substance: titanium oxide (TiO_2)
property: physical properties of anatase

energy gap

E_g	3.23 eV	80G

Real and imaginary parts of the refractive index: Fig. 2. Optical absorption spectrum: Fig. 1.

defects

Very little systematic work has been reported on defects in anatase; evidence has however been adduced to support the argument that defects similar to the "A" centre in rutile can be formed on irradiation [77M].

phonon wavenumbers

Under the space group D_{4h}^{19} the local site vibrational fundamentals transform as $a_{1g} + a_{2u} + 2b_{1g} + b_{2u} + 3e_g + 2e_u$, of which a_{1g}, b_{1g}, and e_g are Raman active.

(in cm^{-1}, RT values)

ν/c	144 vvs	Mode: e_g	w: weak, m: medium,	67B
	144		s: strong, vs: very strong	78O
	197 w	e_g	Weak second order peaks also	67B
	197		seen at 316,696 and 796 cm^{-1}	78O
	400 m	b_{1g}	[67B]. The e_g band at 197 cm^{-1}	67B
	399		is considerably softened from	78O
	515 mw	b_{1g}	the value reported from a	67B
	513		rigid-ion calculation [79K];	78O
	519 mw	a_{1g}	for temperature dependence,	67B
	519		see Fig. 3, for pressure dependence,	78O
	640 m	e_g	see Fig. 4	67B
	639			78O

Above 25.6 kbar a transition to a new form of TiO_2 is observed which may have the PbO_2 or $CaCl_2$-structure [79O]. A similar transition has been reported for rutile.

transport properties

Resistivities of as grown crystals very variable: $10^4...10^{12}$ Ω cm [78V] at RT. Some typical data are shown in Fig. 5. For the more conducting samples two regions of behaviour are found: for T > RT, $\log \rho \propto E_A/kT$, where $E_A \approx 0.38$ eV. For T < RT, random hopping behaviour is found, with $\log \rho \propto (T_0/T)^{1/4}$ and $T_0 \approx 22$ K [78V].

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Fig. 1.

TiO_2, anatase and rutile. Low resolution spectra (optical density vs. wavenumber) [58B].

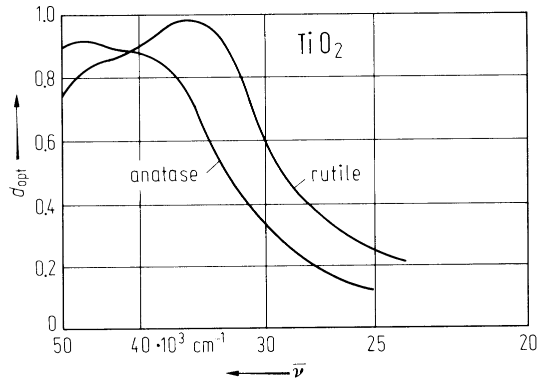

Fig. 2.

TiO_2. Optical properties of anatase films grown anodically on Ti metal in 1 N sulfuric acid [77B].

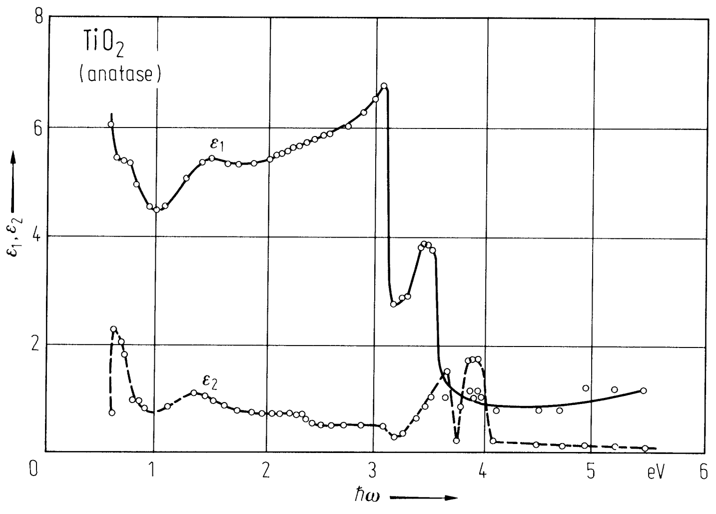

Fig. 3.

TiO_2. Raman shift vs. temperature for anastase modification [78O].

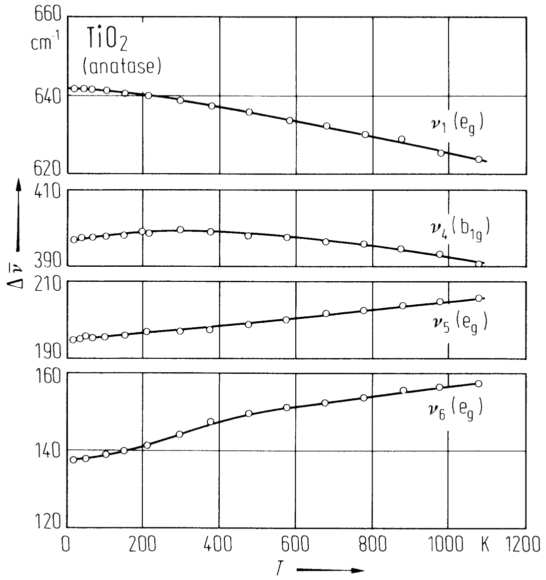

Fig. 4.

TiO_2. Raman wavenumbers vs. pressure at 298 K for anatase modification [78O].

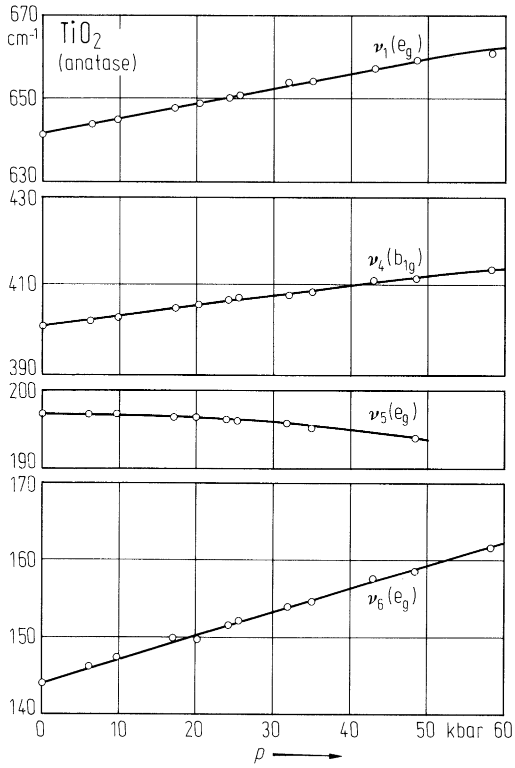

Fig. 5.

TiO_2. Electrical resistivity of anatase modification vs. temperature. Curves *1*...*3*: ρ vs. $10^3/T$ for three (unoriented) samples of differing dopant level; curves *1*', *2*': ρ vs. $(1/T)^{1/4}$ for the two (unoriented) samples of lower resistivity [78V].