substance: NbO_2
property: band structure, optical spectra

No calculation of low-temperature phase band structure has been reported. The high-temperature rutile phase has been calculated using an APW technique [79P]. Reduced Brillouin zone: Fig. 1, band structure: Fig. 2, density of states: Fig. 3.

The optical spectrum has been reported in preliminary form [76L] and a comparison of the theoretical joint density of states for the rutile form with experimental data is shown in Fig. 4 for both the low-temperature and the rutile form stabilized to room temperature by addition of 20% Ti. The transitions below 3.4 eV are assigned to d–d transitions on Nb, and O 2p – Nb 4d charge transfer only occurs at energies above this.

The He I and XPE spectra are shown in Figs. 5 and 6. Comparison with RuO_2 and MoO_2 is also facilitated by the empirical band structure diagram for the LT form shown in Fig. 7. The d bands are quite narrow, that in NbO_2 being ca. 1 eV.

References:

76L Lu, S. S. M., Shin, S. H., Pollak, F. H., Raccah, R. M.: Proc. 13th Int. Conf. Semicond. Rome 1976, p. 330.

78B Beatham, N.: D. Phil. Thesis, Oxford 1978.

79P Posternak, M., Freeman, A. J., Ellis, D. E.: Phys. Rev. B19 (1979) 6555.

Fig. 1.

NbO_2. Brillouin zone of the rutile form [79P].

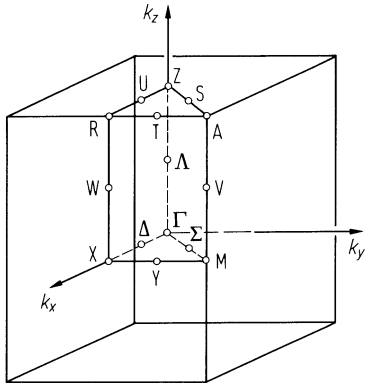

Fig. 2.

NbO_2. Band structure of the rutile form [79P].

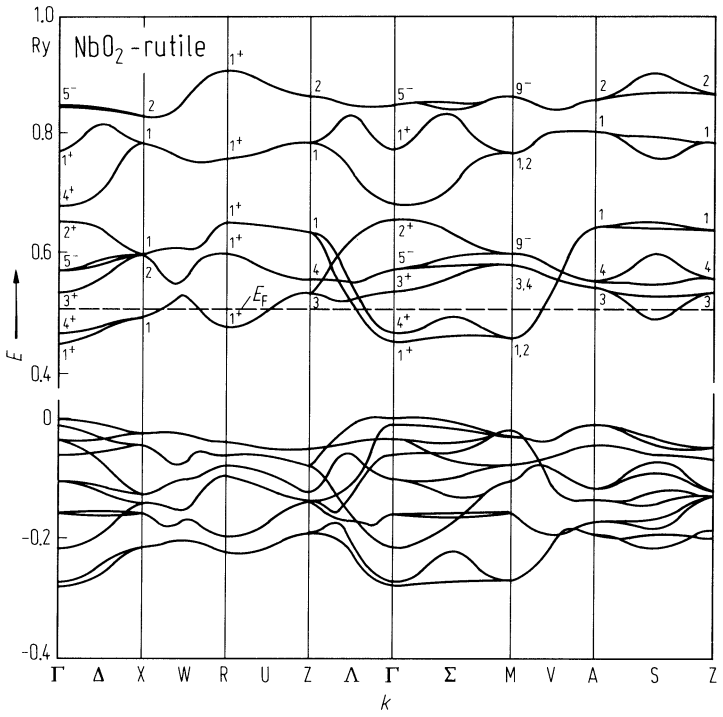

Fig. 3.

NbO_2. Density of states for metallic rutile form NbO_2 [79P].

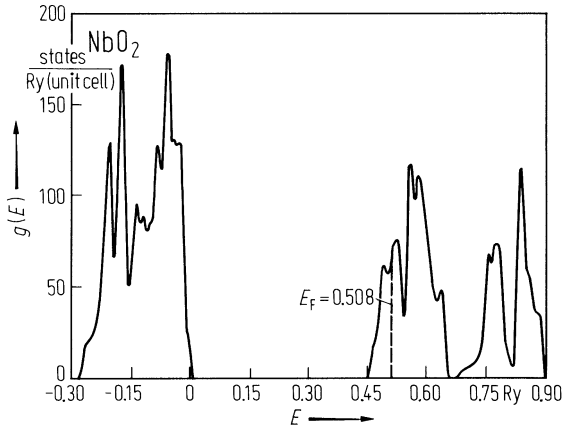

Fig. 4.

