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Perovskite compounds containing cation inducing probable disorder is very attractive owing to the fact that positional disorder is often at the origin of the relaxor phenomena. The complex perovskite AA'(BB')O<sub>3</sub> are known to exhibit normal and/or relaxor ferroelectric behaviour. Many investigations have been devoted to the study of relaxation parameters in such materials in order to achieve their use in satisfactory capacitors and actuators [1,2]. However, most of these materials are lead-based ceramics which present a disadvantage due to the toxicity of PbO. So, for environmental and health reasons, manufacture of such materials are more and more constrained to eliminate the lead content from these compounds. In this way, we have investigated new lead free compositions in BaSc<sub>1/2</sub>Ta<sub>1/2</sub>O<sub>3</sub>-BaTiO<sub>3</sub> systems. We present here the dielectric study and correlate the results obtained with the structure of these new lead-free materials.

Samples of the (1-x) BaSc<sub>1/2</sub>Ta<sub>1/2</sub>O<sub>3</sub>-x BaTiO<sub>3</sub> solid solution were prepared from high purly BaCO<sub>3</sub>, TiO<sub>2</sub>, Sc<sub>2</sub>O<sup>3</sup> and Ta<sub>2</sub>O<sub>5</sub> powders using solid state methods. All these materials were previously dried at 120°C for 15 h, weighed, mixed for 1 h and calcined at 1200°C for 15 h. After calcinations, powders were mixed for 1h and pressed under 100 MPa into 8mm diameter and about 1 mm thick. The pellets were then sintered in oxygen atmosphere at 1350°C for 4 h.

Room temperature powder XRD patterns were recorded on a Philips diffractometer X'Pert Pro MPD using CuK $\alpha$ radiation (5°  $\leq 2 \ \theta \leq 80^{\circ}$ ). The X-ray diffraction pattern for ceramics with compositions x=0.025 and 0.05 were investigated. The results obtained suggest that these compositions have respectively tetragonal and cubic symmetry at room temperature.

The dielectric measurements were performed on ceramic discs after deposition of gold electrodes on the circular faces by cathodic sputtering. The dielectric permittivity of the sample was measured under helium atmosphere as a function of both temperature (80–500 K) and frequency  $(10^2-2.10^5 \text{ Hz})$ . For composition close to BaTiO<sub>3</sub>, three dielectric peaks have been observed and correspond at cubic paraelectric to tetragonal ferroelectric, and then to an orthorhombic ferroelectric and finally to a rhombohedral ferroelectric similar to those of pure BaTiO3. For the relative high values of x (incorporation of Sc<sup>3+</sup> and Ta<sup>5+</sup> cations) only one peak occurs with weak frequency dispersion. The tetragonal and cubic symmetry are related to the classical or relaxor ferroelectric behaviour respectively.

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## Keywords: lead-free; ferroelectric; XRD

## FA2-MS05-P05

**Combined Refinement of High Resolution Neutron and Synchrotron Data of PLZT.** <u>Manuel</u> <u>Hinterstein<sup>a</sup></u>, Roland Schierholz<sup>a</sup>, Markus Hölzel<sup>a</sup>, Anatoliy Senyshyn<sup>a</sup>, Jens Kling<sup>a</sup>, Ljubomira Ana

25<sup>th</sup> European Crystallographic Meeting, ECM 25, İstanbul, 2009 *Acta Cryst.* (2009). A**65**, s 202 Schmitt<sup>a</sup>, Hans-Joachim Kleebe<sup>a</sup>, Hans Kungl<sup>b</sup>, Michael Knapp<sup>c</sup>, Hartmut Fuess<sup>a</sup>. <sup>a</sup>Institute for Materials Science and Geosciences, University of Technology Darmstadt, Germany. <sup>b</sup>Institute of Ceramics in Mechanical Engineering, University Karlsruhe, Germany, <sup>c</sup>CELLS, Barcelona, Spain. E-mail: <u>manuel.hinterstein@desy.de</u>

Lead containing oxides with perovskite structure like PbZr<sub>1</sub>,  $_x Ti_x O_3$  (PZT) are widely used as sensors and actuators. Especially, solid solutions near the rhombohedral-tetragonal morphotropic phase boundary (MPB) possess eminent piezoelectric characteristics and are widely used in a donor or acceptor doped modification with improved electrical properties. Despite extensive studies the microstructure of the morphotropic phase boundary (MPB) in ferroelectric PZT is still under discussion. Whereas some groups (Noheda *et al* [1]) fitted diffraction data by monoclinic symmetry, other groups describe the MPB as composed of a complicated system of micro- and nanodomains [2].

Extensive studies have been performed on donor doped  $Pb_{0.985}La_{0.01}(Zr_{1-x}Ti_x)O_3$  (PLZT) across the entire compositional range of the MPB. Temperature dependent measurements at the beamline B2 in Hamburg provide an insight into the phase composition in the vicinity of the MPB and will be compared with undoped PZT. These results are complemented by high resolution neutron powder diffraction data collected at SPODI at the FRM II in Munich at low temperatures that describe the compositional dependent structural evolution from the rhombohedral to the tetragonal side of the phase diagram. The observed superstructure reflections reveal new structural aspects of the low temperature phases. A study of combined neutron and synchrotron high resolution powder diffraction data refinement (MS beamline at the SLS in Villingen) gives a detailed overview of the structural changes across the MPB. Results will be discussed together with transmission electron microscopic observations. The authors appreciate the financial support of the German Research Foundation (DFG) through the Sonderforschungsbereich 595 "Electric Fatigue in Functional Materials".

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Keywords: synchrotron powder diffraction; neutron high-resolution diffractometry; piezoelectric ceramics

## FA2-MS05-P06

**Probing the Giant Piezoelectric Effect at the Atomic Scale in PbZn<sub>1/3</sub>Nb<sub>2/3</sub>O<sub>3</sub>**. <u>Jérôme Rouquette</u><sup>a</sup>, Ali Al-Zein<sup>a,b</sup>, Julien Haines<sup>a</sup>, Philippe Papet<sup>a</sup>, Claire Levelut<sup>b</sup>, Hichem Dammak<sup>c</sup>, Olivier Mathon<sup>d</sup>. <sup>a</sup>ICG UMR CNRS 5253, PMOF, Montpellier, France. <sup>b</sup>LCVN UMR CNRS 5587, Montpellier. <sup>c</sup>SPMS UMR CNRS 5580, ECP, Châtenay-Malabry, France. <sup>d</sup>ESRF, Grenoble, France E-mail: Jerome.Rouquette@univ-montp2.fr