MS33.O03

Coexistence of magnetic and atomic position modulations in CaMn7O12

R. Przeniosło[1], W. Sławiński[1], D. Wardecki[1], I. Sosnowska[1], L. Keller[2], M. Bieringer[3]

[1]Faculty of Physics, University of Warsaw, Poland, [2]Laboratory for Neutron Scattering, Paul Scherrer Institut, Villigen, Switzerland, [3]University of Manitoba, Faculty of Chemistry, Winnipeg, Canada

The rhombohedral CaMn7O12 manganite is an important material which shows magnetoelectrioc coupling with very high values of the electric polarization [1]. These outstanding properties motivated many experimental studies and also theoretical analysis. The mechanism which leads to these extraordinary properties has not been explained up to now. A fundamental information needed for such studies is the crystal structure and the magnetic ordering. CaMn7O12 has a complex structure with a magnetic moments modulation below TN=90K [1,2], a modulation of the atomic positions below TC=250K [2] and also orbital ordering. The magnetic modulation propagation vector qm is related with the atomic positions modulation vector qp by the relation qp=2qm [2]. This 2:1 relation is valid across a large range of temperatures and show the importance of spin-lattice coupling. The crystal and magnetic structure of CaMn7O12 was studied by neutron powder diffraction at the instrument DMC at SINQ [3]. The magnetic and atomic position modulations are described by using the superspace group formalism. This approach is especially important for description of both modulations with the same model [2]. The resulting magnetic ordering model obtained in [3] is more precise as compared with earlier works [1,2]. The present results [3] differ from those published by other authors [1]. The important difference is that in the present studies the angle, Phi, between Mn3+ and Mn4+ magnetic moments located in the same (001) planes (Phi = 0.99(2)Pi), i.e. the moments are antiparallel, whereas Johnson et al. [1] determined this angle as Phi=0.84(4) Pi. This angle is an important parameter of the model Hamiltonians describing the electronic and magnetic properties of CaMn7O12.

[1] *R. D. Johnson, L. C. Chapon, D. D. Khalyavin, et al. Phys. Rev. Lett., 2012, 108, 067201.,* ***[2]*** *W. Sławinski, R. Przeniosło, I. Sosnowska et al.: Acta Crystallogr. B, 2012, 68, 240.,* ***[3]*** *R. Przeniosło, D. Wardecki, W. Sławinski, I. Sosnowska and L. Keller, Physica B, 2013, 438, 27*

Keywords: perovskite, modulated structures, X-ray and neutron diffraction