Morphotropic Phase Boundary, Defects and Domain Walls

Dragan Damjanovic
Group for Ferroelectrics and Functional Oxides
Swiss Federal Institute of Technology in Lausanne – EPFL
Lausanne, Switzerland
dragan.damjanovic@epfl.ch

In this tutorial the following fundamental topics of physics and chemistry of ferroelectric materials will be discussed:

(i) **Morphotropic phase boundary (MPB).** MPB is one of the most important concepts in the field of complex ferroelectric materials (usually oxides). Technologically important piezoelectric materials are made of solid solutions that exhibit a region in the phase diagram where properties are enhanced. This region is in turn associated with a change of the crystal symmetry of the solid solution with changing composition, which is known as MPB. We will start with an introduction and present early ideas why properties may be enhanced at MPB. Then, recent discoveries that led to a deeper insight into fundamental mechanisms and processes taking place at MPB will be discussed, including free energy flattening, polarization rotation, monoclinic phases, crystal anisotropy, hierarchical domain structure, domain engineering and enhanced domain wall displacement. We will also present examples of MPB in nonferroic piezoelectric materials.

(ii) **Defects and Domain Walls.** Domain walls are a defining property of ferroelectrics. They can be mobile and contribute significantly to dielectric, elastic and piezoelectric properties of ferroelectric materials. Point defects (electronic and atomic) are unavoidable in a real material and can affect properties in many ways. Technologically important soft and hard ferroelectric piezoelectrics are obtained by engineering interaction of atomic point defects with domain walls, polarization and strain. We will start with an introduction into defect chemistry of perovskites and formation of domain walls and then focus on interaction of defects with domain walls, polarization and strain. As with the previous section, we will start with earlier ideas and then discuss new experimental and theoretical results that led to a deeper insight and current understanding of the problem. We will consider $Pb(Zr,Ti)O_3$, $BiFeO_3$ and $BaTiO_3$-based materials.