Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Phase diagrams of epitaxial $BaTiO_3/SrTiO_3$ superlattices from first principles[1] SERGEY LISENKOV, LAURENT BELLAICHE, University of Arkansas — The fabrication of artificial superlattices (SL) consisting of alternating layers of two or more ferroelectric oxides is nowadays possible. Such heterostructures may possess properties that dramatically differ from those of bulk ferroelectrics, since, e.g., physical properties of ferroelectric SL should be very sensitive to the epitaxial strain arising from the substrate on which the SL is grown. Determining the temperature-misfit strain diagram of SL is thus of considerable importance. Here, a first-principles-based effective Hamiltonian approach (that has been recently developed and successfully tested for disordered or ordered $Ba_xSr_{1-x}TiO_3$ systems [1]) is used within Monte-Carlo simulations to determine such phase diagram in epitaxially grown (001) $BaTiO_3/SrTiO_3$ SL of different period. We found that, unlike in the short SL, that exhibit a phase diagram that resemble that of (001) $BaTiO_3$ thin films under short-circuit-like conditions, original domain patterns with unusual inhomogeneous atomistic features occur in the longer SL. The reason behind such dramatic difference is revealed. [1] L. Walizer *et al,*, *Phys. Rev. B*, **73**, 144105, (2006).

[1]Supported by ONR grants N00014-01-1-0365, N00014-04-1-0413, N00014-01-1-0600, by NSF grant DMR-0404335, by DOE grant DE-FG02-05ER46188.

Sergey Lisenkov
University of Arkansas

Date submitted: 15 Nov 2006 Electronic form version 1.4