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PURDUE MATERIALS ENGINEERING

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Seeing the unseen: Local atomic disorder of ferroelectric oxides from pair distribution functions and local structure response to electric fields

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Dielectric and ferroelectric 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, piezoelectric microelectromechanical systems (MEMS), vibrational energy harvesters, and ultrasound imaging devices. In these materials, changes in the crystallographic structure under application of externally applied electric fields (*e.g.*, phase transitions, lattice strain) significantly influence the properties. However, most established characterization techniques such as diffraction cannot resolve the structures of many newly explored material compounds and systems because the structures exhibit local-scale chemical or positional disorder that does not influence the diffraction patterns. New characterization techniques are required in order to fully characterize increasing structural complexity at the nanoscale in these functional materials. One such approach, the pair distribution function (PDF) which describes atom-atom distances from ~2 Å to >50 Å, has gained attention as a method to study the local structure of such complex materials. In this talk, I first introduce several prior studies demonstrating the ability of PDF to obtain structural information inaccessible via conventional Bragg diffraction. We then present our own measurements on $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) and $(1\text{-}x)BaTiO_3\text{-}xBi(Zn_{0.5}Ti_{0.5})O_3$ (BT-BZT) which evidence significant local structure distortions from the average structure. In NBT, PDF studies have revealed the effect of unique local environments of Bi^{3+} and Na^{+}. In BT-BZT, a high energy density dielectric at x >0.10, a unique behavior of permittivity vs. temperature is linked to local structure effects that are observable in the PDF. Results from a newly developed technique of *in situ* electric-field PDF are then presented for several established and emerging compositions. The local structure response of various systems is found to be different, reflecting unique electromechanical behaviors in different systems. Notably, we observe the reorientation of disordered Bi^{3+} displacements in NBT during application of electric field, a dipolar mechanism that has not been previously characterized *in situ*.

Dr. Jacob Jones (Purdue BSME '99, MSME '01, PhD Materials '04) is a Professor in the Department of Materials Science and Engineering and Director of the Analytical Instrumentation Facility at North Carolina State University. His research interests include electromechanics, mechanical behavior of materials, and crystallography. Jones' group applies advanced in situ X-ray and neutron scattering methods in order to study real-time processing-structure-property relationships of materials. Much of his recent work has focused on the mechanics of electrically-active domain walls in solids and their contribution to the piezoelectric, dielectric and elastic properties. However, the X-ray tools and techniques developed in pursuit of these efforts are also widely applied to materials synthesis and the response of solids to other perturbing fields (e.g., magnetic, mechanical). Since 2004, Jones has published 130 papers on these topics and his research has been supported by the National Science Foundation, the Army Research Office, National Institute of Standards and Technology, and various industrial and other laboratory sponsors. He has received numerous research awards including the National Science Foundation CAREER award (2007), a PECASE - Presidential Early Career Award for Scientists and Engineers (2009), the IEEE Ferroelectrics Young Investigator Award (2011), and the 2010 and 2012 Edward C. Henry "Best Paper" awards from the Electronics Division of the American Ceramic Society. Jones has also been selected to be elevated to the grade of Fellow of The American Ceramic Society, a recognition to be given October 5, 2015 at the 117th Annual Meeting of the American Ceramic Society.