NbO_2. Joint density of states for (a) the rutile and (b) the low-temperature forms compared to experimental values of ε_2 shown as perpendicular lines [76L].

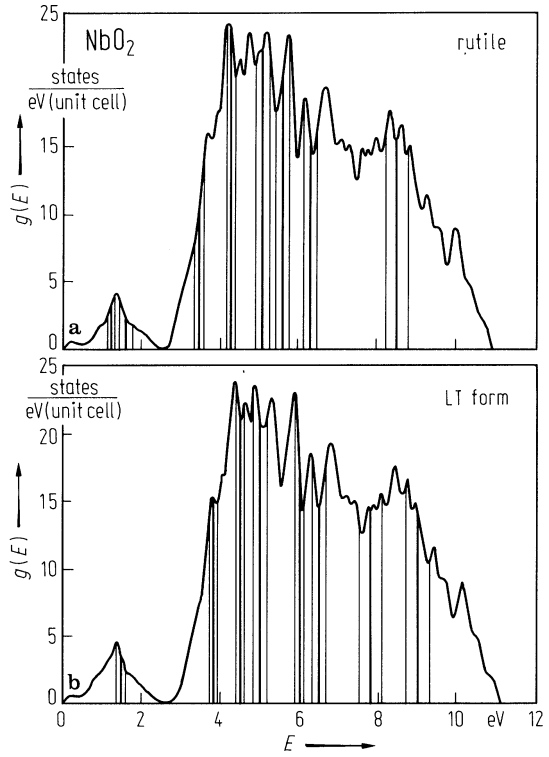

Fig. 5.

NbO_2. He I and He II spectra (intensity vs. electron kinetic energy) of NbO_2 and Nb_2O_5 at RT [78B].

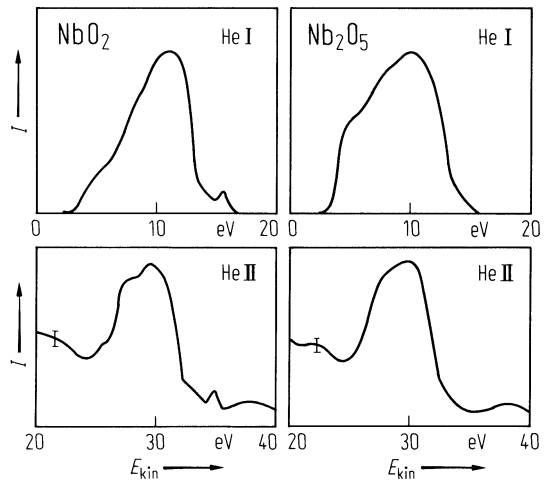

Fig. 6.

NbO_2. XPE spectrum (intensity vs. electron kinetic energy) of the valence band region (at RT) and comparison with MoO_2 and RuO_2 [78B].

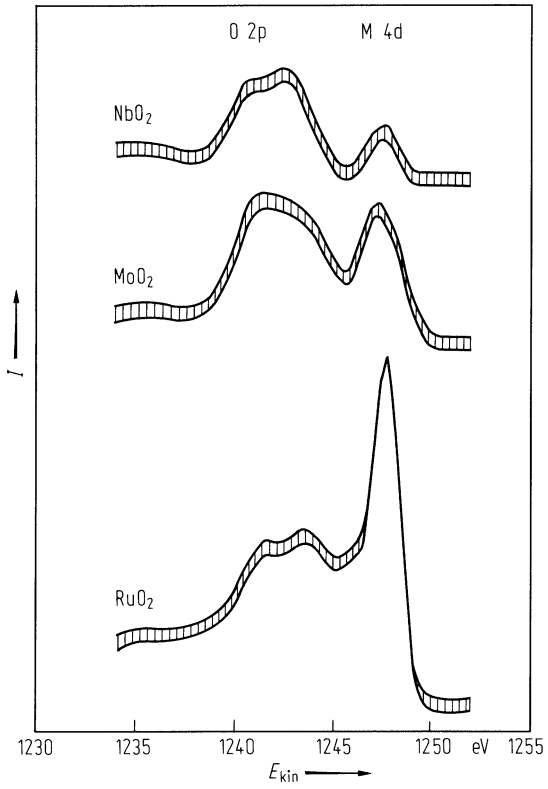

Fig. 7.

NbO_2. Empirical band scheme (low temp. form) and comparison with MoO_2 and RuO_2 [78B]. Numbers in brackets refer to number of states per formula unit (Nb_2O_4 etc.).