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The Effect of Grain Boundary Charge on Ferroelectric Transitions in Nanograin $BaTiO_3$ I-WEI CHEN, XIAOHUI WANG, YUDI WANG, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA19104-6272, USA — We have recently reported dense polycrystalline $BaTiO_3$ that has sub-100 nm grains. As grain size decreases, the electrical field due to grain boundary charge extends to an increasingly larger fraction of the grain giving rise to a size effect that is fundamentally different from those previously considered in the literature. Using Ginsberg Landau theory we have modeled this effect on ferroelectric transition, polarization/phase distribution and dielectric/piezoelectric responses, and compared it with the experimental results of $BaTiO_3$ (XRD, TEM, and $\varepsilon(T)$). Such nanograin ferroelectric ceramics, currently available at sub-10 nm grain size, are of considerable interest for the next-generation microelectronic component applications. A related grain boundary effect on phase transition has also been reported in coarse grain and bicrystal $SrTiO_3$.

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