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$Li_{0.95}Mn_{2.05}O_4$ under high pressure and at elevated temperature in DAC

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A displacive crystal distortion to lower symmetry that cooperatively removes a localized-electron orbital degeneracy so as to leave the atoms in the centre of symmetry of their distorted sites has been observed in many manganese oxides. Moreover, strong Jahn-Teller electron-phonon coupling has been proposed as the crucial component which localizes the e_g electrons as polarons. High pressure and high temperature are a means to tune such an interplay between lattice and electronic degrees of freedom in the lithium manganese spinel [1,2].

The $Li_{0.95}Mn_{2.05}O_4$ spinel sample was obtained from the appropriate amounts of thoroughly mixed powders of α-Mn_2O_3 and Li_2CO_3 (99.0% Merck) by thermal treatment in air at 1048 K. After heating, the specimen was quenched rapidly in solid CO_2. Structural analyses showed the expected stoichiometry of the obtained powder and confirmed that no spurious phases were present.

The structural properties of $Li_{0.95}Mn_{2.05}O_4$ under pressure and at elevated temperature were studied up to 13 GPa by X-ray powder diffraction at the MSPD-BL04 beamline [3] of the ALBA Synchrotron Light Source using monochromatic radiation (λ = 0.4246 Å). Diffraction patterns were recorded on image plates and then integrated [8] to yield intensity vs 2θ diagrams.

For HP/HT experiments, sample was loaded in the 140-µm-diameter hole of an rhenium gasket inside a membrane-type diamond anvil cell (DAC) with a polydimethyl-siloxane oil of type 'Rhodorsil 47V1000' (VCR) as the pressure transmitting medium, which behaves hydrostatically up to 3 GPa (similar to the 4 : 1 methanol–ethanol mixture) and quasi-hydrostatically up to 10 GPa with a small maximum of nonhydrostaticity at 6 GPa [4]. Gold has been chosen as a pressure standard because of its moderate compressibility, chemical inertness, and large X-ray scattering power [5]. A small lump of gold with a purity of 999.9 (four nines fine) and an average particle size of 30 µm was put in the hole of a rhenium gasket.

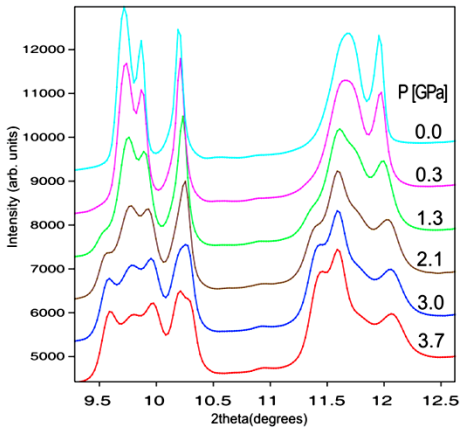

Figure 1. Pressure-induced evolution of XRD pattern.

$Li_{0.95}Mn_{2.05}O_4$ was studied by synchrotron X-ray diffraction isothermally at ambient temperature and at 107 °C under pressures up to 12 GPa. Usually the cooperative Jahn–Teller (JT) distortion is continuously reduced with increasing pressure. However, we obtained a strong indication that the JT effect and the concomitant orbital order are induced with pressure even if in the initial sample the cooperative Jahn–Teller distortion has been suppressed with temperature.

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