Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Competing Atomic and Molecular Mechanisms of Thermal Oxidation of Si vesus SiC XIAO SHEN, Vanderbilt University, BLAIR R. TUTTLE, Penn State Behrend College, SOKRATES T. PANTELIDES, Vanderbilt University — Thermal oxidation is a universal process in solids and is of practical importance in semiconductor technology. The oxidation of Si and SiC provide a unique opportunity for studying the oxidation mechanism because the products are the same oxide SiO_2. The oxidation of Si follows a linear-parabolic law with molecular oxygen identified as the oxidant. The oxidation of SiC obeys the same linear-parabolic law as Si but with different rates and temperature dependences. Using results from first-principle calculations, we first show that an atomic oxygen mechanism can account for the oxidation of Si-face SiC. We then discuss implications of the results and identify the determining factors in the competition between atomic and molecular mechanism. This work is supported by NSF GOALI grant DMR-0907385.

Xiao Shen
Vanderbilt University

Date submitted: 07 Nov 2011 Electronic form version 1.4