Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

DFT Simulations of the Growth of Thin Films on Si and Ge
COLLIN MUI[1], YE XU, CHARLES MUSGRAVE, Stanford University — Germanium is currently being explored as a replacement for silicon for future CMOS technology nodes. Consequently, how its surface chemistry affects thin film growth on Ge substrates is of both technological and scientific interest. We have predicted the mechanisms and energetics for several reactions for growing thin films on both the Ge and Si (100)-2x1 surfaces including ALD of Hafnium oxide, H desorption, oxidation by water, and hydrogenperoxide, nitridization by ammonia and various organic functionalizations. From these results we have determined the various characteristics of the reactivity of various species towards both Si and Ge and have begun establishing guidelines for understanding the reactivity of Ge surfaces versus Si. For example, although it is commonly suggested that processing of Ge devices can be done at lower temperatures, often higher activation barriers are found for Ge and thus processing temperatures are often higher than for Si. Furthermore, intermediates and products of reaction on Ge are less stable than their analogues on Si. Finally, we have found that Ge in general tends to be more selective in its reactivity than Si because of its typically higher activation barriers.

[1]Present address: Novellus Inc.

Charles Musgrave
Stanford University

Date submitted: 06 Dec 2004 Electronic form version 1.4