Role of Nanostructure in Ferroelectric Capacitors

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Along the way to develop lead-free dielectric materials, it was discovered that nanoparticles of Barium Titanate performed three times better than macroscopic materials in supercapacitors. This spiked a flurry of interest to discover how the material worked. Here we show that the answer to this question lies in the nature of the "microstrain" defined by the classical Williamson-Hall analysis of neutron or X-ray powder diffraction data. While classical XRD shows the material is cubic, X-ray pair distribution function measurements clearly show the local structure is lower symmetry than cubic. This apparent inconsistency is resolved by examining 3D Bragg coherent diffraction images of selected nanocrystals, which show the existence of ~50 nm-sized domains, interpreted as tetragonal twins, which cause the average crystalline structure to appear cubic [1]. The ability of these twin boundaries to migrate under the influence of electric fields explains the dielectric anomaly for the nanocrystalline phase. This talk will explain how X-ray coherence is used for imaging and how this could be a routine complement to powder diffraction measurements for other industrial materials, such as cements, 3D printed structures or semiconductor devices.

[1] "Structural investigation of the metastability of barium titanate nanoparticles grown under hydrothermal conditions", Ana F. Suzana, Sizhan Liu, Jiecheng Diao, Longlong Wu, Tadesse A. Assefa, Ross Harder, Wonsuk Cha, and Ian K. Robinson, Advanced Functional Materials 2208012 (2023)