Short-range distortions and long-range cubic order in barium titanate nanoparticles

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Barium titanate (BTO) is an important material for energy storage, serving as a high permittivity dielectric in electrostatic capacitors. Barium titanate nanoparticles integrated into a polymer composite could also serve as a versatile dielectric medium for some applications. However, the behavior of discrete BTO nanoparticles needs to be understood better to maximize the performance of composite dielectrics. To that end, high-energy synchrotron X-ray diffraction patterns (XRD) of BTO nanoparticles were collected and analyzed using atomic pair distribution functions (PDFs). Our PDF data show that barium titanate (BTO) nanoparticles ≤ 100 nm in diameter exhibit a distortion of their unit cell. Fits to PDFs over temperatures of 20° to 220°C suggest that Ti atom displacements from the center of the unit cell are comparable to or even greater than those in bulk BTO. Furthermore, these Ti displacements persist at temperatures well above 120°C where the tetragonal to pseudo-cubic phase transition occurs in bulk. Raman spectra acquired over an identical temperature range confirm that BTO nanoparticles ≤ 100 nm in diameter exhibit a distorted unit cell even above 120°C. At the same time, these identical BTO nanoparticles exhibit long-range order consistent with a cubic lattice, as recorded by laboratory XRD Bragg reflections between temperatures of 20° and 150°C. Fitting the PDFs over their full range of 6 nm reveals a long-range structure with a reduced lattice distortion that still manages to support tetragonal Raman lines yet is sufficiently close to cubic to yield apparent Bragg peak singlets.

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