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Analysis of Chemical Reactions between Radical Growth Precursors Adsorbed on Plasma-Deposited Silicon Thin-Film Surfaces TAMAS BAKOS, MAYUR VALIPA, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — The dominant precursor in the plasma deposition of hydrogenated amorphous silicon (a-Si:H) thin films is the SiH_3 radical. In this presentation, we report results of first-principles density functional theory calculations on the crystalline $\text{Si}(001)-(2\times 1)\text{:H}$ surface and molecular-dynamics simulations on a-Si:H surfaces for the interactions between SiH_3 radicals adsorbed on Si thin-film surfaces. The analysis reveals that two SiH_3 radicals may either form disilane (Si_2H_6) that desorbs from the surface or undergo a disproportionation reaction producing an SiH_2 radical that is incorporated in the film and a silane molecule that is released in the gas phase. The corresponding activation barriers depend on the local atomic coordination of the surface Si atoms; Si_2H_6 formation is barrierless if both radicals are bonded to overcoordinated surface Si atoms and exhibits barriers in excess of 1 eV for two chemisorbed SiH_3 radicals.

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