

The intermediates of Thermal Decomposition of 1,3-Disilabutane to Silicon Carbide on Si(100) Surface

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1,3-Disilabutane (1,3-DSB) is an excellent precursor for SiC film growth by CVD, but, the decomposition mechanism is not clear. In this study, 1,3-DSB was exposed on Si(100) surface under 100 K in the UHV chamber and thermally decomposed up to 1300 K. and desorbed species detected by Reactive Ion Scattering (RIS), Auger Electron Spectroscopy (AES), Temperature Programmed Desorption (TPD), and Temperature Programmed RIS (TPRIS) during thermal decomposition. RIS method, physisorbed 1,3-DSB was detected under 100 K. the surface temperature increased, physisorbed 1,3-DSB desorbed molecularly at 114 K and 126 K in the TPD. This TPD result was caused by multi-layered 1,3-DSB. Multi-layered 1,3-DSB desorbed at lower temperature than first layered 1,3-DSB. TPRIS results showed that 1,3-DSB partially decomposed to C₂SiH₄ and disappeared over 125 K on the surface. This intermediate more decomposed to the second intermediate, CSiH₄, over 180 K and it existed on the surface in the temperature range of 180 K to 900 K in the TPRIS experiments. TPD and AES results showed that CSiH₄ lost hydrogen and became SiC above 900 K. The adsorption geometries and relative energies of the intermediates, C₂SiH₄ and CSiH₄, were calculated by DFT method.