

substance: Nb₂O₅

property: phase diagram, modifications

phase diagram: Fig. 1, detailed diagram for the NbO_x system (2.42 < x < 2.50): Fig. 2. In addition to the phases Nb₂O₅ and NbO₂, oxides of composition Nb₃₂O₇₉, Nb₁₂O₂₉, Nb₂₅O₆₂ and Nb₂₂O₅₄ have been reported, as well as a number of intergrowth phases.

crystal structure of Nb₂O₅

Structurally the chemistry of Nb₂O₅ is more complex than any other binary transition metal oxide.

reported modifications of the Nb₂O₅ structure

(first column: crystal form according to [66S], second column: alternative notations and references)

TT	"pseudo-hexagonal" [55F], monoclinic [72T], δ or γ'-form [57H, 63T]
T	γ-form [57H, 63T], T-form [41B]
B	ζ-form [57H, 63T]
M	M-form [41B], β or α'-form [57H, 63T]
H	H-form [41B], α-form [57H, 63T]
N	—
P	η-form [64L]
ε	ε-form [59R]
I-high	—
II	—
OXI...OXVI	—
—	R-form [66G]

All save the TT, ε, I, II and OXI to OXVI forms have been studied crystallographically. With the notable exception of the B- and T-forms, the essential structural principle is the sheared ReO₃ or NbO₂F structure [70W]; where idealized projections are shown, as in Figs. 3...5 the pseudo-cubic axes of the parent structures are used.

References:

- 41B Brauer, G.: Z. Anorg. Allgem. Chem. 248 (1941)1.
55F Frevel, L. K., Rinn, H. W.: Anal. Chem. 27 (1955) 1329.
57H Holtzberg, F., Reisman, A., Berry, M., Berkenblit, M.: J. Am. Ceram. Soc. 79 (1957) 2039.
59R Reisman, A., Holtzberg, F.: J. Am. Ceram. Soc. 81 (1959) 3182.
63T Terao, N.: Jpn. J. Appl. Phys. 2 (1963) 156.
64L Laves, F., Petter, W., Wulf, H.: Naturwiss. 51 (1964) 633.
66G Gruehn, R.: J. Less-Common Met. 11 (1966) 119.
66S Schäfer, H., Gruehn, R., Schultz, F.: Angew. Chem. Int. Ed. Engl. 5 (1966) 40.
69C Chang, L. L. Y., Phillips, B.: J. Am. Ceram. Soc. 52 (1969) 527.
70M Mertin, W., Anderson, S., Gruehn, R.: J. Solid State Chem. 1 (1970) 419.
70W Wadsley, A. D., Anderson, S.: Perspectives in Structural Chemistry, Dunitz, J. D., Ibers, J. A. (eds.) New York: Academic Press 3 (1970) 1.
72T Tamura, S.: J. Mater. Sci. 7 (1972) 298.
74M Marucco, J. F.: J. Solid State Chem. 10 (1974) 211.

Fig. 1.

Nb-O. Phase diagram [69C].

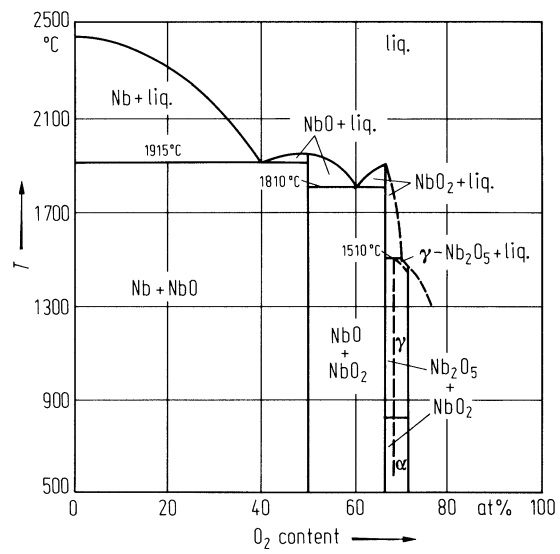


Fig. 2.

