Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Deciphering the Structure of Etched Si(100) Surfaces BRANDON S. ALDINGER, ANKUSH GUPTA, IAN T. CLARK, Dept. of Chemistry & Chemical Biology, Cornell University, MARC F. FAGGIN, Dept. of Chemistry and Chemical Biology, Cornell University, RICHARD G. HENNIG, Materials Science and Engineering, Cornell University, MELISSA A. HINES, Dept. of Chemistry and Chemical Biology, Cornell University — A simple aqueous etchant has recently been shown to create near-atomically flat Si(100) surfaces. We use a combination of STM, vibrational spectroscopy, and density functional theory to propose a new model for the etched silicon surface structure. This model contradicts long-standing interpretations of the spectrum of H-terminated Si(100). Broadness in the absorbance bands previously attributed to roughened surfaces is actually caused by variations in the interadsorbate stress. Also, etchant pH is shown to have a surprisingly large effect on morphology. The low pHs used in many industrial processes are shown to cause pronounced roughening and nanoscale hillock formation. The interpretation of these relatively simple H/Si(100) spectra sheds light on the chemical mechanisms that lead to much more complicated Si(100) morphologies.

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Date submitted: 12 Jan 2010 Electronic form version 1.4