state conversion. Ordering of the spin states is manifested in the corresponding superstructure reflections; these can be traced in a diffraction experiment as a function of external stimuli. By mapping reciprocal space with an area detector and synchrotron light, we have studied the temperature dependence of the superstructure reflections for $NdBaCo_2O_{5.5}$ and $TbBaCo_2O_{5.48}$. We have found that above the metal-insulator transition there are two different Co ions in the asymmetric unit, one sitting in a pyramidal and one in an octahedral environment. Below the transition temperature there are four structurally different Co ions. This observation agrees with the "spin blockade" mechanism suggested for the metal-insulator transition in cobaltites. We also present results of structural analyzes illustrating how the corresponding powder diffraction measurements could easily overlook the correct structure. A symmetry analysis bracketing the observed phase transitions within the context of Landau theory is also given.

Keywords: cobaltites, spin transition, spin ordering

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Investigation of the crystal symmetry of $BiMnO_3$: Electron diffraction study

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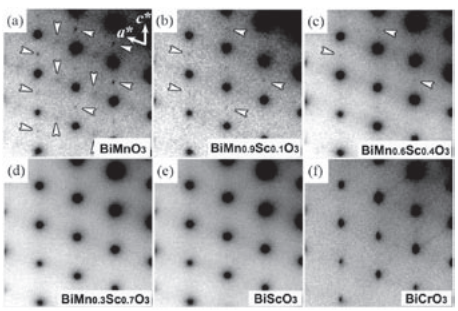
$BiMnO_3$ has been considered as a multiferroic material due to the ferroelectric and ferromagnetic properties. The crystal symmetry is, however, controversial today. We investigated the crystal symmetry of $BiMnO_3$ by Convergent-Beam and Selected-Area Electron Diffraction (CBED and SAED, respectively). CBED, which was used in order to discriminate the crystal axes of $BiMnO_3$, showed that $BiMnO_3$ belongs to space group $C2/c$. In the [010] SAED pattern, however, the very weak but sharp h0l (l=2n+1) reflections were observed indicating the noncentrosymmetric long-range ordered structure ($C2$) [1]. This implies that the weak reflections had quite little influence on the CBED patterns [2]. The h0l (l=2n+1) reflections could not be detected in structurally related $BiScO_3$ and $BiCrO_3$ indicating centrosymmetric $C2/c$, respectively [1]. This strongly suggests that the noncentrosymmetric long-range ordered structure ($C2$) of $BiMnO_3$ is attributed not only to Bi^{3+} ions with lone electron pair but also to Mn^{3+} ions, that is, to correlation between Bi^{3+} and Mn^{3+} ions.



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Keywords: ferroantiferro-magnetic ferroelectrics, perovskite oxides, electron diffraction

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Structural and magnetic phase transitions in the complex perovskite systems $BiMn_7O_{12}$ and $LaMn_7O_{12}$

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By means of neutron powder diffraction as a function of temperature, we have investigated the nuclear and magnetic structures of the new systems $(BiMn_3^{+3})(Mn_3^{+4})O_{12}$ and $(LaMn_3^{+3})(Mn_3^{+4})O_{12}$. Single-phase powder samples of both phases were recently synthesized under high pressures at the IMEM-CNR in Parma. In both systems, the A' cation is trivalent, thus all of the Mn B-cations are expected to be trivalent. Both systems crystallize in the $A'A_3B_4O_{12}$ complex perovskite structure consisting of a pseudo-cubic network of corner-shared BO_6 octahedra. This system may display a rich manifold of charge, spin and orbital orderings characteristic of mixed-valence systems. In both systems, we have determined precisely the nuclear and magnetic structures as a function of temperature, between room temperature and 2K. We have observed two magnetic transitions at low temperature in the La compound, involving crystallographically different Mn ions. Between 65K and 20K, the propagation vector k is (0,0,0), and only the Mn ions in the B-site are ordered. Below 20K, additional magnetic reflections appear, the lattice is no longer body centered, and magnetic moments of manganese atoms belonging to the A site are ordered. The magnetic structure has been solved by simulated annealing techniques, with help of symmetry analysis. It will be discussed in comparison with the Na analog which had been studied before. For the Bi compound, the effect of the lone pair of Bi on the structure will be discussed, as well as the magnetic structures observed at low temperature.

Keywords: magnetic structures, perovskite structures, neutron powder diffraction

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Coupling of Tb- and Mn-magnetic orders in multiferroic $TbMnO_3$

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While ferroelectricity and magnetism are chemically incompatible, it has recently been shown that inversion and time-reversal symmetry can be broken simultaneously if magnetic spins order in a cycloidal arrangement as in $RMnO_3$. It has been also shown that although the magnetic ordering of Mn-spins drives multiferroicity, R-ions strongly modulate it and thus significantly influence multiferroic properties. Irrespective of the mechanism that drives multiferroic behavior, the magnetic coupling between R- and Mn-spins needs to be understood in order to arrive at a detailed and quantitative model of multiferroics. Here we report on diffraction measurements which demonstrate that the Tb- and Mn- magnetic ordering in multiferroic $TbMnO_3$ remain