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Subtle role played by H in Si thin-film growth from radicals: key atomic-scale mechanisms revealed by DFT calculations F. MONTALENTI, S. CEREDA, LEO MIGLIO, F. ZIPOLI, M. BERNASCONI, L-NESS and Materials Science Department, University of Milano-Bicocca, Milan (Italy), M. CERIOTTI, Department of Chemistry and Applied Biosciences, ETH Zurich — Breaking silane molecules and creating reactive radicals in the gas phase is an efficient strategy for growing Si films at high growth rates and/or moderate temperatures. In a seminal experimental paper [1], the possibility of obtaining crystalline growth down to T$\sim$200°C, was clearly demonstrated under high dilution of radicals in H. Several interpretations, in some cases controversial, have been given for explaining this evidence. Here we shall show that a clear understanding can be reached by relying on DFT calculations. Starting by a fully hydrogenated Si(001)(1×2) surface, typical of low-temperature growth, we first illustrate the role played by SiH_3 in removing adsorbed H, therefore creating empty sites for further SiH_3 adsorption [2]. The adsorbed sylil, however, is frozen in its initial, non-epitaxial configuration, so that crystalline growth cannot take place. We demonstrate that further incoming hydrogen can easily transform silyl into SiH_2 which, in turn, incorporates into epitaxial sites crossing a barrier of only $\sim$1 eV [3], compatible with Ref. [1] conditions. [1] C.C. Tsai et al., J. Non-Cryst. Solids 114, 151 (1989). [2] S. Cereda et al., Phys. Rev. B 75, 235311 (2007), Phys. Rev. Lett. (in press).

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