substance: Ti_2O_3
property: optical spectra

Near infrared reflectance: Fig. 1, visible and UV reflectance; Fig. 2, XPE spectrum: Fig. 3.

IR reflectance shows a feature extending from 1200 to 3000 cm^{-1} whose polarization dependence suggests that it is the $a_1 - e_\pi$ transition. ε_2 exhibits considerable structure at ca. 1 eV which may contain both $a_1 - e_\pi$ and $e_\pi - e_\pi^*$ transitions, the latter playing a role due to a_1/e_π mixing for $k \neq 0$. At 3.0 eV further structure is found and assigned to $a_1 - a_1^*$. Peaks $C^\perp$ and $C^\parallel$ are assigned to $a_1 - e_\sigma$ though both O – Ti charge transfer and Ti d – s transitions should also be considered. The XPE spectrum reveals at ≈ 300 K a d-band of width 1...1.5 eV, in agreement with the above analysis, showing that Ti_2O_3 is clearly a semiconductor at 300 K. However, at 580 K there is a clear metal-like Fermi edge.

Fig. 4 shows the temperature dependence of the $a_1 - e_\pi$ and mixed $a_1 - e_\pi$, $e_\pi - e_\pi^*$ transitions. Thermoreflectance [79B] and resonant Raman spectra [75S] show the presence of an additional small feature at 2.3...2.4 eV assigned variously to $a_1 - e_\pi^*$ and $e_\pi - e_\pi^*$, and [79B] confirms the assignment of the structure near 3.0 eV to $a_{1g}...a_{1g}^*$. The thermoreflectance [79B] also assign structure at 1.8 eV to plasmon resonance.

References:

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76S Sinha, A. P. B., Honig, J. M.: J. Solid State Chem. 19 (1976) 391.
78L1 Lucovsky, G., Allen, J. W., Allen, R.: Phys. Semicond. Proc. Int. Conf. 14th 1978.
78L2 Lu, S. S. M., Pollak, F. H., Raccah, P. M.: Phys. Rev. B17 (1978) 1970.
79B Bianconi, A., Stizza, S., Bernardini, R., Nannarone, S.: Phys. Status Solidi (b) 93 (1979) 5767.

Fig. 1.

Ti_2O_3. Imaginary part of the dielectric constant vs. photon energy in the near infrared for both polarization directions at 300 K. Solid lines from [78L1], dots from [78L2].

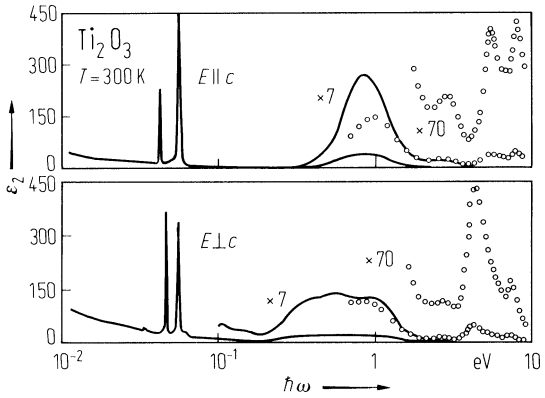

Fig. 2.

Ti_2O_3. Imaginary part of the dielectric constant vs. photon energy in the visible and uv region for both polarization directions at 300K [78L2].

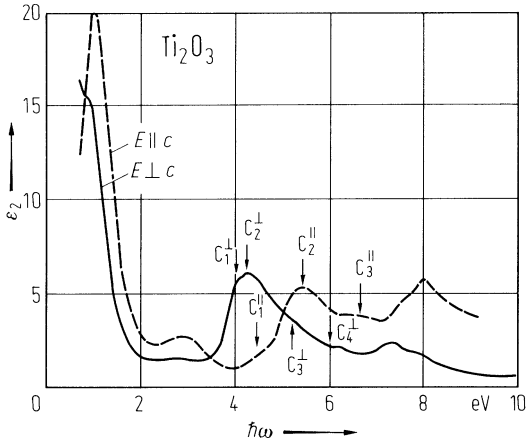

Fig. 3.

Ti_2O_3. XPE spectrum (relative intensity vs. electron binding energy) at (a) 300 K and (b) 580 K [76S]. Two lines are upper and lower limits to the spectral noise.

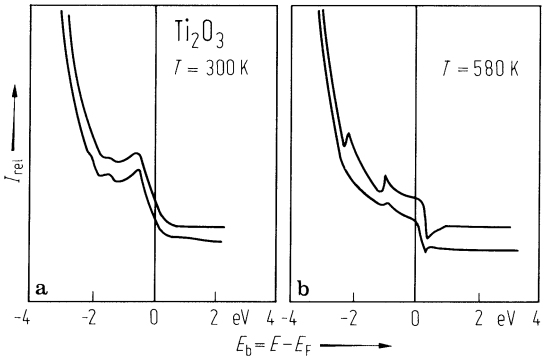

Fig. 4.

Ti_2O_3. Energy of the $a_1 \rightarrow e_\pi$ transition ($E \perp c$) and the mixed $a_1 \rightarrow e_\pi$, $e_\pi \rightarrow e_\pi^*$ transition ($E \parallel c$). Full circles: optical data, open circles: dc conductivity [78L1].