ITN-EJD

Marie Skłodowska-Curie Project

Cluster Lead-free piezoelectrics

PhD position at ICMCB and LIST, n°2015-06-MC

***Beginning*: October, 1st, 2015**
***Dead line for application*: May, 31st, 2015**

Crystal growth and characterization of lead free piezoelectrics in the pseudo-ternary system $BaZrO_3$-$BaTiO_3$-$CaTiO_3$

Piezoelectric materials convert mechanical stress into electrical charges and conversely. They are key functional materials which are pivotal to "smart" technologies including biomedical devices, ultrasensitive sensing, sonars and equipment for scientific research such as the atomic force microscope (AFM). For decades, the most widely used piezoelectric has been a solid solution between $PbTiO_3$ and $PbZrO_3$ perovskites, commonly called PZT. However, due to the toxicity of lead, the use of PZT-based materials is more and more restricted in many countries. Despite intense investigations carried out to find lead-free alternatives[1,2], the piezoelectric performances of PZT remain unbeaten.

Recently, it has been shown that $Ba(Ti_{0.8}Zr_{0.2})O_3$-$(Ba_{0.7}Ca_{0.3})TiO_3$ solid solution (in short BCTZ) is a very promising contestant as it exhibits a very large piezoelectric response[3]. It has been soon recognized that the phase diagram and instabilities of BCTZ and thus the origin of the outstanding features of BCTZ are different from those of PZT. In particular, the role of oxygen polyhedral rotations on the mechanism of polarization appears important but remains hardly understood. In-depth investigations are expected to provide a better understanding of how to optimize the electromechanical response of BCTZ and related compounds and more generally guide us toward the design of new optimized lead-free piezoelectrics.

The objective of this PhD is to achieve better understanding of the microscopic mechanisms able to produce a large electromechanical response in BCTZ and related materials, in order to guide the rational design of new lead-free piezoelectric compounds.

The experimental work will focus on growth and characterization of large, cm-size single crystals (see figure) in the $BaZrO_3$-$BaTiO_3$-$CaTiO_3$ system[4]. In particular, challenging rich-$BaZrO_3$ and rich-$CaTiO_3$ compositions of the phase diagram will be explored through their single crystal growth. This approach promises a crucial advance compared to previous investigations on polycrystalline ceramics, where the intrinsic properties remain often obscured by grain boundaries and secondary phases. Moreover, large-sized single crystal will allow their structural characterization by synchrotron, neutron and light scattering techniques. The investigation of crystals cut along desired crystallographic axes will allow identifying axis of high piezoelectric response. Improving the understanding of both the structural and physical properties will provide the necessary input for advanced modeling of these single crystals (interaction with PhD project n°2015-07-MC).

[1] Properties of epitaxial films made of relaxor ferroelectrics. S. Prosandeev, D. Wang and L. Bellaiche, Phys. Rev. Lett. 111, 247602 (2013).
[2] Thermotropic phase boundaries in classic ferroelectrics. T.T.A. Lummen et al., Nature Comm. 5, 3172 (2014).
[3] Large Piezoelectric Effect in Pb-Free Ceramics. W. Liu and X. Ren, Phys. Rev. Lett. 103, 257602 (2009)
[4] Continuous cross-over from ferroelectric to relaxor state and piezoelectric properties of $BaTiO_3$-$BaZrO_3$-$CaTiO_3$ single crystals, F. Benabdallah, P. Veber, M. Prakasam, O. Viraphong, K. Shimamura , M. Maglione, J. Appl. Phys. 115, 144102 (2014)

BCTZ boule grown at ICMCB[4]

This project will benefit from the complementary expertise of:

- **Institute for Condensed Matter Chemistry Bordeaux (ICMCB, CNRS, University of Bordeaux)** where single crystals of BCTZ will be performed by using top-seeded solution growth. Growth of targeted compositions will be followed by cutting of single crystals along suitable crystallographic directions; and by chemical, morphological and crystallographic characterization. Investigation of dielectric, piezoelectric and pyroelectric properties

- Luxembourg Institute of Science and Technology (LIST) where advanced characterization of the chemical composition and both the local and average crystal structure will be performed, as well as the determination of the phase diagram by using Raman spectroscopy, X-ray diffraction, diffuse scattering and absorption using synchrotron radiation. Simultaneously to dielectric investigations performed at ICMCB, a particular attention will be paid on the dielectric aging and fatigue of crystals at LIST. Finally, pair distribution functions will be investigated at both synchrotron and neutron sources, for understanding the local structure namely in terms of octahedral tilts

- **FEE GmbH, Forschungsinstitut für mineralische und metallische Werkstoffe-Edelsteine/Edelmetalle** where the crystal growth of large sized single crystals will be carried out as well as their orientation and cutting.

This interdisciplinary project will bring results to the broader community of scientists who are interested in fundamental research in growth of single crystals of lead-free materials as well as their structural and physical properties characterization.
We are looking for a motivated applicants appreciating scientific challenges, with excellent and appropriate skills in the fields of:

- Crystal growth
- Solid-state physics
- Materials science
- Physical chemistry

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