substance: MnO
property: phase diagram, crystal structure, lattice parameters

phase diagram: MnO–Mn_3O_4 boundary: Figs. 1...3 and [59D, 67S, 67H, 70F].

crystal structure: rocksalt structure at room temperature, rhombohedral structure at 4.2 K ($T_{tr} \approx 117$ K).

lattice parameters

a	4.4475(2) Å	RT	space group O_h^5 - Fm3m	70M
a	4.4316(3) Å	*T* = 4.2K	from neutron diffraction	58R
α	90.624(8)°			

Temperature dependence of lattice parameters: Figs. 4, 5. The distortion below T_N = 117 K is apparently an exchange striction which compresses the crystal along <111>, increasing the nearest neighbour and decreasing the next-nearest neighbour distances (Fig. 6). Under high pressure a transformation to tetragonal or lower symmetry is observed. Variation of *a*/*a*(0) with pressure: Fig. 7.

References:

58R Roth, W. L.: Phys. Rev. 110 (1958) 1333.
59D Davies, M. W., Richardson, F. D.: Trans. Faraday Soc. 55 (1959) 604.
65R Rodbell, D. S., Osika, L. M., Lawrence, P. E.: J. Appl. Phys. 35 (1965) 666.
66C Clendenen, R. L., Drickamer, H. G.: J. Chem. Phys. 44 (1966) 4223.
67H Hed, A. Z., Tannhauser, D. S.: J. Electrochem. Soc. 114 (1967) 314.
67S Schwertfeger, K., Muan, A.: Trans. AIME 239 (1967) 1115.
68B Bloch, D., Cherbit, P., Georges, R.: Compt. Rend. 266B (1968) 430.
70F Fender, B. E. F., Riley, F. D.: "Chemistry of Extended Defects in Nonmetallic Solids", Eyring, L., O'Keeffe, M. (eds.), Amsterdam: North-Holland Publ. Comp., 1970, p. 54.
70M Morosin, B.: Phys. Rev. B1 (1970) 236.

Fig. 1.

MnO. Ratio of oxygen to manganese concentration vs. oxygen partial pressure in the range 1200 ...1650ºC [67S].

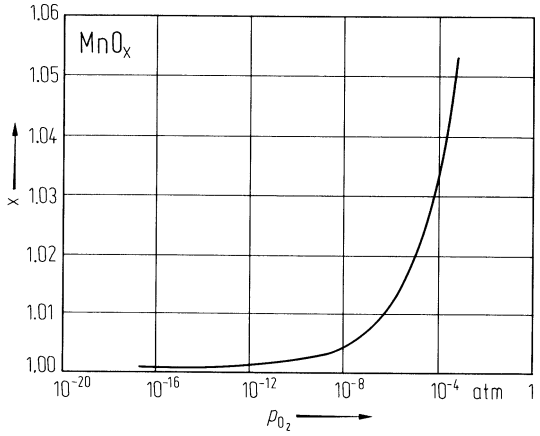

Fig. 2.

MnO. Oxygen partial pressure vs. reciprocal temperature for the system Mn – Mn_3O_4 [67S].

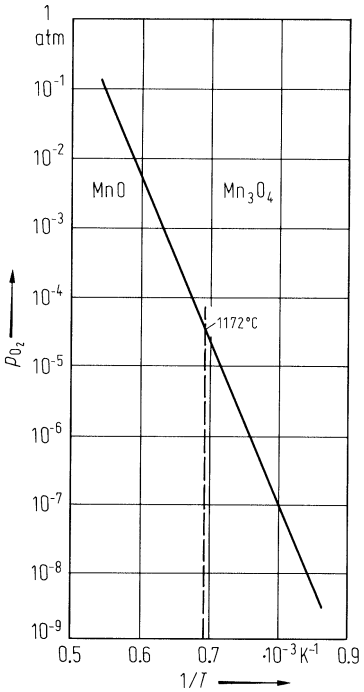

Fig. 3.

MnO_x. Part of the Mn – O phase diagram. Dot-dashed lines are oxygen isobars [67H]. L: liquid, S: solid, SS: solid solution, F: eutectic point; p_{O2} in atm.

