Oral Presentation

Gas-phase Reaction Kinetics of 1-Methylsilacyclobutane in a Hot-wire Chemical Vapor Deposition Reactor

Ismail Badran and Yujun Shi

Department of Chemistry, University of Calgary
2500 University Drive, Calgary, Alberta, T2N 1N4, Canada   ism45@yahoo.com
Tel: 1-403-2108674; Fax: 1-403-2899488

Thin films made of silicon carbide (SiC) play an important role in the manufacturing of solar cells, lithium-ion batteries, and microelectronics. Recently, there was a growing interest in fabricating SiC's using hot-wire chemical vapor deposition (HWCVD). Particularly, using single-source precursors that contain both carbon and silicon. 1-methyl-1-silacyclobutane (MSCB) is a four-membered ring compound that is characterized by its high ring-strain which facilitate its thermal decomposition on the hot-wire. In order to utilize MSCB in an industrial HWCVD reactor, its reaction kinetics in the gas phase needs to be comprehended.

Vacuum ultraviolet laser (VUV) single photon ionization (SPI) in tandem with time-of-flight mass spectrometry (TOF-MS) was used to study the kinetics of MSCB under typical HWCVD conditions. A new analytical method was developed solely for this study. MSCB was synthesized in situ. The steady state approximation was assumed in order to derive rate constants formulations, in which the kinetic data were analyzed and fit.

Results: The rate constants for the individual decomposition routes along with their respected activation energies were determined. Both the temperature and pressure dependence on the rate constant were investigated. The activation energies for the HWCVD decomposition of MSCB were lower than the theoretically calculated ones, or the ones obtained from the thermal pyrolysis, indicating a catalytic behavior on the hot-wire. However, the activation energies were slightly higher than the ones obtained from the HWCVD primary decomposition under a collision-free environment. This infer that the reactions inside the HWCVD reactor were a mix between a heterogeneous decomposition on the hot-wire, followed by homogeneous secondary reactions in the gas-phase. The study shapes a new methodology to study the kinetics of the complex reactions involved in the HWCVD reactor.