

# ICMAT 2025

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## Coherent X-ray Scattering of domains in Ferroelectric Capacitor Materials

### References:

[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)

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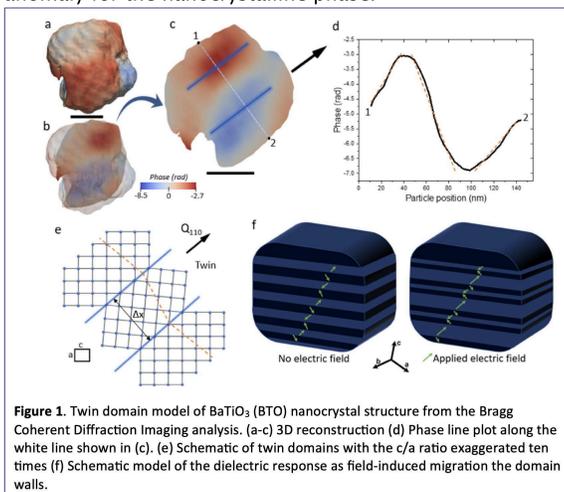
### Abstract:

**Background and Objectives:** 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.

**Methods:** 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.

**Results:** 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].

**Discussion and Conclusion:** 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<sub>3</sub> (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 of the domain walls.

Author Disclosure Information:

**I. Robinson:** None.

**Topics (Complete):** Synchrotron Radiation: Analytical Techniques and Applications

**Presentation Preference (Complete):** Oral Presentation

**Status:** Complete

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