Dielectrics and Ferroelectrics: New Scattering Methods and Statistics Lead to New Physical Insight

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Dielectric and piezoelectric materials are used to store and convert electrical and mechanical energy, making them essential to a broad range of applications and devices including impact and displacement sensors, actuators, capacitors, microelectromechanical systems, vibrational energy harvesting, diesel fuel injectors, sonar, and ultrasound. In these applications, the dielectric and piezoelectric coefficients define the performance and the limits of device operation. However, the true origin of the material response, and thus the property coefficients, are not well understood because of the numerous and complex microstructural and crystallographic contributions to these properties (e.g., ionic and dipolar polarizability, ferroelastic domain wall motion, interphase boundary motion, the intrinsic piezoelectric effect, etc.)

This talk will first demonstrate the use of advanced \textit{in situ} X-ray and neutron scattering methods (including diffraction and pair distribution functions from total scattering) to discern the underlying mechanics and physics at play in electro-active materials such as dielectrics and piezoelectrics, ultimately revealing the contribution of these various mechanisms to the property coefficients. In all cases, direct measurements of the contribution from lattice deformation (e.g., piezoelectric) and the motion of intragranular interfaces (e.g., ferroelectric domain walls, interphase boundaries) are quantitatively related to the property coefficients using micromechanics-based formulations.

The second part of this talk will include an introduction to an alternative statistical framework for analysis of diffraction data, that of Bayesian statistics in conjunction with a Markov Chain Monte Carlo (MCMC) algorithm. This analysis approach is applied to modeling doublets from ferroelastic degenerate reflections and quantifying the extent of domain wall motion in ferroelectrics on a probability basis. We have also applied these approaches to full-pattern profile fitting. The parameters in the new models represent structure using probability distributions, treating solutions probabilistically with improved uncertainty quantification.