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Barium Titanate Nanoparticles: Short-range Lattice Distortions with Long-range Cubic Order[1] RICHARD C. HASKELL, Harvey Mudd Coll., CHENYANG SHI, Columbia U., SIMON J.L. BILLINGE, Columbia U. Brookhaven Nat. Lab, ERIC PUMA, Pomona Coll., SUN HWI BANG, NATHANIEL J.H. BEAN, JEAN-CLAUDE DE SUGNY, ROBERT G. GAMBEE, ADRIAN HIGHTOWER, Harvey Mudd Coll., TODD C. MONSON, Sandia Nat. Lab, Albuquerque — Small barium titanate (BTO) nanoparticles ($\leq$ 100 nm) exhibit a distortion of the lattice unit cell as inferred from high-energy synchrotron X-ray diffraction patterns (XRD) analyzed using atomic pair distribution functions (PDFs). Fits to PDFs at 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 the bulk material and persist at temperatures well above 120°C where the tetragonal to pseudo-cubic phase transition occurs in the bulk. Raman spectra acquired over a temperature range of 20° to 220°C confirm that small BTO nanoparticles exhibit a distorted unit cell even above 120°C. On the other hand, small BTO nanoparticles exhibit a long-range order consistent with a cubic lattice as recorded by laboratory XRD Bragg reflections at temperatures of 20° to 150°C. We have reconciled these seemingly contradictory data sets by fitting the PDFs over their full range of 6 nm to reveal a long-range structure with a reduced lattice distortion that still manages to support tetragonal Raman lines but is sufficiently close to cubic to yield apparent Bragg peak singlets.

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