substance: Ta_2O_5
property: transport properties and non-stoichiometry

Ta_2O_5 is almost a line phase, and direct measurements of non-stoichiometry have only proved possible at the lowest oxygen partial pressures (Fig. 1).

Transport parameters vs. oxygen partial pressure: conductivity: Fig. 2a, transport number for ionic conductance, t_i: Fig. 2b, Seebeck coefficient: Fig. 3, for resistance vs. temperature, see Fig. 4.

The Seebeck coefficient shows a change from n- to p-type behaviour with increasing p_{O2}.
The logarithm of the oxygen pressure at the p-n transition varies linearly with reciprocal temperature [62K]. At higher oxygen pressures t_i goes through a maximum and σ through a minimum. Activation energies vary with p_{O2} (in atm) at log $p_{O2} = -16$, $E_A \approx 1.9$ eV (T = 900...1400°C) whereas at higher p_{O2} E_A is lower (Fig. 4).

The resistivity has a marked maximum with p_{O2} at the p-n transition.

Interpretation is bedevilled by the significant ionic contribution. Two regions may be distinguished:

$n >> I, p$ ($\sigma \propto p_{O2}^{-1/6}$) and $p, n << I$ ($\sigma \propto p_{O2}^{-1/4}$). Further analysis showed [74S]:

(a) the ratio of ionic and electron mobilities is activated with E_A = 2.0 eV (T = 900...1400°C),

(b) the ionic conductivity is activated with E_A = 1.8 eV (T = 900...1400°C),

(c) $\mu_n \approx 0.05$ cm^2/V s, $\mu_{ion} \approx 2 \cdot 10^{-3}$ cm^2/V s at 1100°C for a ceramic sample,

(d) Seebeck data suggest motion by electrons in a very narrow conduction band,

(e) if the minimum in conductivity corresponds to $n = p$, then the activation energy for the electron conductivity is 1.8 eV, assuming unactivated mobility and $E_g \approx 3.6$ eV.

Anodic thin amorphous film measurements at 300 K have led to very small values of $\mu_n \approx 10^{-12}$ cm^2/V s [73A, 74J] with the Fermi level apparently pinned 0.44 eV below the conduction band. The interpretation of these results is controversial [76Y, 78G].

ac conductivity results (Fig. 5) were analyzed in terms of a power law (real part of admittance proportional to ω^n) At low temperatures (near RT) n = 0.95, but for higher temperatures and lower frequencies, n decreases [77J]; at 380 K and $\nu < 1$ Hz, n = 0.3 [79S1]. The value of n is consistent with random range hopping models with $E_A \approx 0.3$ eV.

Photoconductivity (Fig. 6) shows a threshold at ≈ 1.5 eV and a strong peak at 2.1 eV [73T, 74T]. The results have been interpreted in terms of an impurity level situated ca. 2.1 eV below the conduction band edge.

References:

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76Y Young, P. L.: J. Appl. Phys. 47 (1976) 235.
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Fig. 1.

Ta_2O_5. Oxygen vacancy concentration vs. (reciprocal) temperature at $p_{O_2} = 10^{-16}$ atm [74S].

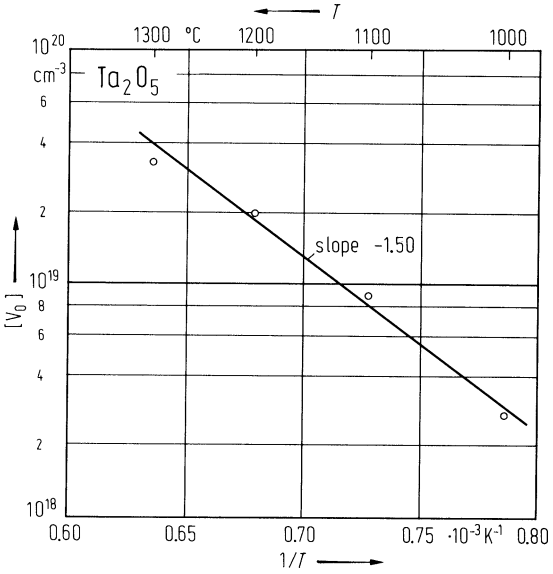

Fig. 2.

Ta_2O_5. (a) Conductivity vs. oxygen partial pressure at 10 kHz at various temperatures, (b) ionic transfer number t_i (defined as $t_i = \sigma_i/\sigma_{tot}$; σ_i = ionic conductivity) vs. oxygen partial pressure at various temperatures for polycrystalline samples [74S].

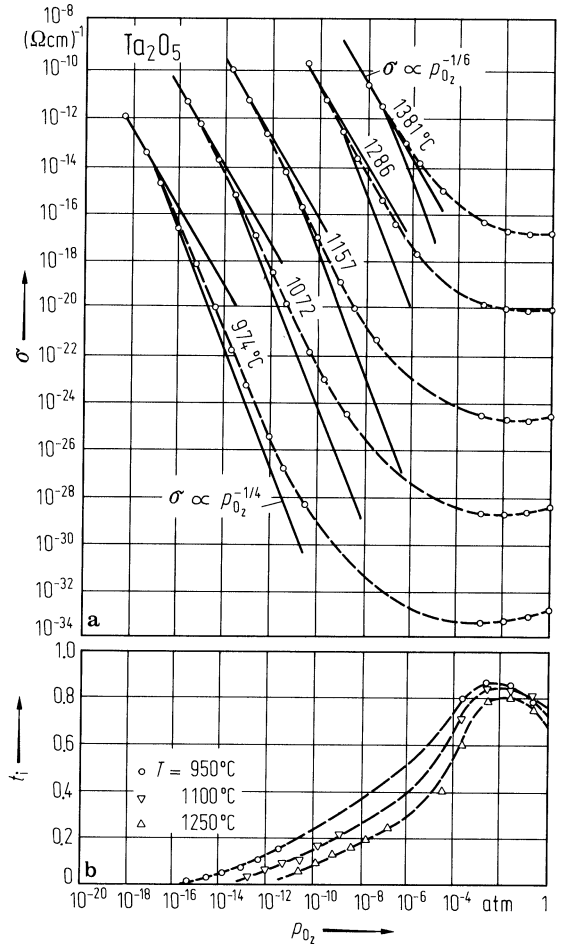

Fig. 3.

