Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Size-dependent infrared phonon modes and ferroelectric phase transition in $BiFeO_3$ nanoparticles[1] PENG CHEN, XIAOSHAN XU, CHRISTOPHER KOENIGSMANN, ALEXANDER C. SANTULLI, STANISLAUS S. WONG, JANICE L. MUSFELDT, University of Tennessee — One emergent property of ferroelectric nanoparticles is the sized-induced structural distortion to a high-symmetry paraelectric phase at small particle sizes. Finite length scale effects can thus be advantageously employed to elucidate ferroelectric transition mechanisms. In this work, we combine infrared spectroscopy with group theory and lattice dynamics calculations to reveal the displacive nature of the ferroelectric transition in $BiFeO_3$, a room temperature multiferroic. Systematic intensity and frequency trends in selected vibrational modes show that the paraelectric phase is $Pm\bar{3}m$ and the lowest frequency A_1 feature is the soft mode that drives the first order transition. Finite length scale effects are also evident in the electronic structure with a red shifted band gap in nanoscale $BiFeO_3$ compared with that of the rhombohedral film, a result that can impact the development of ferroelectric photovoltaics and oxide- based electronics. Taken together, these findings demonstrate the foundational importance of size effects for enhancing the rich functionality and broad utility of transition metal oxides.

[1]This work is supported by the U.S. Department of Energy.

Peng Chen
University of Tennessee

Date submitted: 14 Dec 2010 Electronic form version 1.4