Bragg coherent diffraction for investigation of nanostructure in industrial materials

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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, shown in Fig 1, which reveal 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.
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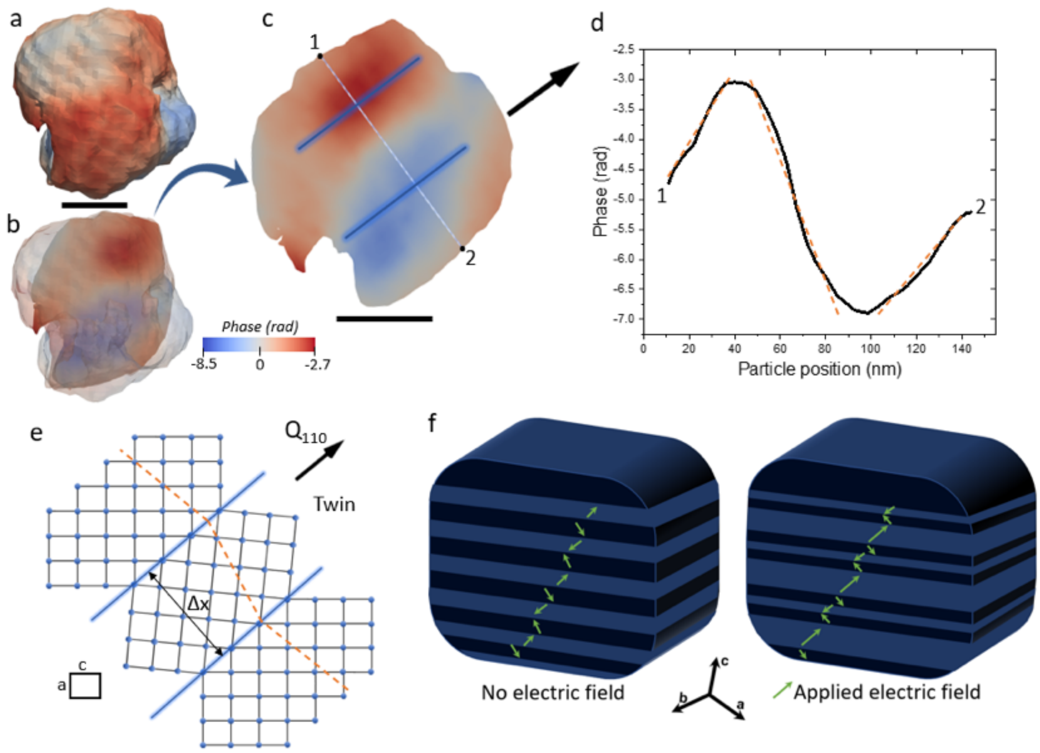

Figure 1. Twin domain model of $BaTiO_3$ (BTO) nanocrystal structure from the Bragg Coherent Diffraction Imaging analysis. (a) 3D reconstruction of one nanocrystal mapped out as a phase isosurface. (b) Translucent copy showing the position of the cross sectional slice shown in (c); (d) Phase line plot along the white line shown in (c). (e) Schematic of a twin domain (central portion of the crystal); the c-a difference is exaggerated ten times for illustration purposes. The shaded blue lines represent the merohedral twin boundaries. The orange dashed line in (d) and (e) represent the modulations caused by the presence of the twin, having a distinctive slope. (f) Schematic model of the dielectric response as field-induced migration the domain walls within the crystal. Green arrows represent the local direction of the polarization.

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