

HIGH PRESSURE-ENHANCED MAGNETIC ORDERING AND MAGNETOSTRUCTURAL COUPLING IN GEOMETRICALLY FRUSTRATED SPINEL Mn_3O_4

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High-pressure effects on the crystal and magnetic structures of Mn_3O_4 have been studied by X-ray and neutron powder diffraction techniques at high pressures up to 37 and 20 GPa and supplemented by the DFT calculations. Upon compression, the crystal structure transforms from the initial tetragonal hausmannite phase of $I4_1/amd$ symmetry into the orthorhombic $CaMn_2O_4$ -type ($Pbcm$ symmetry) phase via the intermediate orthorhombic $CaTi_2O_4$ -type ($Bbmm$ symmetry) phase. In the tetragonal phase, the application of pressure, $P > 2$ GPa leads to a suppression of low-temperature incommensurate and commensurate antiferromagnetic (AFM) orders with a propagation vector $k = (0, \sim 0.5, 0)$ and the expansion of the Yafet-Kittel-type ferrimagnetic phase, becoming the only ground state. The magnetic ordering temperature increases rapidly from 43(2) K at $P = 0$ GPa to 100(5) K at $P = 10$ GPa. In the orthorhombic $CaMn_2O_4$ -type phase, the AFM order on the sublattice of Mn^{3+} spins with a propagation vector $k = (1/2, 0, 0)$ is formed below $T_N = 275$ K. Considering the whole studied pressure range, the magnetic ordering temperature demonstrates a colossal rise in more than 6 times. The pressure behavior of the competing magnetic interactions has been established using density-functional-theory calculations and thereby the underlying mechanism of the observed magnetic phenomena has been discussed.

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