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**Precursor-Surface Reactions in Plasma Deposition of Silicon Thin Films** TAMAS BAKOS, MAYUR VALIPA, DIMITRIOS MAROUDAS, Department of Chemical Engineering, University of Massachusetts, Amherst — Device-quality hydrogenated amorphous silicon (a-Si:H) thin films are usually grown by plasma deposition under conditions where the $SiH_3$ radical is the dominant deposition precursor. In this presentation, we report results of first-principles density functional theory calculations on the interactions of the $SiH_3$ radical with the crystalline Si(100)-(2×1):H surface in conjunction with molecular-dynamics simulations of a-Si:H thin film growth by $SiH_3$ radicals, which elucidate the pathways and energetics of surface reactions that govern important film properties. In particular, we show that an $SiH_3$ radical can insert into strained surface Si-Si dimer bonds, abstract surface H through an Eley-Rideal mechanism, and passivate surface dangling bonds; these reactions follow exothermic and barrierless pathways that lead to a temperature-independent growth rate in agreement with experimental measurements. We also identify a thermally activated surface H abstraction process, in which the $SiH_3$ radical diffuses through overcoordinated surface Si atoms until it encounters a favorable site for H abstraction; the diffusion and H-abstraction steps have commensurate activation barriers. This mechanism explains partly the reduction of the film H content at elevated substrate temperatures.

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