

Abstract Submitted
for the SHOCK13 Meeting of
The American Physical Society

Pressure-induced phase transition in γ -MnOOH WOLFGANG H. MORGENROTH, BJOERN WINKLER, Goethe-Universitaet Frankfurt, Altenhoferallee 1, 60438 Frankfurt a.M., Germany, VICTOR MILMAN, Accelrys, 334 Science Park, Cambridge CB4 0WN, UK — At ambient conditions manganite, γ -MnOOH, crystallizes in space group $P2_1/c$ (Kohler et al. 1997). A high pressure study by Suzuki (2006) up to 9 GPa gave a bulk modulus of 91(2) GPa, when the data was fitted with a 2nd order Birch-Murnaghan equation of state. Preliminary DFT calculation predicted a phase transition to an orthorhombic space group at pressures above 15 GPa. In order to test the prediction, natural γ -MnOOH was ground to powder and compressed in a DAC up to 70 GPa. Lattice parameters were determined from X-ray patterns recorded at the Extreme Conditions Beamline P02.2@PETRA III. A structural phase transition into an orthorhombic phase was observed at 47 GPa. The bulk modulus of the ambient pressure phase is 98(3) GPa with $K' = 7.7(3)$. Currently, DFT+U calculations are carried out to understand the compression mechanism and the phase transition. Funding by the BMBF (project 05K10RFA) is gratefully acknowledged. We thank DESY Photon Science for beam time and Hanns-Peter Liermann and his team for support. Kohler T. et al, J Solid State Chemistry, 1997, 133, 486-500. Suzuki A., SPring-8 Exp. Report, 2006, 2006A1464.

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Date submitted: 20 Feb 2013

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