substance: VO_2
property: electronic properties

Calculations of the electronic structure: cluster type [76L, 75S], tight binding type [71M, 73M, 77A], APW type [72M, 73C1, 73C2], band structure types [77G], calculation of Hubbard-*U*: [73H, 78S], semi-empirical band structures [69B, 73G]. Photoelectron spectrum [78V] shows a shift of the V 3d band by 0.3 eV to lower binding energies at T_{tr}. Other PE data show the development of a clear Fermi edge above T_{tr} [80B].

low-temperature phase (semiconducting)

Brillouin zone: Fig. 1, energy bands: Fig. 2, density of states: Fig. 3. For E_g-values see document (absorption coefficient).

high-temperature phase (metallic)

Brillouin zone: Fig. 4, energy bands: Fig. 5, density of states: Fig. 6, semi-empirical band-: Fig. 7

Hubbard self-energy ("Hubbard-*U*")

U	0.5(5)...0.7(5) eV	theoretical estimates	79S
	1.22 eV		78S
	2 eV		73H
	1.1 eV	experimental upper limit	79S
	0.92 eV	photoconductivity	80K

References:

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Fig. 1.

VO_2. a) Brillonin zone for monoclinic VO_2; b) the k_1 plane of the zone shown in a) [73C2]. $\boldsymbol{K}_{1,2,3}$: reciprocal lattice vectors; $\boldsymbol{k}$ arbitrary vector.

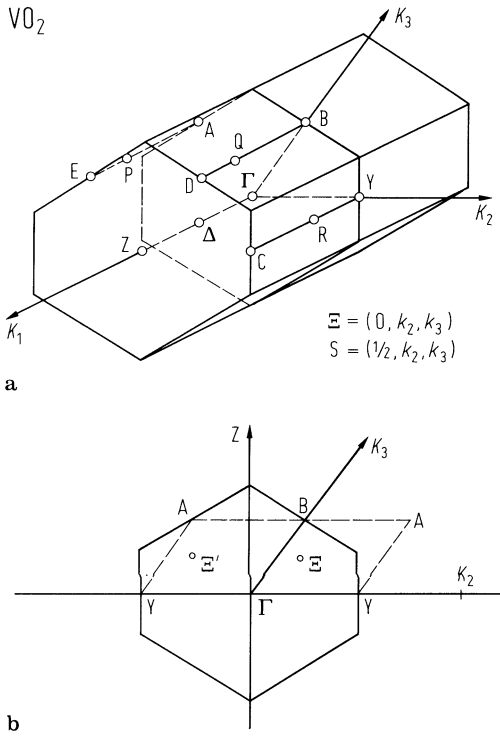

Fig. 2.

VO_2. Energy bands for the d-band region for monoclinic VO_2 [73C2].

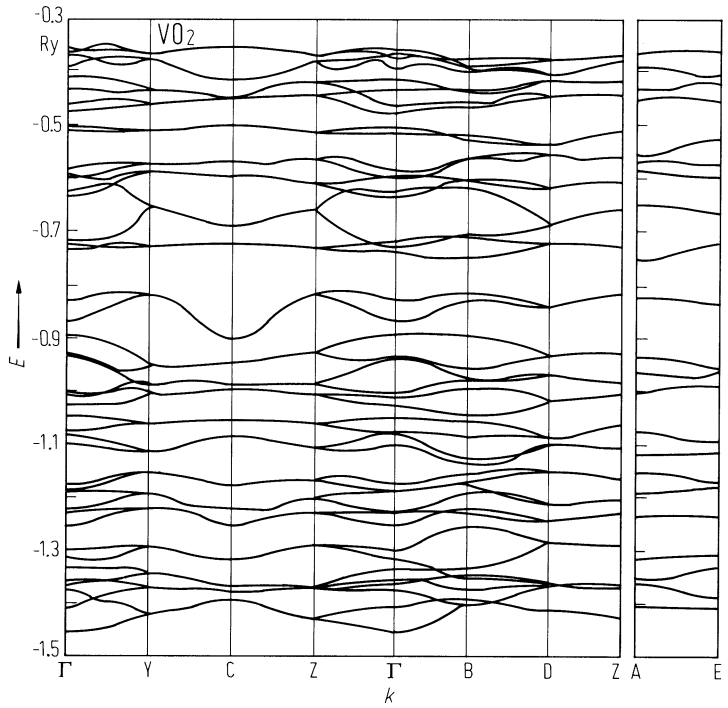

Fig. 3.

VO_2. Density of states corresponding to the energy bands of Fig. 2 [73C2].

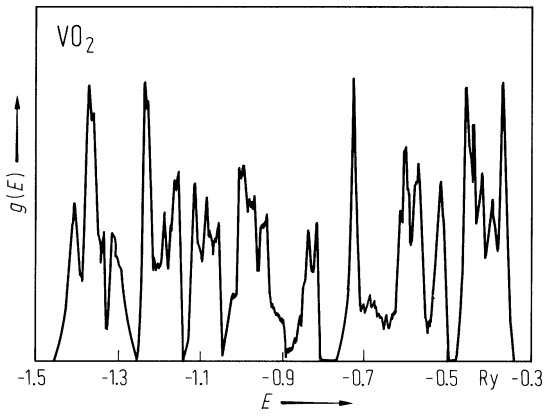

Fig. 4.

TiO_2, rutile. (a) Unit cell, (b) Brillouin zone [77V]. Distances in Å.

