Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Kinetic Monte Carlo Simulation of Plasma Deposition of Silicon Thin Films SUMEET PANDEY, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — We report results from kinetic Monte Carlo simulations of plasma deposition of silicon thin films under conditions that render the SiH_3 radical the dominant deposition precursor. The transition probabilities for the various kinetic events accounted for in the simulations are based on first-principles density functional theory (DFT) calculations of the corresponding optimal pathways on the H-terminated Si(001)-(2×1) surface and on molecular-dynamics simulations on hydrogenated amorphous silicon film surfaces. The relevant surface transport and reaction processes include SiH_3 diffusion, SiH_3 chemisorption and insertion into Si-Si bonds, surface H abstraction reactions, surface hydride dissociation reactions, as well as SiH_4 and Si_2H_6 desorption into the gas phase. Surface etching is predominantly observed over the 373-640 K temperature range. The surface compositions obtained are in good agreement with experimental measurements on films deposited under similar growth conditions. At 500 K, surface SiH_2 formed by surface trihydride dissociation reactions is the dominant surface hydride species.

Sumeet Pandey
University of Massachusetts, Amherst

Date submitted: 27 Nov 2007 Electronic form version 1.4