

**MS37-P3 Oxygen Diffusion and Structural and Properties in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_{4+d}$  and  $\text{La}_2\text{CoO}_{4+d}$**  J. Schefer<sup>a</sup>, M. Ceretti<sup>b</sup>, L. Le Dreau<sup>c</sup>, R. Sura<sup>a,d</sup>, C. Prestipino<sup>d</sup>, W. Paulus<sup>b</sup>, L. Keller<sup>a</sup>, K. Conder<sup>a</sup>, E. Pomjakushina<sup>a</sup>, B. Pederson<sup>a</sup> *Laboratory for Neutron Scattering & Laboratory for Developments, Paul Scherrer Institut, CH-5232 Villigen PSI*, <sup>b</sup>*Chimie et Cristallographie de Matériaux (C2M), Université de Montpellier 2, FR-34095 Montpellier Cedex 5*, <sup>c</sup>*Bruker AXS France, FR-77447 Marne-La-Vallée Cedex 2*, <sup>d</sup>*University of Rennes1, Sciences Chimiques de Rennes, Campus de Beaulieu, FR-35042 Rennes*, <sup>e</sup>*Forschungs-Neutronenquelle Heinz Maier-Leibnitz, DE-85747 Garching*  
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The understanding of oxygen ion conduction in solids at moderate temperatures is a key issue for the development of oxygen membranes in solid oxide fuel cells [1] or for oxygen sensors. The  $\text{K}_2\text{NiF}_4$  structure [2], e.g.  $\text{La}_2\text{MO}_{4+d}$  ( $M=\text{Co},\text{Cu}$ ) will undergo oxygen intercalation at ambient temperature. In  $\text{La}_2\text{CoO}_{4+d}$  the oxygen intercalation is influenced by the strontium induced defects and therefore changes with strontium content [3]. Oxygen diffusion in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_{4+d}$  need to be examined with high quality single crystal samples grown by our groups using mirror furnace technique, as there is no porosity and grain boundaries likely control equilibration rates. The knowledge of the structural properties is essential for the diffusion studies and for the application of first-principle studies, e.g. in  $\text{La}_2\text{CuO}_{4+x}$  [4]. In order to predict the oxygen diffusion mechanism in the case of Sr doped  $\text{La}_2\text{CuO}_4$  we investigated single crystals of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_{4+d}$  ( $0 \leq x \leq 0.15$ ) by using neutron and X-ray diffraction measurements using TriCS@SINQ, PSI, RESI@FRM-2 and ID11@ESRF to relate structural changes to oxygen diffusion properties.

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**Keywords:** oxygen diffusion, structure, fuel cell materials

**MS37-P4 Bimodal domain configuration and wedge formation in tetragonal  $\text{Pb}[\text{Zr}_{1-x}\text{Ti}_x]\text{O}_3$ .** <sup>a</sup>Ljubomira Ana Schmitt, <sup>b</sup>David Schrade, <sup>c</sup>Hans Kungl, <sup>a</sup>Bai-Xiang Xu, <sup>d</sup>Ralf Mueller, <sup>c</sup>Michael J. Hoffmann, <sup>a</sup>Hans-Joachim Kleebe, <sup>a</sup>Hartmut Fuess, <sup>a</sup>*Institute of Materials and Geo-Sciences, Technische Universität Darmstadt, Germany*, <sup>b</sup>*I W S Beratende Bauingenieure, 65510 Idstein / Ts., Germany*, <sup>c</sup>*Institute of Ceramics in Mechanical Engineering, University of Karlsruhe, Germany*, <sup>d</sup>*Institute of Applied Mechanics, Department of Mechanical and Process Engineering, TU Kaiserslautern, Germany*  
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In the present study the domain structure, bimodality of domains and wedge-shape formation of domain tips are investigated in tetragonal  $\text{Pb}[\text{Zr}_{0.375}\text{Ti}_{0.625}]\text{O}_3$  and  $\text{Pb}[\text{Zr}_{0.45}\text{Ti}_{0.55}]\text{O}_3$  ferroelectrics by transmission electron microscopy (TEM) [1].

The strict alternation of broad and narrow microdomains is denoted as bimodality [2].

Finite element method (FEM) calculations predicted the stability of the experimentally observed domain configuration for different boundary conditions concerning electrical as well as mechanical state [1]. FEM simulations showed that bimodal domain structures can be explained either by the electric conditions imposed by the polarization direction of neighbouring domains or by mechanical stress induced by clamping due to neighbouring domain walls as well as adjacent grains.

TEM investigation of a specific bimodal domain configuration, composed of four different domains, revealed the presence of a distinct domain wall. This wall was composed of alternating tiny charged and broad uncharged areas. Thereby the polarization vectors were arranged in a head-to-side, tail-to-side or head-to-tail manner, respectively.

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**Keywords:** ferroelectric materials; transmission electron microscopy; domain structure