Fundamentals of Ferroelectrics and Piezoelectrics

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This tutorial is aimed primarily at experimentalists who are relative newcomers to the field of ferroelectricity and wish to achieve greater insight into their data through the application of basic models of ferroelectricity.

Using an alternative pedagogical approach to most textbooks, the initial emphasis will be on visualizing the interrelation between electrical and mechanical properties via simple crystal chemical concepts and then progressing to the Landau-Ginzburg-Devonshire (LGD) thermodynamic theory. Initially, from a static ionic model, we will show how the elastic non-linearity of interatomic bonds leads to the fundamental form of electromechanical coupling known as electrostriction. In special cases the non-linearity results in spontaneous polarization and ferroelectricity. The same framework will be used to develop the relationship between the three primary properties of piezoelectric materials: the elastic compliance, the dielectric permittivity and the piezoelectric charge coefficient. Extending the treatment into the time and frequency domains leads to the lattice dynamics analysis of ferroelectrics, whilst consideration of the thermodynamics of the analysis provides a pathway to the LGD thermodynamic theory of ferroelectrics. The latter part of the tutorial will then focus on a practical guide to using thermodynamic theory, employing case studies, ranging from the classic example of $BaTiO_3$ through to relaxors and thin films. Finally, we will try to answer the question: "Where do I start with LGD ?".

You will be most comfortable here if you are happy using computational applications such as Mathematica or Matlab to process simple mathematical functions that would be familiar to most high school students. If you are eager to find an alternative to LDA and GGA for the exchange correlation approximation, then you are probably in the wrong tutorial !

I am happy to answer questions either before or after the tutorial at: a.j.bell@leeds.ac.uk