

Role of Nanostructure in Multilayer Capacitors

Ian Robinson, Ana F. Suzana, Sizhan Liu, Jiecheng Diao, Longlong Wu, Tadesse A. Assefa, Milinda Abeykoon, Ross Harder, Wonsuk Cha and Emil S. Bozin

London Centre for Nanotechnology, University College, London
Brookhaven National Laboratory
Argonne National Laboratory

Multilayer Ceramic Capacitors use lead-free dielectric materials, such as Barium Titanate (BTO). It was discovered that the dielectric constant of nanoparticle BTO performed three times better than macroscopic materials. 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.

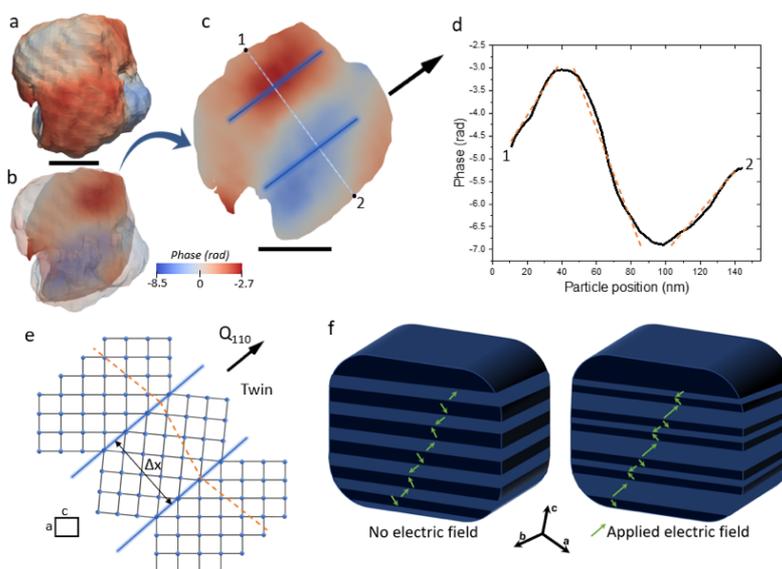


Figure 1. Twin domain model of BaTiO₃ (BTO) nanocrystal structure from the Bragg Coherent Diffraction Imaging analysis. (a-c) 3D reconstruction (d) Phase line plot along the white line shown in (c). (e) Schematic of twin domains with the c/a ratio exaggerated ten times (f) Schematic model of the dielectric 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)