Crystal and Magnetic Structure of MnO to 9 GPa by Neutron Diffraction

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Manganese oxide (MnO) is a representative of the archetypal 3d-monoxide series which have been investigated for decades. At ambient conditions it is a paramagnetic Mott-Hubbard insulator with an fcc crystal structure. Similar to NiO, CoO, and FeO type-II antiferromagnetic order occurs below the Néel temperature (T_N=120 K for MnO), accompagnied by a small rhombohedral distortion. Simultaneous measurements of magnetic and crystal structure parameters under pressure allow a deep insight into the interatomic forces in one the most famous and simplest highly correlated electron systems.

To this end we have carried out powder neutron diffraction studies to 9 GPa under hydrostatic conditions (resolution: $\Delta d/d$=0.6%). We find an increase of T_N by a rate of dT_N/dP=+4.0 K/GPa when defined relative to the point where the magnetic moment reaches 50% of its maximal (0 K) value (Fig.1). This value is ca. 20% larger than deduced from published macroscopic measurements in the kbar range (+3-3.5 K/GPa [1]), but considerably smaller than determined from inelastic x-ray scattering to 100 GPa (+6.0 K/GPa) [2].

The rhomohedral distortion α increases with pressure at a rate of $d\alpha/dP$= +0.015 deg./GPa, in good agreement with ab initio predictions [3]. The transition is known to be first-order in volume [4] and magnetization [5]. Below 1 GPa we observe indeed a discontinuous volume change of $\Delta V/V \approx 4x10^{-4}$ at T_N. Under pressure, this value appears to derease to below the resolution level of our measurement.

An additional effect of pressure is an increase of the temperature range where antiferromagnetic fluctuations can be observed above T_N. This might be an indication of a pressure-induced crossover of the transition from first-order to second-order, by comparison with similar findings in NiO where the transition is already continuous at ambient pressure [4,6].

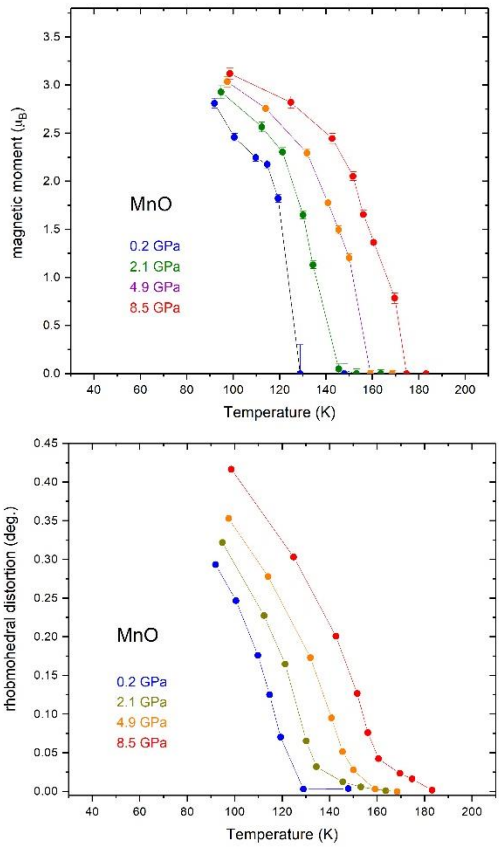

Figure 1. Pressure dependence of refined magnetic moment (top) and rhombohedral distortion (bottom). Preliminary analysis.

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