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Size Effect on Ferroelectric Transitions in Nanograin Barium Titanate Polycrystals I-WEI CHEN, YUDI WANG, University of Pennsylvania, TIEYU SUN, XIAOHUI WANG, Tsinghua University — Data of dielectric constants and polarization of <100 nm $BaTiO_3$ are now available which allows a definitive assessment of the origin of the size effect in these ceramics of multiple polarization transitions. There are three effects to be considered. First, when the grain size is below 500 nm, the ferroelectric transition is not accompanied by the formation of multiple domain walls, implicating a large residual stress that causes an increase in the temperatures of subsequent tetragonal/orthorhombic and orthorhombic/rhombohedral transitions. Second, when the grain size of $BaTiO_3$ is below 50 nm, screening of grain boundary charge due to defect segregation is ineffective, implicating a large internal field even above T_c. Such a field shifts the temperatures of different transitions differently, favoring the phase of a larger polarization. Third, the dead layer at the grain boundary that clamps the polarization is significant when the grain size decreases to a few nm. It uniformly lowers all the transitions by the same temperature. These effects on transition temperatures and dielectric constant will be compared with the experimental data to assess their relative importance.

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