Mn_3O_4のポストスピネル相の巨大原子変位および、その磁性

Giant atomic displacement and the magnetism of Mn_3O_4 postspinel

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Manganates display strong coupling between lattice, spin and orbital degrees of freedom which can lead to magnetic frustration and Jahn-Teller distortion. Mn_3O_4 spinel [1] transforms into a $CaMn_2O_4$-type post-spinel phase at high pressure which can be quenched back to ambient conditions [2]. Figure 1 shows the magnetic structure of Mn_3O_4 postspinel, which was obtained from low temperature neutron diffraction data (collected at SNS, ORNL). Mn_3O_4 postspinel exhibits an atomic displacement of approximately 0.25 Å at a magnetic phase transition at 210 K [2]. This giant atomic displacement is due to the coupled effect of built-in strain in the metastable structure with the orbital realignment of the Mn^{3+} ion [2]. We also studied the pressure dependence of the transition temperature (210 K) using neutron diffraction technique, and found that it increases linearly at a rate of 5 K/GPa above 3 GPa, suggesting that postspinel structure of Mn_3O_4 is only metastable at modest pressures.

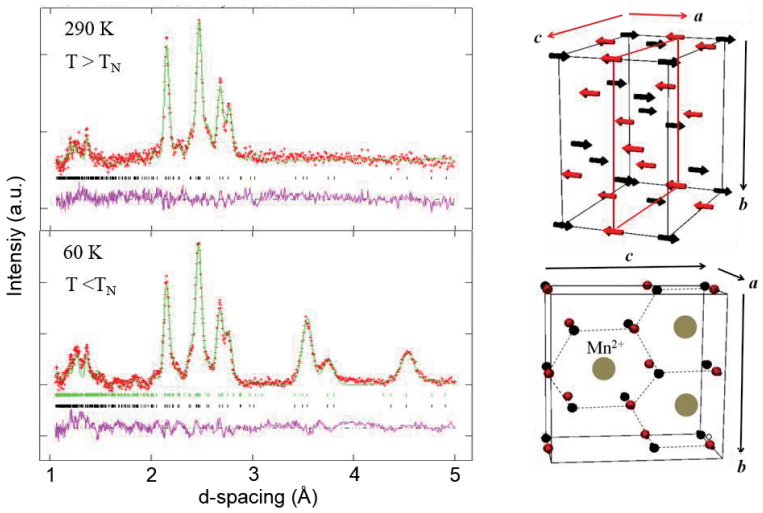

Figure 1. Neutron powder diffraction profile and the magnetic structure of Mn_3O_4 postspinel

[1] G. Aminoff, Z. Kristallogr. **64**, 475 (1927).

[2] S. Hirai, A.M. dos Santos, M.C. Shapiro, J.J. Molaison, N. Pradhan, M. Guthrie, C.A. Tulk, I.R. Fisher, and W.L. Mao, Phys. Rev. B **87**, 014417 (2013).