MS16-O2 Exotic phases and strain in model perovskite under pressure

Bouvier Pierre[1]

1. Institut Néel, CNRS/UJF, 25 rue des Martyrs BP166, Grenoble, 38042 France

email: pierre.bouvier@neel.cnrs.fr

Over the past 10 years, many efforts have been devoted to the (re-)examination of structural distortions in perovskites under high-pressure in order to identify general rules for their evolutions and interactions with reducing volume. I will present structural characterization of various model perovskites such as $PbTiO_3$ [1,2], $SrTiO_3$ [3], $CaTiO_3$ [4] and the multiferroic $BiFeO_3$ [5,6]. Through those example, I will show that the use of single crystal x-ray diffraction and Raman spectroscopy allows precise determination of symmetry adapted strains and order parameters and will discuss the appearance of either new kinds of large cells structures or the unusual emergence of a polar phase at high pressure.

1. Ferroelectricity of perovskite under pressure, I.A.Kornev, L.Bellaiche, P.Bouvier, P.-E.Janolin, B.Dkhil, J.Kreisel, Phys. Rev. Letters, **95** (2005) 196804/1-4.

2. High pressure effect on $PbTiO_3$, P.E.Janolin, P.Bouvier, J.Kreisel, I.A.Kornev, L.Bellaiche, W.Crichton, M.Hanfland, B.Dkhil, Phys. Rev. Letters, **101** (2008) 237601/1-4.

3. Pressure-temperature phase diagram of $SrTiO_3$ up to 53 GPa, M.Guennou, P.Bouvier, J.Kreisel, D.Machon, Phys. Rev B **81**, 054115 (2010).

4. High-pressure investigations of $CaTiO_3$ up to 60 GPa, M.Guennou, P.Bouvier, B.Krikler, J.Kreisel, R.Haumont, G.Garbarino, Phys. Rev B, **82** (2010) 134101/1-10.

5. Effect of high pressure on the multiferroic $BiFeO_3$, R. Haumont, P. Bouvier, A. Pashkin, K. Rabia, S. Frank, B. Dhkil, W. A. Crichton, C. A. Kuntscher, J. Kreisel, Phys. Rev. B **79**, 184110 (2009).

6. Multiple high-pressure phase transitions in $BiFeO_3$, M.Guennou, P.Bouvier, G.S.Chen, B.Dkhil, R.Haumont, G.Garbarino, J.Kreisel, Phys. Rev. B **84**, 174107 (2011).

Keywords: perovskite, high-pressure, single crystal, structure, Raman

MS16-O3 Dynamics of oxygen vacancies in strontium titanate

M. Zschornak[1,2], J. Hanzig[1], H. Stöcker[1], C. Richter[1,3], M. Nentwich[1], E. Mehner[1], F. Hanzig[1], S. Jachalke[1], S. Gorfman[4], B. Khanbabaee[4], T. Leisegang[1], D. Novikov[3], S. Gemming[2,5], D.C. Meyer[1]

1. Institute of Experimental Physics, TU Bergakademie Freiberg, Germany.
2. Institute of Ion Beam Physics and Materials Research, HZ Dresden-Rossendorf, Germany.
3. Deutsches Elektronen-Synchrotron (DESY) Photon Science, Hamburg, Germany.
4. Department of Physics, University of Siegen, Germany.
5. Institute of Physics, TU Chemnitz, Germany.

email: matthias.zschornak@physik.tu-freiberg.de

Strontium titanate ($SrTiO_3$) is an oxide crystallizing with cubic perovskite-type of structure that exhibits a high tunability of electronic properties by means of defects. Apart from dopants, especially intrinsic defects and predominantly oxygen vacancies may severely alter the crystal's properties.

We have investigated the dynamics of oxygen vacancies in $SrTiO_3$ causing structural as well as symmetry changes under influence of an external electric field. Defect migration and separation in the crystal induce remarkable electronic modifications, accompanied with whole regions of a new metastable phase exhibiting repealed centrosymmetry, polar character and pyro- as well as piezoelectricity. These structural changes have been thoroughly studied by means of in-situ X-ray Diffraction, I-V characteristics, Raman, Sharp-Garn and Resonant X-ray Scattering. Structural dynamics in response to the electric field occur on two different time-scales, due to slow ionic transport on the one hand and rapid electronically driven atomic displacements on the other. Theoretical models have been developed to account for the experimental findings and will be presented in conjunction to the experimental results.

Keywords: oxides, perovskites, structural symmetry, defects, migration, electroformation, DFT