

DIFFUSE MAGNETIC SCATTERING ABOVE T_c IN QUASI-2D**La_{1.2}Sr_{1.8}Mn₂O₇**T. Chatterji¹ R. Schneider² J. Hoffmann² D. Hohlwein² R. Suryanarayanan³ G.Dhalenne³ A. Revcolevschi³¹Institut Laue-Langevin Diffraction/Science 6 Rue Jules Horowitz
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We have investigated the magnetic diffuse scattering from the colossal magnetoresistive (CMR) bilayer manganite La_{1.2}Sr_{1.8}Mn₂O₇ above the magnetic phase transition temperature. La_{1.2}Sr_{1.8}Mn₂O₇ is ferromagnetic with a Curie temperature of about 128 K. It belongs to the $n = 2$ Ruddlesden-Popper phase with a modified bilayer perovskite structure in the $I4/mmm$ space group. The magnetic diffuse scattering above T_c shows rod-like intensity distribution along c^* indicating the quasi-2D bilayer character of the system. The strong magnetic correlations of the Mn atoms in the a-b plane and also that between the two planes of the bilayers persist even at room temperature, which is about 2.3 x T_c. The diffuse magnetic scattering has been successfully modelled by using only two exchange interactions in the quasistatic mean-field approximation. By fitting the intensity data to mean-field model calculations, using a least-squares fitting procedure, we have been able to determine the in-plane exchange interaction J_a and interplane exchange interaction J_c of the bilayer. The exchange interactions J_a and J_c, obtained from the least squares fit, are J_a = 2.789(2) and J_c = 1.395(6) meV at room temperature. The interactions so determined are somewhat smaller than that (J_a = 4.8(1), J_c = 1.7(1) meV) determined by us from the measurements of the spin-wave dispersions at 1.5 K. The reduction of the exchange interactions at higher temperature is partly due to their renormalization at higher temperature. However, the anisotropy of the orbital occupancy may contribute to the reduction of the ratio J_a/J_c at higher temperature.

Keywords: NEUTRON DIFFRACTION, DIFFUSE SCATTERING, EXCHANGE INTERACTION**CHARGE ORDERING THAT ONLY SUCCEEDS AFTER NATURES SECOND ATTEMPT**P. Karen¹ P.M. Woodward² J. Lindén³¹University of Oslo Department of Chemistry POB 1033 Blindern OSLO 0315
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Double-cell perovskites RBaFe₂O₅ (R = rare earth element) are the last contribution to the family of Verwey phases. As paramagnetic mixed-valence (Fe^{2.5+}) conductors at high temperatures, they have iron atoms in identical square-pyramidal coordinations of tetragonal symmetry. Below Neel temperature of some 400 K, antiferromagnetic order of iron spins occurs, accompanied by orthorhombic distortion. Moessbauer spectra show that this magnetostriuctive distortion sets the frame for the first attempt to separate the mixed valence, at around 300 K. Two specific magnetic- and electric-field tensor orientations emerge under this partial local separation of charges that otherwise is best detected calorimetrically (ΔS around -0.7 Jmol⁻¹K⁻¹). The second attempt to order charges occurs some 40 K below, having all symptoms of the classical Verwey transition: a sudden change in volume, entropy, and electrical conductivity. A large orthorhombic distortion allows disproportionation of bond lengths sufficient for bond-valence separation of approximately 0.75. The entropy change is by an order of magnitude larger than for the first attempt and increases towards heavier R. A long-range charge order is detected by synchrotron x-ray diffraction. Powder neutron diffraction registers a subtle change in the spin arrangement, within the overall antiferromagnetic order, that is essential for the transition: The double-exchange mediated intervalence transfer of the high-temperature phase switches to the G-type antiferromagnetic interaction in the charge-ordered counterpart. Increasing oxygen non-stoichiometry in RBaFe₂O_{5+w} decays the Verwey transition. Moessbauer spectra then account for the valence and spin states of iron under disruption of the long-range order of the separated charges.

Keywords: VERWEY TRANSITION MIXED VALENCE CHARGE ORDERING**PHASE TRANSITIONS IN SrLaCuRuO₆ AND SrLaNiRuO₆ DOUBLE PEROVSKITES**

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The SrLaMRuO₆ family (M= Cu, Mn, Co) has been studied during the last decade. All compounds present a perovskite structure, some are B-site cation ordered (M=Co) and some are not (M=Mn). The Mn compound was reported to have a disordered double perovskite structure (space group *Pnma*). However, in a more recent study using electron diffraction it was found to have ordered B-site cations. It was also reported a first order phase transition at 480 K leading to a structure with *R-3c* space group. We have studied SrLaCuRuO₆ in relation to the concept of pseudosymmetry, used to predict phase transitions. Starting point for the pseudosymmetry calculations were the known structural data. The calculations indicated a possible high-temperature phase. We have synthesized and analyzed the Ni compound since we expected the same behavior as in the Cu. Preliminary results for the room temperature phase of the compounds are consistent with an ordered perovskite structure, which in the case of the Cu compound is in contradiction with the published work. The Cu material was known to be the only double perovskite of BII BV type and with a disordered structure. By means of high temperature x-ray powder diffraction we studied the structural evolution of the title compounds. In both cases a phase transition was observed at about 620 K. The high temperature phase was indexed as trigonal (*R-3*).

Keywords: PHASE TRANSITION POWDER DIFFRACTION DOUBLE PEROVSKITE**STRUCTURE MODEL OF ATOMS BEHAVIOUR OF PbMg_{1/3}Nb_{2/3}O₃ AND PbZn_{1/3}Nb_{2/3}O₃ IN FERROELECTRIC RELAXOR PHASE**A. R. Lebedinskaya¹ M. F. Kupriyanov²¹Azov - Black Sea State Agro - Engineering Academy Department of Physics
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In this report we present the results of the experimental and theoretical study of the local structure of single crystals PbMg_{1/3}Nb_{2/3}O₃ (PMN) and PbZn_{1/3}Nb_{2/3}O₃ (PZN) as a function of temperature (103 K, 183 K, 203 K) using X-ray scattering and a special procedure of processing the experimental structure amplitudes taking into account the sensitivity of structure amplitudes to the shifts and Debye-Waller factors of the atoms for both compounds. It has been established unusual features connected with the appearance of the metastable spontaneous polarization regions in both materials and evolution to a ferroelectric state. Abnormally large value of Debye-Waller factor for Pb atom at low temperatures indicates a possible considerable disorder in shiftings of these atoms in this relaxors and can be an indication of relaxor behavior in similar compounds. Analysis of the temperature dependence of Debye-Waller factor of Nb atoms showed that Nb atom displacement from the centre of oxygen octahedron is independent of the temperature for both compounds. The local structure and possible mechanisms of structure evolution in two relaxors will be discussed in comparison with some other Pb-containing relaxor ferroelectrics of perovskite-type compounds.

Keywords: PEROVSKITES, RELAXOR, ORDERING