Origin of the Enhanced Dielectric Response of Ferroelectric Materials seen by Coherent X-ray Scattering

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The dielectric constant of nanoparticle Barium Titanate (BTO) performed three times better than macroscopic materials in Multilayer Ceramic Capacitors, which make use of these lead-free dielectric materials. Various models have been proposed for the enhancement. Here we use Bragg Coherent Diffraction Imaging (BCDI) to understand 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. 3D BCDI of selected nanocrystals, shown in Fig 1, reveals 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.

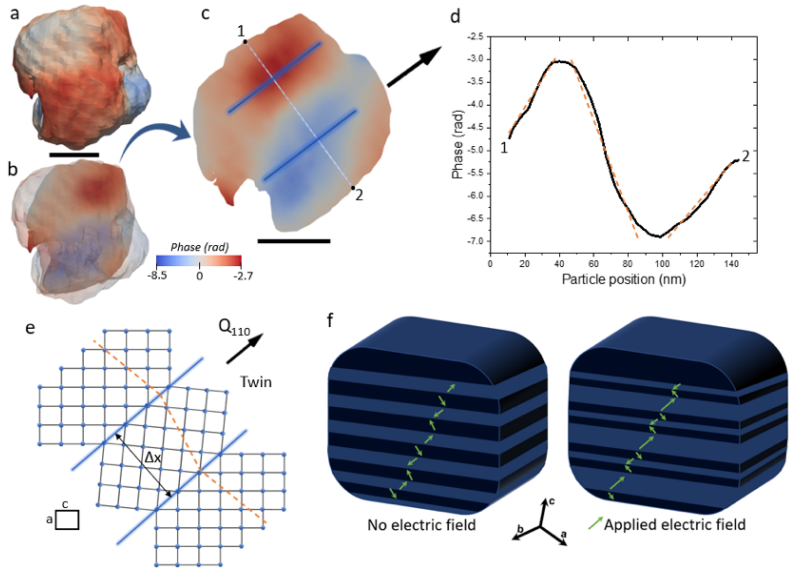

Figure 1. Twin domain model of $BaTiO_3$ (BTO) nanocrystal structure from the Bragg Coherent Diffraction Imaging analysis. (a-c) 3D reconstruction (d) Phase line plot along the white line shown in (c). (e) Schematic of twin domains with the c/a ratio exaggerated ten times (f) Schematic model of the dielectric response as field-induced migration the domain walls.

[1] Ana F. Suzana, Sizhan Liu, Jiecheng Diao, Longlong Wu, Tadesse A. Assefa, Milinda Abeykoon, Ross Harder, Wonsuk Cha, Emil S. Bozin and Ian K. Robinson, Advanced Functional Materials 2208012 (2023)