Executive Summary

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Project "Electro-mechanical coupling in lead-free piezoelectric materials"

Many devices employ elements that are based on interconversion of mechanical and electrical energies. Examples include ink-jet printers, fuel injection actuators in cars, transducers for ultrasonic imaging and therapy in medicine, sensors and actuators for vibration control, accelerometers, sample stages in scanning microscopes, parking transducers, and sonars. In many of these applications the active material is based on Pb (e.g., $Pb(Zr,Ti)O_3$ or PZT) which is toxic and the devices are therefore subjected to legislations that restrict use of hazardous substances. The physical effects that convert electrical energy into mechanical and vice-versa are known as piezoelectricity, electrostriction and flexoelectricity. The piezoelectric effect is the most widely used in applications.

The ultimate goal of this project's is to develop lead-free alternatives to lead-based compositions that currently dominate the market worth some 24 billion dollars/year. To reach this goal it is essential to understand various physical processes that contribute to the electro-mechanical coupling in materials. These contributions include lattice response to external fields, domain wall motion in ferroelectric materials, instabilities related to morphotropic phase boundary (MPB)), field induced phase transitions, defects, internal fields and non-homogeneities. Although presently little used compared to piezoelectric effect, electrostriction and flexoelectricity are considered in this project as possible alternatives to the piezoelectric effect, thus broadening the spectrum of lead-free candidates for electro-mechanical devices.

The work was carried out partly in collaboration with groups in Germany, Slovenia, Australia, United States and New Zealand. Our research was focused on selected lead-free compositions ($(Na_{1/2}Bi_{1/2})TiO_3$-$BaTiO_3$, $(Ba,Ca)(Ti.Zr)O_3$, $BiFeO_3$, and $(Ba,Sr)TiO_3$) and their solid solutions.

The achievements include: (i) analysis of morphotropic phase boundary systems which resulted in a new concept of composition-temperature phase diagram with enhancement of the electro-mechanical properties based on polarization extension in addition to the more conventional polarization rotation mechanism; (ii) demonstration that donor and acceptor dopants affect properties of $(Na_{1/2}Bi_{1/2})TiO_3$-$BaTiO_3$-based materials differently than properties of PZT; (iii) revelation of contributions of grain-to-grain interactions to the piezoelectric effect in polycrystalline materials; (iv) demonstration that electrical conductivity of moving domain walls contributes to the dynamic piezoelectric effect and frequency dispersion of the piezoelectric coefficient in $BiFeO_3$; (v) uncovering of macroscopic symmetry breaking in $(Ba,Sr)TiO_3$ and its possible role in the flexoelectric response in this material; (vi) demonstration that enhanced piezoelectric response in $(Ba,Ca)(Ti.Zr)O_3$ is accompanied by significant elastic softening; (vi) demonstration of electric-field control of morphotropic phase boundary; and others. These results will help further development of electro-mechanically active lead-free materials.

The project has resulted in more than 20 publications, four of which are, according to Web of Science, highly cited papers in fields of Physics and Materials Science. The papers were published in journals covering a broad range of topics, including Nature Materials, Advanced Functional Materials, Physical Review Letters, Physical Review B, Applied Physics Letters, Journal of Applied Physics, Journal of American Ceramic Society and others. The work was presented at over 20 international conferences, seminars and workshops as an invited contribution, four of which were plenary presentations.