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Atomic-Scale Analysis of SiH₃ Diffusion on Surfaces of Plasma-Deposited Amorphous Si Thin Films MAYUR VALIPA, University of California, Santa Barbara, TAMAS BAKOS, University of Massachusetts, Amherst, ERAY AYDIL, University of California, Santa Barbara, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — Under conditions of low SiH₄ dissociation during plasma-assisted deposition of hydrogenated amorphous silicon (a-Si:H) thin films, the dominant deposition precursor is the SiH₃ radical. Device-quality a-Si:H films grown under these conditions are remarkably smooth as the SiH₃ radical is very mobile on the films' surfaces and fills surface valleys during its diffusion. In this presentation, we discuss atomic-scale mechanisms of SiH₃ diffusion on a-Si:H surfaces based on molecular-dynamics simulations of SiH₃ radical impingement on a-Si:H film surfaces. The computed average activation barrier for radical diffusion on the a-Si:H surface is 0.16 eV; this low barrier is due to the weak adsorption of the radical onto the a-Si:H surface and its migration predominantly through over-coordination defects. The mechanisms and energetics of SiH₃ migration reported for the a-Si:H surface are consistent with our density functional theory calculations on crystalline Si surfaces. The diffusing SiH₃ radical also incorporates preferentially into surface valleys on the a-Si:H film when it transfers an H atom and forms a Si-Si backbond.

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