Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

An ab initio study of strained PZT films SCOTT BECKMAN, KARIN RABE, DAVID VANDERBILT, Rutgers University — The potential for creating ferroelectric-based devices such as ferroelectric random-access memories (FeRAMs) has led to an intense interest in ferroelectric perovskite thin films, alloys, and superlattices. Engineering of FeRAMs requires the control of both the spontaneous polarization and the barrier for polarization reversal. The two parameters that are simplest to modify are the composition, which is controlled during the film deposition, and the epitaxial strain, which is controlled by substrate selection. Here, using *ab initio* methods, we investigate how the ferroelectric properties of $PbZr_{(x)}Ti_{(1-x)}O_3$ (PZT) depend upon epitaxial strains ranging from $-0.02 \leq \epsilon \leq +0.02$. Compositions ranging from $0.0 \leq x \leq 0.5$ are examined by the creation of special quasirandom structures. In agreement with the literature,[1] the effect of strain on the polarization is found to be small. We also compute the strain dependence of the barrier for polarization reversal, and discuss the results in the context of experimental measurements of coercive fields and polarization retention.[1]

[1]H.N. Lee, S.M. Nakhmanson, M.F. Chisholm, H.M. Christen, K.M. Rabe, and D. Vanderbilt, Phys. Rev. Lett. 98, 217602 (2007).

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Date submitted: 26 Nov 2007 Electronic form version 1.4