. K., Nagender Naidu, S. V., Iyengar, L.: J. Am. Ceram. Soc. 53 (1970) 124.
79M Meagher, E. P., Lager, G. A.: Can. Mineral. 17 (1979) 77.

Fig. 1.

TiO_2, anatase and rutile. Thermal expansion coefficients vs. temperature [70R].

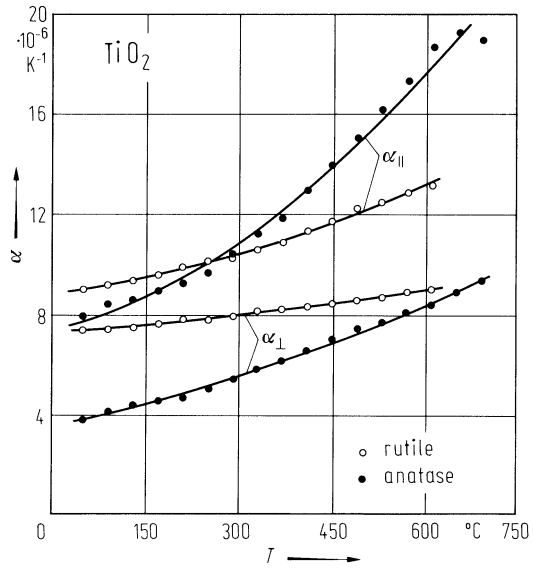

Fig. 2.

TiO_2, rutile. Crystal structure [79M].