Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

On the Growth Mechanisms of Plasma Deposited Amorphous Silicon Thin Films DIMITRIOS MAROUDAS, SUMEET PANDEY, TEJINDER SINGH, University of Massachusetts, Amherst — We present a theoretical study of the growth mechanism of plasma deposited amorphous silicon (Si) thin films based on kinetic Monte Carlo simulations according to a transition probability database constructed by first-principles density functional theory calculations. Based on the results of the study, we propose a comprehensive mechanism of amorphous Si thin film growth by plasma deposition under conditions that make the silyl radical the dominant deposition precursor. The growth mechanism consists of various surface kinetic events including radical-surface interactions, adsorbed radical-radical interactions, radical surface diffusion, and surface hydride dissociation reactions. Of particular importance to the Si film growth process and the resulting surface composition is the radical dissociative adsorption mediated by Si over-coordination defects along the reaction pathway. The proposed mechanism explains the experimentally measured surface composition of plasma deposited Si films under the deposition conditions considered.

Dimitrios Maroudas
University of Massachusetts, Amherst

Date submitted: 21 Nov 2008 Electronic form version 1.4