Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Ordered Oxygen Vacancy Structure on the Rutile TiO_2 (100) Surface OLIVER WARSCHKOW, School of Physics, University of Sydney, Australia, YINGMIN WANG, ARUN SUBRAMANIAN, LAURENCE D. MARKS, MARK ASTA, Department of Materials Science and Engineering, Northwestern University, Evanston IL, DONALD E. ELLIS, Department of Physics and Astronomy, Northwestern University, Evanston IL — We report the structure of a c(2x2) reconstruction of the Rutile TiO_2 (100) surface obtained by a combination of transmission electron diffraction (TED), direct methods analysis and density functional calculations. The surface layer is found to be Ti2O3 stoichiometric and characterized by an ordered array oxygen vacancies in the subsurface layer. Annealed under oxygen flow, the structure is metastable but relatively long-lived, suggesting that oxygen uptake from the gas-phase is kinetically hindered. A density functional theory construction of the surface phase diagram supports this interpretation. We compare and contrast our reconstruction with similarly reduced reconstructions reported in the literature for the TiO_2 (110) surface.

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Date submitted: 05 Jan 2005 Electronic form version 1.4