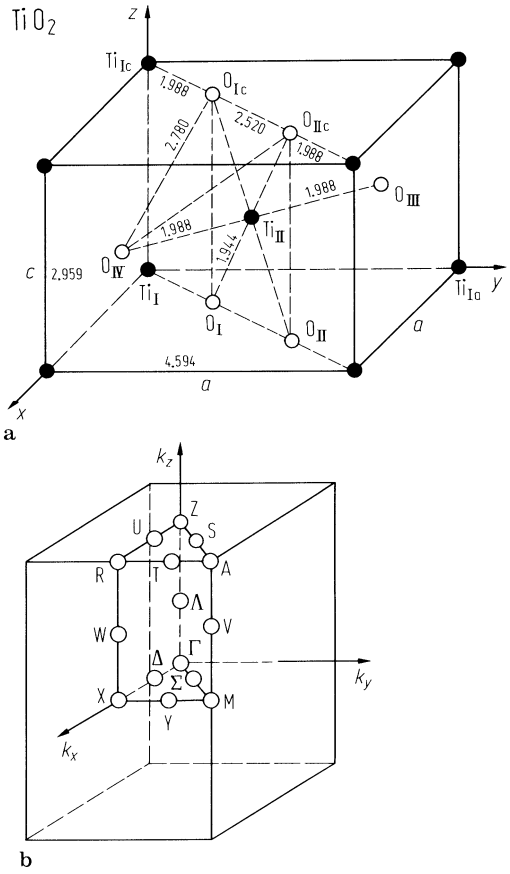

Fig. 5.

VO_2. Energy bands for the d-band region for rutile (metallic) VO_2 [73C1].

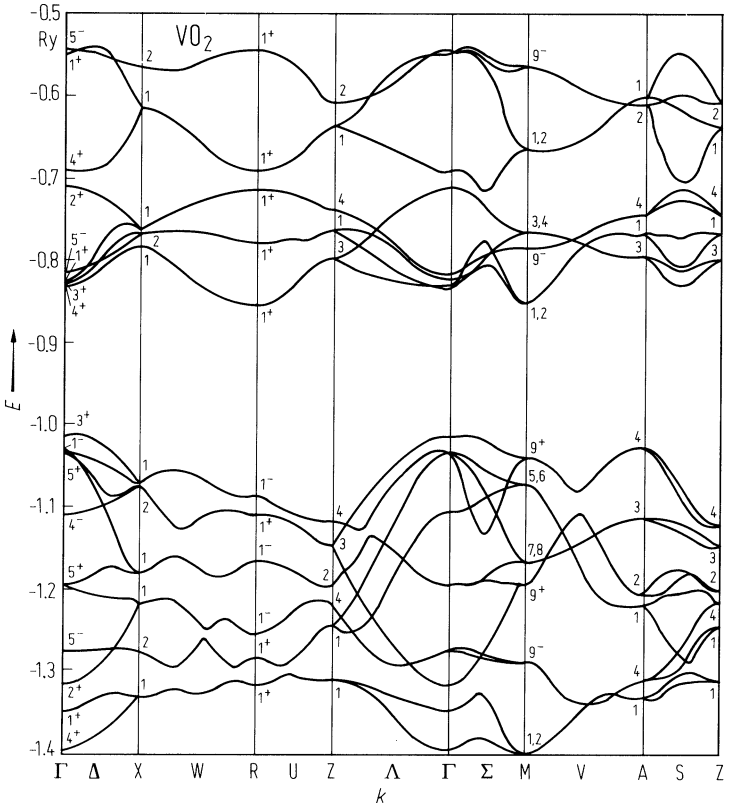

Fig. 6.

VO_2. Density of states corresponding to the energy bands of Fig. 5 [73C1]. $g(E)$ in states Ry^{-1} (unit cell)$^{-1}$ (?).

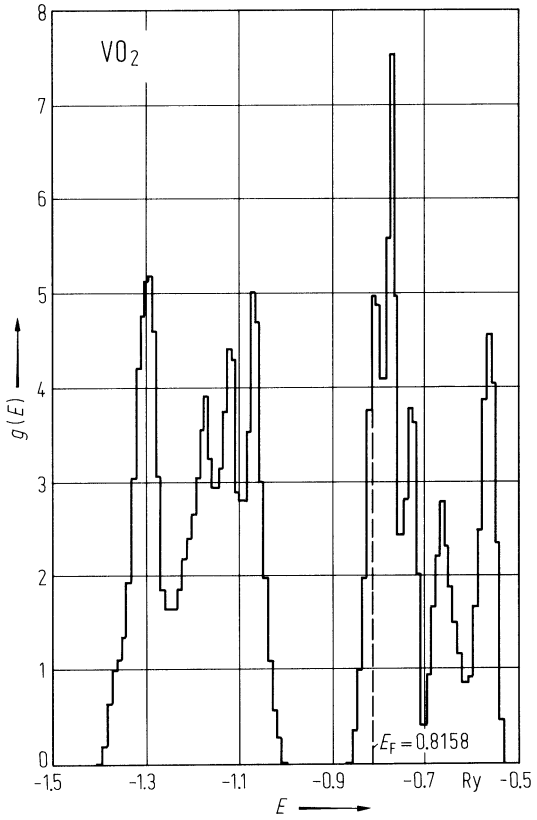

Fig. 7.

VO_2. Phenomenological band structure (a) for $T > T_{tr}$, (b) details of the d-band region for $T > T_{tr}$, (c) details for the d-band region for $T < T_{tr}$ [73G].