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A comparative study of dissociation pathways of silane & germane on Si (001) using cluster & slab formalism in density functional theory. ABIR DE SARKAR, LI QIANG, HWAY CHUAN KANG, DAVID J. SROLOVITZ — Si-Ge thin films are of enormous importance in view of their wide gamut of applications in electronic, opto-electronic, photonic devices, etc. Therefore, a concrete understanding of the elementary processes that lead to film growth is indispensable for an optimum control of film growth. Thin films are typically grown by chemical vapor deposition (CVD) using gas phase precursors like silane & germane. Dissociation of the gas phase precursor (e.g. silane, germane) on the substrate (e.g. Si, Ge) is the first and the most crucial elementary step in film growth. In order to obtain a clear understanding and insight into this mechanism, we have investigated the different possible pathways for silane and germane dissocation on Si(001). (001) surface of Si is typically and preferably used as substrate in film growth. Both germane and silane have been found to exhibit a preference for the intradimer mode of adsorption to the interdimer mode of adsorption on Si(001) surface. Germane shows a lower barrier for dissociative adsorption and the difference of barriers between these 2 modes of adsorption is higher for silane. Unlike the barriers for hydrogen desorption from Si-Ge surface (where the cluster approach predicts a higher barrier), the barriers predicted by the slab formalism for dissociative adsorption has been observed to be higher than the cluster values.

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