# Functional Strains and Domains in Crystalline Materials

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From X-ray diffraction measurements, the "microstrain" is defined by the classical Williamson-Hall analysis of neutron or X-ray powder diffraction data. With the development of strain-sensitive imaging methods, such as Bragg Coherent Diffraction Imaging (BCDI), we can now spatially resolve the strain field and add detail to the understanding of strain. Nanoparticles of Barium Titanate perform three times better than macroscopic materials in supercapacitors, causing a flurry of interest to discover how the material worked. 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 BCDI images of selected nanocrystals, which show the existence of ~50 nm-sized internal 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 [2]. In other examples, a striped array domain structure was identified in magnetite microcrystals, which is driven by the structural phase transition at low temperature [3]. Finally, a pronounced phase domain structure was found to be introduced in solid-state electrolyte materials, which may account for their functional improvement in ion conductivity.

[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)

[2] Electric Field Driven Domain Wall Dynamics in $BaTiO_3$ Nanoparticles, Jialun Liu, David Yang, Ana F. Suzana, Steven J. Leake, Ian K. Robinson, Physical Review B 111 054101 (2025)

[3] Symmetry Breaking during Low-Temperature Domain Formation in micron-sized Magnetite Crystals Yue Dong, David Yang, Jialun Liu, Aly Abdeldaim, Wei Wang and Ian Robinson, submitted to Physical Review B (2025)