

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Spontaneous polarization
in one-dimensional Pb(ZrTi)O₃ nanowires¹ IVAN NAUMOV, HUAXIANG
FU, Department of Physics, University of Arkansas — Formation of spontaneous
polarization in one-dimensional structures is the key phenomenon that reveals col-
lective behaviors in systems of reduced dimension, but has remained unsolved for
decades. Here we report *ab initio* studies on finite-temperature structural proper-
ties of infinite-length nanowires of Pb(Zr_{0.5}Ti_{0.5})O₃ solid solution. Whereas existing
studies have ruled out the possibility of phase transition in 1D chains, our atomistic
simulations demonstrate an unambiguous otherwise. We show that phase transitions
in 1D wires occur on a remarkable macroscopic length scale, but not necessarily on
an infinite length scale as assumed in the general theories of 1D phase transition.
Such phase transitions are characterized by large longitudinal d_{33} , χ_{33} responses and
a large c/a strain. The long rang ordering in PZT nanowires is explained by use of
depolarizing effects associated with finite thickness of wires. Our results suggest no
fundamental constraint that limits the use of ferroelectric nanowires and nanotubes
arising from the absence of spontaneous ordering.

¹This work was supported by the Office of Naval Research and the Army

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Date submitted: 26 Nov 2005

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