NbO_x . Details of the phase diagram in the region $\text{Nb}_{12}\text{O}_{29}$ – Nb_2O_5 [74M].

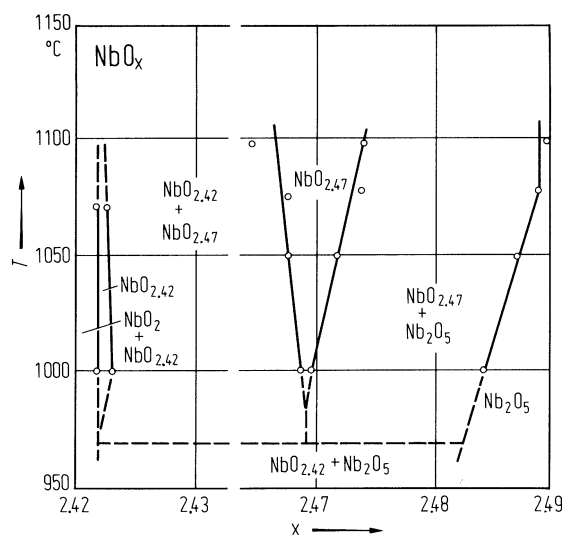


Fig. 3.

P-Nb₂O₅. Idealized structure [70W].

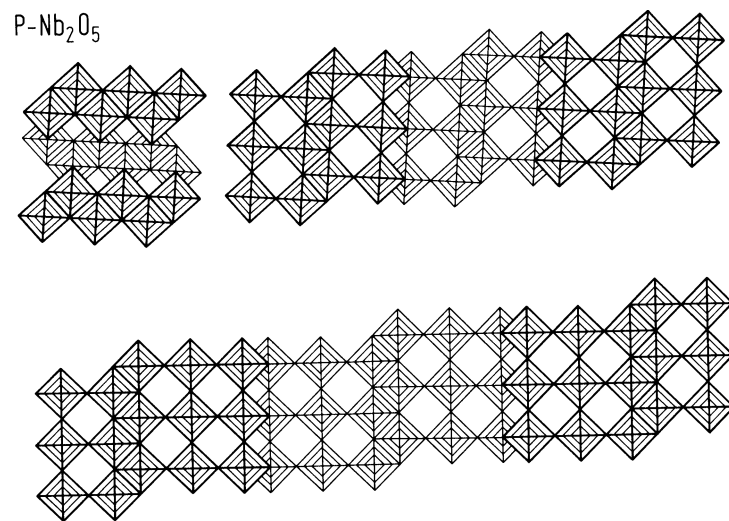


Fig. 4.

N- and M- Nb_2O_5 . Idealized structure [70M].

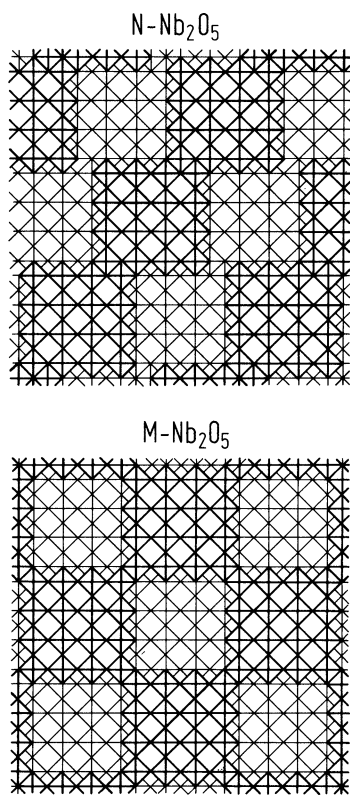


Fig. 5.

H-Nb₂O₅. Idealized structure [70W]. Full circle: are the Nb atoms in tetrahedral sites in the tunnels.

H-Nb₂O₅

