Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Surface and Interface Structures of Crystalline Oxides on Silicon (COS) FRED WALKER, Oak Ridge National Laboratory, MARCO BUONGIORNO-NARDELLI, North Carolina State University, RODNEY MCKEE, Oak Ridge National Laboratory — The structure of the Sr-covered Si(001) surface (the precursor to COS heteroepitaxy) is a matter of on-going scientific debate with experiment and theory casting opposing views. Real space Z-contrast imaging shows that half of the silicon atoms on the (001) surface are absent, and this has presented us with the intriguing question – "Where does the silicon go?". A metallic surface termination of silicon was required in the layer-sequenced heteroepitaxy of COS. What has been common to all experimental realizations of the layer-sequenced COS structure, is the presence of hydrogen evolving from the metal sources during the film growth. We report here that this hydrogen has inadvertently played a pivotal role in defining the silicon termination and thus the evolution of the interface structure for COS. We will describe the thermodynamic basis for this hydrogen effect along with experimental and theoretical characterization of the structural details. Research sponsored jointly by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy at Oak Ridge National Laboratory under contract DE-AC05-00OR22725 with UT-Battelle, LLC and at the University of Tennessee under contract DE-FG02-01ER45937. Calculations have been performed on CCS supercomputers at Oak Ridge National Laboratory.

Fred Walker
Oak Ridge National Laboratory

Date submitted: 30 Nov 2005 Electronic form version 1.4