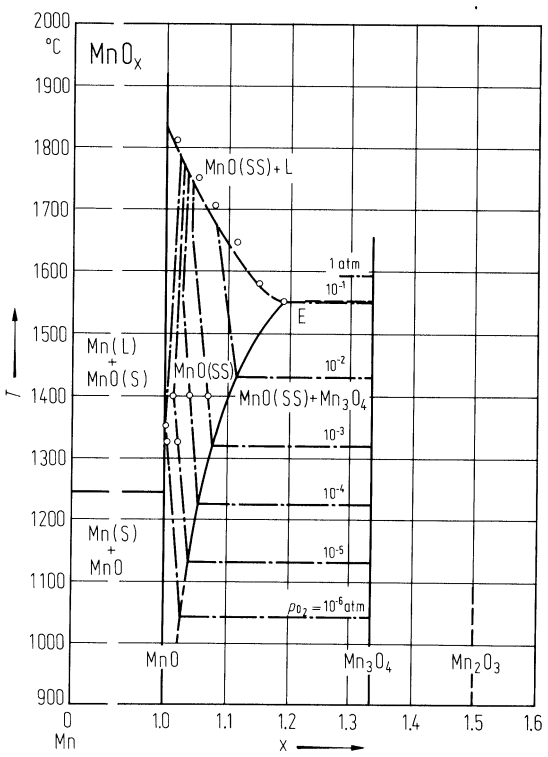

Fig. 4.

MnO. Lattice constant and unit cell volume vs. temperature. Solid line: predicted from Debye Model; circles: experimental points [70M].

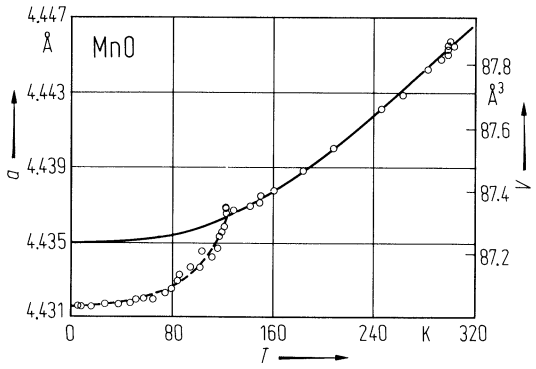

Fig. 5.

MnO. Angle Δ of the pseudocubic cell ($\alpha = \pi/2 + \Delta$) vs. temperature [65R, 70M].

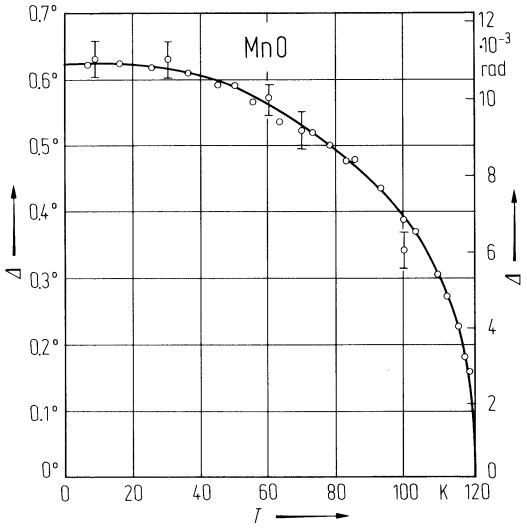

Fig. 6.

MnO. Distance *d* between parallel and antiparallel spin neighbours vs. temperature for $T < T_N$ [68B].

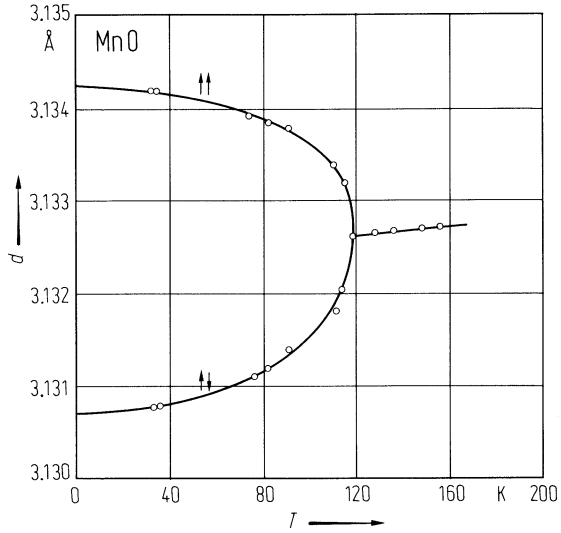

Fig. 7.

MnO. Lattice constant vs. pressure [66C].