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Twin Structure of Solid Oxide Electrolytes. Taras Tataryn[a], Dmytro Savytskii[a], Leonid Vasylechko[a], Carsten Paulmann[b,c], Ulrich Bismayer[c]. [a]*Lviv Polytechnic National University, Lviv, Ukraine.* [b]*HASYLAB, DESY, Hamburg, Germany.* [c]*Min.-Petrogr. Institut, Universität Hamburg, Hamburg, Germany.*
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An increasing interest in electrolyte materials for advanced energy applications demands understanding of their *real* structure and its influence on the physical properties. It is therefore relevant to investigate both the crystal- and micro-structures, since the considered properties depend on domain walls and their distribution (twin structures) [1]. ZrO_2 doped with Sc, and $LaGaO_3$ doped Sr and Mg, are considered as prospective solid electrolytes for application in solid oxide fuel cells (SOFCs). The present work is devoted to structure investigations of ZrO_2 doped with 10 mol % Sc_2O_3 (ZSO-10) and $La_{0.95}Sr_{0.05}Ga_{0.9}Mg_{0.1}O_{3-\delta}$ (LSGM-05) and determination their twin structures in their ferroelastic phases.
In order to study the thermal evolution of their crystal structures investigations were carried out at the synchrotron powder diffractometer B2 (HASYLAB/DESY). High-temperature diffraction data were collected in the Debye-Scherrer capillary geometry using the on-line image plate detector OBI and the STOE furnace. Data analysis was carried out by the Rietveld method using the WinCSD program package. Domain orientations were determined by the Laue method. The white beam synchrotron experiments have been carried out using the Kappa-diffractometer at F1 (HASYLAB) equipped with a MAR CCD system and a gas-stream heating device.
The powder diffraction examinations revealed that the rhombohedral structure (space group $R\bar{3}$) of ZSO-10 transforms into the high-temperature cubic structure (space group $Fm\bar{3}m$) at 873 K, while LSGM-05 transforms at 500 K from orthorhombic to monoclinic and at 670 K to rhombohedral phase. Analysis of the Laue patterns confirms that the ZSO-10 crystal was twinned relatively to intersecting (101) and (100)/(001) mirror planes in the rhombohedral phase, while LSGM-05 was twinned relatively to intersecting $(01\bar{1})$ and $(21\bar{1})/(2\bar{1}1)$ mirror planes in the orthorhombic phase. In both crystals the twin structure tends to form typical "chevron-like" wall configurations that allow for a stress-free co-existence of four different orientation states. These four orientation states occur because they perfectly match geometrically and no additional stress occurs at the intersections of domain walls throughout the full temperature range of the corresponding phases [2]. The work was supported by WTZ (UKR 07/009) and Ukrainian Ministry of Science (project "Segnet").

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Keywords: crystal structure; ferroelastic; electrolytes

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Molecular Alignment of Ferroelectric Liquid Crystals by Polyimide Thin Film. Ahmet Yildirim[a], Suleyman Yilmaz[a]. [a]*Harran University, Department of Physics, Osmanbey Campus, 63400, Sanliurfa, Turkey.*
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In presented study, the photoinduced alignment of ferroelectric liquid crystals onto photochemically stable polyimide thin films was studied. The molecular alignment quality of ferroelectric liquid crystal display cells depends mainly on the difference between the ferroelectric liquid crystal surface energy and the aligning substrates surface energy; however, the structure and thickness of ferroelectric liquid crystal layers are also very important. The effect of the thickness of photoaligning polyimide thin film on the alignment quality and multiplex operation of passively addressed ferroelectric liquid crystal display cells has been investigated.
This method has been replaced by photoresist coating and etching, whereas other techniques have been used photomask for alignment. The empty cell of liquid crystal is prepared by the attentive procedures in very sensitive conditions and the thickness of cell gap is measured by the rotational interferometric system. This application encouraged and motivated us to further studies, which will be applied by lithograph application by changing on the UV exposing time and the percentage of the chemical etching.

Keywords: liquid crystals; liquid-crystal displays; ferroelectric materials

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Tensor Distinction of Domains in Ferroic Crystals. Daniel B. Litvin. *Penn State Berks P.O.Box 7009, Reading, PA 19610-6009, USA.*
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Ferroic crystals contain two or more domain states and may be distinguished by the values of components of tensorial physical properties of the domains. We extend Aizu's global tensor distinction of all domains which arise in a ferroic phase transition from phases invariant under time reversal to include those domains which arise in transitions from magnetic and non-magnetic phases. For determining possible switching of domains, a domain pair tensor distinction is also given for all pairs of domains which arise in each ferroic phase transition.

Keywords: ferroic domain structures; domain switching; physical properties electrical magnetic

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Ferroelectric Properties and Structural Relationship in $BaSc_{1/2}Ta_{1/2}O_3$-$BaTiO_3$ System. Kamel Taïbi[a], Nouari Bensemma[b], Ahmed Kerfah[a], Achoura Guehria-Laidoudia[a], Annie Simon[c]. [a]*Faculté*

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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_3 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 $BaSc_{1/2}Ta_{1/2}O_3$-$BaTiO_3$ 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) $BaSc_{1/2}Ta_{1/2}O_3$- x $BaTiO_3$ solid solution were prepared from high purity $BaCO_3$, TiO_2, Sc_2O^3 and Ta_2O_5 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 CuKα radiation (5° ≤ 2 θ≤ 80°). 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 Hz). For composition close to $BaTiO_3$, 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^{3+} and Ta^{5+} 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

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Combined Refinement of High Resolution Neutron and Synchrotron Data of PLZT. Manuel Hinterstein[a], Roland Schierholz[a], Markus Hölzel[a], Anatoliy Senyshyn[a], Jens Kling[a], Ljubomira Ana Schmitt[a], Hans-Joachim Kleebe[a], Hans Kungl[b], Michael Knapp[c], Hartmut Fuess[a]. *[a]Institute for Materials Science and Geosciences, University of Technology Darmstadt, Germany. [b]Institute of Ceramics in Mechanical Engineering, University Karlsruhe, Germany, [c]CELLS, Barcelona, Spain.*
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Lead containing oxides with perovskite structure like $PbZr_{1-x}Ti_xO_3$ (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

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Probing the Giant Piezoelectric Effect at the Atomic Scale in $PbZn_{1/3}Nb_{2/3}O_3$. Jérôme Rouquette[a], Ali Al-Zein[a,b], Julien Haines[a], Philippe Papet[a], Claire Levelut[b], Hichem Dammak[c], Olivier Mathon[d]. *[a]ICG UMR CNRS 5253, PMOF, Montpellier, France. [b]LCVN UMR CNRS 5587, Montpellier. [c]SPMS UMR CNRS 5580, ECP, Châtenay-Malabry, France. [d]ESRF, Grenoble, France*
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