of the interesting topics of condensed matter research. It has drawn renewed interest in connection with the potentially useful electronic materials such as colossal magnetoresistive and multiferroic materials. One of the dominant effects of this coupling is the spontaneous exchange striction associated with the magnetic ordering at lower temperatures. We have investigated magnetoelastic effects in multiferroic YMnO3 and HoMnO**3** below antiferromagnetic phase transition by neutron powder diffraction. YMnO3 and HoMnO3 belong to the family of hexagonal manganites RMnO3 (R = Sc, Y, Er, Ho, Tm, Yb, Lu) that show multiferroic behaviour. These hexagonal manganites are paraelectric at high temperatures with centrosymmetric space group *P63/mmc*. Below about 1000 K they undergo paraelectric-to-ferroelectric transition to the non-centrosymmetric structure with the space group *P63cm*. At further lower temperatures of the order of about 100 K the magnetic hexagonal manganites order with a non-collinear antiferromagnetic structure with the propagation vector k = 0. We have done neutron powder diffraction experiments on YMnO3 and HoMnO3 on a high-intensity powder diffractometer. The lattice parameter *a* of the hexagonal unit cell of YMnO3 decrease in an usual way at lower temperatures and then shows abrupt anomalous contraction below *TN = 70* K whereas the lattice parameter *c* increases continuously with lowering temperaure and then shows abrupt anomalous increase below *TN*. The unit cell volume *V* also undergoes abrupt contraction below *TN*. By fitting the background thermal expansion of a nonmagnetic lattice with Einstein-Grueneisen equation we determined the lattice strains □*a*, □*c* and □*V* due to the magnetoelastic effects as functions of temperature. We have determined the temperature variation of the ordered magnetic moment of Mn ion by fitting the measured Bragg intensities of the nuclear and magnetic reflections with the known crystal and magnetic structure models and have established that the lattice strains due to the magnetoelastic effect in YMnO3 couples with the square of the ordered magnetic moment or the square of the ordered parameter of the antiferromagnetic phase transition. We have determined the small structural modifications at the antiferromagnetic phase transition due to the magnetostriction effects and related these with the ferroelectric polarisation. Similar results have been obtained for multiferroic HoMnO3. We have compared the present results with those obtained by us [1], [3] in parent compounds LaMnO3 and NdMnO3 of the colossal magnetoresistive (CMR) manganites and also in the whole series of model insulating antiferromagnets MF2 (M = Cr, Mn, Fe, Co, Ni, Cu). This has led us to conclude that the compounds with magnetic ions having considerable unquenched orbital moments behave anomalously compared to those with spin-only moments.

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Keywords: antiferromagnetism, ferroelectricity, neutron diffraction

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Symmetry-mode analysis of the alumina phase diagram

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The oxides and oxyhydroxides of aluminum present a notoriously complex structural family with at least 13 different structural phases. Of particular interest and importance are the phase sequences involving the boehmite, γ, and α phases due to their industrial and technological applications. Much time and effort have been spent mapping out the myriad transition sequences that have been observed within this family, which can vary substantially with only slight changes in the synthetic conditions, initial crystallite size, and/or hydrothermal history. Yet, the detailed transformation mechanisms that relate them are not well understood. Using symmetry principles as a guide, we have uncovered candidate mechanisms that help to explain a variety of transitional phases observed along common phase pathways leading to α alumina.

Keywords: alumina, phase transformation mechanism, symmetry-mode analysis

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Atomic scale description of the macroscopic piezo-ferroelectric properties of high performance lead zirconate titanate (PZT)

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Materials science can be defined as an interdisciplinary field involving the properties of matter and its applications. This scientific field investigates the relationship between the structure of materials and their macroscopic properties. In this framework the "in situ" atomic-scale structural description of the origin of the ferroelectric properties as a function of the applied electric field ***E***, i.e. switching of the spontaneous polarization P_S with an electric field, corresponds to a perfect example of such a goal. Piezoelectricity is inherent to ferroelectricity and the structural investigations of such a material as a function of an applied electric field will create a strong piezoelectric strain ($d_{kij} = \frac{\partial \eta_{ij}}{\partial E_k}$, where d_{kij} is the piezoelectric coefficient, η_{ij} is the strain and E_k is the applied electric field) which unfortunately makes structural determination difficult due to the existence of an associated strong texturing. In this contribution, a 45°-scattering geometry was used to average the preferred orientation and solve "in-situ" the crystal structure as a function of the applied electric field. Note that this set-up could be used in other studies, involving homogeneous strains as a function of other intrinsic physical parameters, i.e. stress, magnetic field, etc. Hence, we were able to describe microscopically the macroscopic physical properties of the most widely used ferroelectric material, lead zirconate titanate (PZT), which is intensively used for technological applications (sensors and actuators, MEMS systems and high frequency devices). As we will show it is possible to directly correlate structural with macroscopic ferro-piezoelectric properties as a function of the electric field and thus elucidate the structural origin of such properties. Polarization flipping of polar lead atoms for example could unambiguously be characterized by a maximum in the disorder parameter of lead, i.e. *Biso* (Pb) linked to the maximum of the entropy, for the positive-negative value of the coercitive field in the P_S-E hysteresis cylce [1].These results will be useful for the design and optimization of higher performance materials.

[1] M. Hinterstein, J. Rouquette, J. Haines, Ph. Papet, M. Knapp, J. Glaum, H. Fuess, *Phys. Rev. Lett.* (revised version).

Keywords: ferro-piezoelectric PZT, rietveld refinement, "in situ" electric field diffraction