Local scale studies of ferroelectric oxides under electric fields and at the nanoscale

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As increasingly complex materials are developed and the miniaturization of functional materials continues, the ability to characterize intricate structural details is key to developing robust structure-property relationships. This seminar presents two topics where local-scale (nanometer and sub-nanometer) studies of ferroelectric perovskites are able to reveal structural features and *in situ* behavior generally inaccessible to other experimental methods. The primary experimental tool utilized is X-ray or neutron total scattering, which is converted into pair distribution functions (PDFs). A PDF reveals the probability of atom-atom distances (pair correlations) as a function of real-space distance, typically from 1 to <100 Å, for all atoms in a sample. The first topic is a study of the lead(Pb)-free ferroelectric $Na_{1/2}Bi_{1/2}TiO_3$ under static electric fields using *in situ* X-ray total scattering. Analysis of the data at different orientations relative to the electric field vector reveals reorientation of the Bi^{3+} displacements towards the electric field direction. This novel method allows for the observation of 'local scale domain reorientation' as well as changes in ion displacements and bond lengths. The second topic is the study of freestanding nanocrystals of the classical ferroelectric $BaTiO_3$ with cubic and spherical morphologies and sizes from 8 to 100 nm. This project endeavors to elucidate the relationships between particle shape, size, surface termination (i.e., capping ligands) and the "internal" crystal structure, and how these variables affect the size limit of ferroelectricity. In order to probe these nanometer and sub-nanometer-scale features, both neutron and X-ray total scattering / PDFs are employed. Neutron PDFs in particular are sensitive to indications of either stabilization or destabilization of polarization for nanocrystals including Ti-O bond length distributions and the degree of correlation of ferroelectric distortions. Our preliminary results suggest that for larger nanocrystals (>20 nm), the shape does not largely effect the internal crystal structure, in contrast to results in the literature for smaller (5-10 nm) nanocrystals.

Bio:
Tedi-Marie Usher-Ditzian is currently a Postdoctoral Research Associate in the Chemical and Engineering Materials Division at Oak Ridge National Laboratory in Tennessee, USA. Usher-Ditzian completed her B.S. and M.S. in Materials Science and Engineering at the University of Florida before moving to North Carolina State University where she earned her Ph.D. from the Department of Materials Science and Engineering in 2016. Her current research interests include the structure of materials at the nanoscale, structure-property relationships for functional materials, and X-ray and neutron diffraction and total scattering. Usher-Ditzian is a recipient of the Ludo Frevel Crystallography Scholarship and the International Research Fellowship funded by the International Center for Materials Research at University of California Santa Barbara.