substance: Ta_2O_5
property: crystal structure and related parameters of L-Ta_2O_5

The Ta–O phase diagram appears to show only one thermodynamically stable phase, Ta_2O_5.
Ta_2O_5 exists in two forms, L- or β-Ta_2O_5, stable below 1320ºC, and H- or α-Ta_2O_5, which is the stable form at high temperature. Kinetics of transformation are slow and H-Ta_2O_5 is therefore the form available as crystals at 300 K and for which the data reported below pertain. H-Ta_2O_5 melts at 1872ºC [56R].

L-Ta_2O_5:

crystal structure

Indexing of the diffraction pattern of this oxide proved very difficult. The most intense lines correspond to an orthorhombic lattice, *a*' = 6.20 Å, *b*' = 3.66 Å, *c*' = 3.89 Å [70R1], but numerous weak lines appear contingent on *b*' multiplied by a factor m which is dependent on impurity content and thermal history. A single phase L-form can be equilibrated by heating Ta_2O_5 to 1350ºC for a long period, just below the upwards transition temperature [70R2]. This has m = 11, *a* = 6.198 Å, *b* = 40.290 Å, *c* = 3.888 Å, *V* = 970.9 $Å^3$, *Z* = l1, d_{calc} = 8.31 g cm^{-3} [71S].

Electron microscopy also shows lattice imaging with m = 11. Equilibration of L-Ta_2O_5 at 1000ºC for long periods gives a structure with m = 14, and at intermediate temperatures an apparently infinite number of ordered, or partially ordered intergrowths with m = 11 to 14 are possible. The L-form is also stabilized by small amounts of cation impurity, provided the ionic radius of the impurity is small; examples are W, Ge, B and Al [70R2].

detailed structure: Fig. 1. There is some relationship to T–Nb_2O_5. The structure shown in Fig. 1 in (001) projection would contain 22 Ta and 58 O, so three O atoms have to be eliminated, which the structure achieves by distortion in the planes d_1...d_4 of Fig. 1. Low temperature amorphous films appear to consist of edge-sharing pentagonal bipyramids, and it is the fusion of these, and concomitant elimination of OH and H_20 that leads to the structure of Fig. 1.

For a detailed table of interatomic distances, see [71S].

References:

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70R2 Roth, R. S., Waring, J. L., Brower, W.: J. Res. Nat. Bur. Stand. Sect. A 74 (1970) 485.
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Fig. 1.

L–Ta_2O_5. A (001) projection of the structure. There are three distortion planes in the unit cell located at d_1, d_2 and d_3. The fourth position at d_4 is related by symmetry but is not used in this unit cell. Black dots represent metal atoms and shaded areas oxygen coordination polyhedra [71S]. 11b': unit cell having 11 UO_3 type subcell structure with *b*' = length of VO_3 type subcell.