

## 56d Surface Smoothing Mechanism of Plasma-Deposited Amorphous Silicon Thin Films

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Hydrogenated amorphous silicon (a-Si:H) thin films grown by plasma-assisted deposition from silane-containing discharges are widely used semiconductor materials in the fabrication of solar cells and flat panel displays. Under conditions of low SiH<sub>3</sub> dissociation, the dominant deposition precursor is the SiH<sub>3</sub> radical. The remarkable smoothness of device-quality a-Si:H films grown under these conditions has been used to conclude that the SiH<sub>3</sub> radical is very mobile and can passivate dangling bonds in surface valleys during diffusion, after adsorbing onto the film. However, the fundamental mechanisms underlying SiH<sub>3</sub> radical migration on a-Si:H film surfaces are not well understood and there exists no detailed account of either the role of surface morphology in affecting the incorporation of SiH<sub>3</sub> radicals into the film, or of the preferential locations for growth on the a-Si:H surface.

In this presentation, we report results of molecular-dynamics (MD) simulations on a-Si:H surfaces in conjunction with first-principles density functional theory (DFT) calculations on the crystalline Si(100)-(2x1):H surface that elucidate the mechanism of surface smoothing of a-Si:H thin films. Using MD simulations of impingement of SiH<sub>3</sub> radicals on growth surfaces of rough a-Si:H films, we studied the incorporation of Si atoms from the diffusing SiH<sub>3</sub> radical into the a-Si:H films over the temperature (T) range 500 ≤ T ≤ 773 K. In addition, using DFT calculations, we have carried out analysis of Si incorporation pathways on crystalline Si surfaces that serve as representative models of atomic bonding at film growth surfaces.

We find that the smoothing mechanism of a-Si:H films consists of two steps, namely the fast diffusion of the deposition precursor on the film surface and, subsequently, the incorporation of the deposition precursor in surface valleys of the a-Si:H film. We show that there exists a mobile diffusive state of the SiH<sub>3</sub> radical where the dangling bond of the radical binds to a four-fold coordinated surface Si atom, which becomes five-fold coordinated as a result of the radical's attachment; this overcoordination of a surface Si atom accompanies the radical on its diffusion pathway. Interestingly, our MD simulations indicate that the diffusing SiH<sub>3</sub> radical incorporates into the a-Si:H film only when it transfers an H atom and forms a Si-Si backbond; the transferred H atom can then either be abstracted or diffuse into the bulk a-Si:H film. This H-transfer process is thermally activated and has important implications for the valley filling mechanisms responsible for a-Si:H surface smoothing. Specifically, the H-transfer process does not require the presence of dangling bonds in surface valleys, but leads to preferential Si incorporation in such valleys of the surface morphology due to a lower activation barrier for incorporation in surface valleys compared to hills. The preferential incorporation of Si into surface valleys of the a-Si:H film leads to an effective smoothing mechanism. The results of our DFT analysis for the mechanisms and energetics of Si incorporation are consistent with our MD simulations on the a-Si:H surface.