Explanation of the high-dielectric constant of $BaTiO_3$ used in Multilayer Capacitors

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This invited talk will introduce the "phase domain" concept of disorder in nanocrystals. Domains are accessible by Bragg Coherent Diffraction Imaging (BCDI) which is used to understand the "microstrain" defined by the classical Williamson-Hall analysis of powder diffraction data. As an illustration, we examine why the dielectric constant of nanoparticle Barium Titanate ($BaTiO_3$, BTO) is three times higher than macroscopic material. BTO is used in Multilayer Ceramic Capacitors, which make use of this lead-free nanoscale dielectric material. 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, reveals the existence of ~50 nanometer-sized phase domains, interpreted as tetragonal twins, which cause the average crystalline structure to appear cubic. The ability of these twin boundaries to migrate under the influence of electric fields explains the dielectric advantage of the nanocrystals.