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Surface Smoothening Mechanism of Plasma-Deposited Amorphous Silicon Thin Films MAYUR VALIPA, University of California, Santa Barbara, TAMAS BAKOS, University of Massachusetts, Amherst, ERAY AYDIL, University of Minnesota, Minneapolis, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — An important concern in the plasma deposition of thin hydrogenated amorphous silicon (a-Si:H) films is to obtain smooth surfaces. Under conditions that lead to device-quality a-Si:H films, the dominant deposition precursor is the SiH_3 radical. In this presentation, we report results of molecular-dynamics simulations combined with first-principles density functional theory calculations to elucidate the smoothening mechanism of plasma deposited a-Si:H thin films. We show that SiH_3 may diffuse rapidly on the a-Si:H film surface via overcoordinated surface Si atoms and incorporate into the film preferentially in surface valleys, after H atom transfer and formation of two Si-Si backbonds, with activation barriers for incorporation dependent on the local surface morphology. Experimental data on smoothening and SiH_3 diffusion are accounted for.

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