Ta_2O_5. Seebeck coefficient vs. oxygen partial pressure at various temperatures for polycrystalline samples [74S].

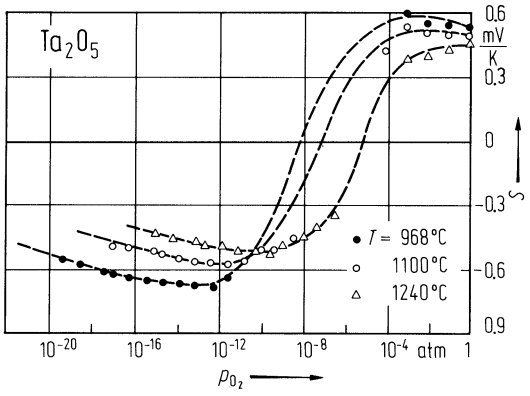

Fig. 4.

Ta_2O_5. Resistance vs. (reciprocal) temperature at p_{O_2} = 1 atm [62K].

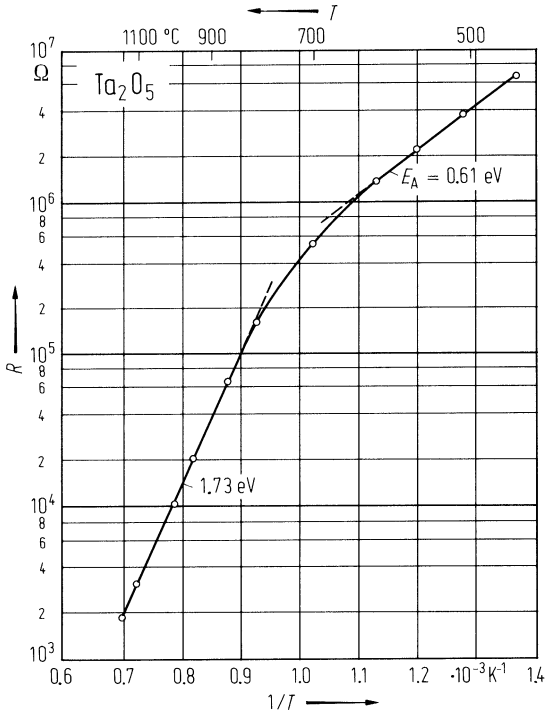

Fig. 5.

Ta_2O_5. (*a*) Conductance vs. frequency of single crystal α-Ta_2O_5 at (*1*) 295 K, (*2*) 320 K, (*3*) 340 K, (*4*) 360 K, (*5*) 380 K, (*b*) capacitance (over *C* at 1 kHz) vs. frequency at various temperatures as in (a) [79S2].

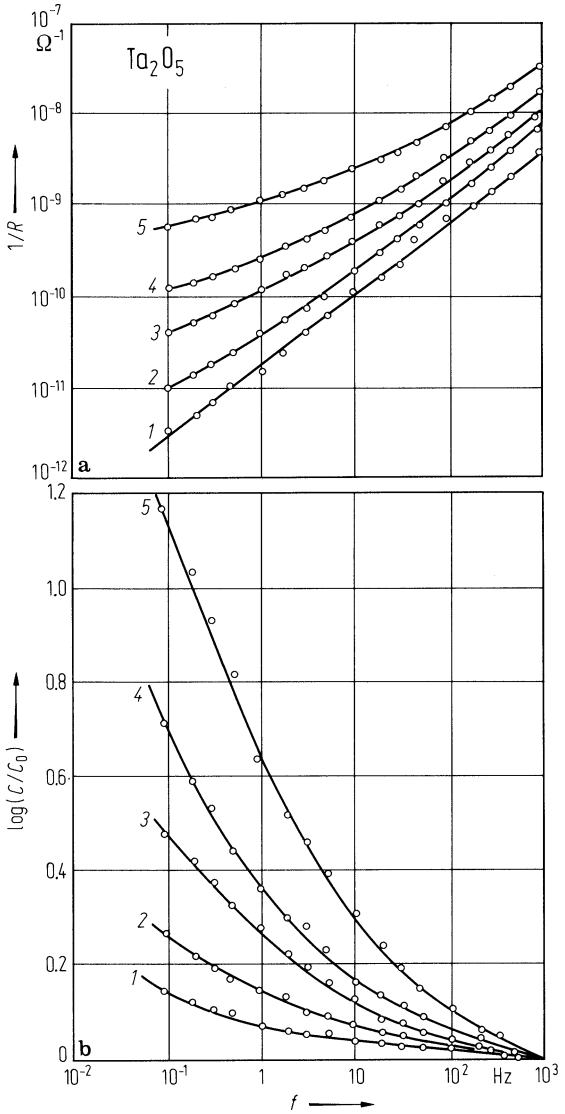

Fig. 6.

Ta_2O_5. Photocurrent (corrected for lamp intensity) vs. photon energy; the sample was irradiated by UV lamp giving the steady-state photocurrents shown [74T].