Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Origin of Colossal Ionic Conductivity in YSZ-STO Superlattices
TIMOTHY PENNYCOOK, MATTHEW BECK, KALMAN VARGA, Vanderbilt University, MARIA VARELA, STEPHEN PENNYCOOK, Oak Ridge National Laboratory, SOKRATES PANTELIDES, Vanderbilt University — An eight order of magnitude increase in the ionic conductivity of yttria-stabilized zirconia (YSZ) has recently been demonstrated in YSZ/strontium titanate (STO) epitaxial heterostructures. YSZ is the preferred electrolyte for solid oxide fuel cells (SOFC), in which the ionic conductivity is the major factor limiting the energy conversion efficiency. A colossal increase in the ionic conductivity, therefore, goes a long way towards increasing SOFC practicality by increasing efficiency overall and reducing the operating temperature necessary for efficient operation. We report density functional calculations that explain this colossal ionic conductivity as the result of a large 7% expansive in-plane strain of the YSZ. Molecular dynamics simulations of strained zirconia yield an activation energy for ionic conduction in agreement with experiment. Additionally, simulated annealing under these strain conditions reveals a new lowest energy structure for which EELS simulations using the Z+1 approximation for the core hole are consistent with electron energy loss spectra from the thin, coherently strained, YSZ layers of the heterostructures. This work is supported by NSF grant DMR-0513048 and DOE Office of Basic Energy Sciences, Division of Materials Science and Engineering.

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Date submitted: 01 Dec 2008 Electronic form version 1.4