Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Intrinsic size effects and topological phase transformations in ferroelectric nanoparticles embedded in dielectric media JOHN MANGERI, Department of Physics, University of Connecticut, YOMERY ESPINAL, Department of Materials Science and Engineering, University of Connecticut, ANDREA JOKISAARI, Center for Hierarchical Material Design, Northwestern University, S. PAMIR ALPAY, SERGE NAKHMANSON, Department of Materials Science and Engineering, University of Connecticut, OLLE HEINONEN, Materials Science Division, Argonne National Laboratory — Self-assembled composite materials comprised of ferroelectric (FE) nanoinclusions dispersed in a dielectric matrix are being actively investigated for a variety of tunable functional properties attractive for a wide range of novel electronic and energy harvesting devices. However, the dependence of these functionalities on shapes, sizes, orientation and mutual arrangement of FE particles is currently poorly understood. In this study, we utilize a time-dependent thermodynamic Landau-Ginzburg-Devonshire approach combined with coupled-physics finite-element-method based simulations to elucidate the behavior of polarization in isolated spherical $PbTiO_3$ or $BaTiO_3$ nanoparticles embedded in the dielectric medium. The equilibrium polarization topology is strongly affected by particle diameter, as well as the choice of inclusion and matrix materials, with monodomain, vortex-like and multidomain patterns emerging for various combinations of size and materials parameters. In turn, this leads to radically different responses under hysteretic field switching, resulting in highly tunable size-dependent FE properties that should be easily observed experimentally.

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Date submitted: 10 Nov 2016 Electronic form version 1.4