2. Models and Data for Semiconductor Processing

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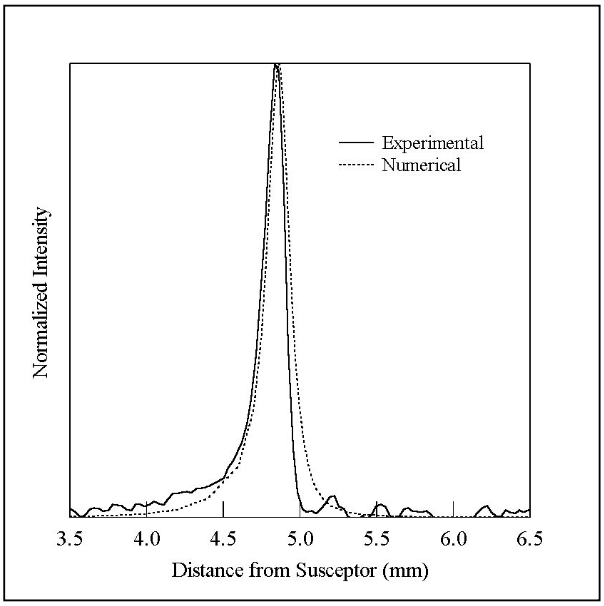
Objective: To provide the necessary information and scientific infrastructure to enable the application of semiconductor process models and controllers that are well-grounded in fundamental physical laws.

Problem: Reactor and process design are often limited to empirical trial and error approaches that tend to converge slowly, if at all, to semi-optimized states. This implies that important industrial processes are not adequately investigated prior to final implementation. This situation manifests itself in more expensive, lower quality products produced by processes that may be less environmentally acceptable.

Approach: Process simulation has the potential to significantly enhance the design phase of process development so as to improve both efficiency and quality. This is because computational power has evolved to the point where highly sophisticated models can be constructed for a variety of complex semiconductor processes. However, the increasing complexity of these models implies a greater need for accurate fundamental thermochemical and kinetic data, which are not presently available. Our approach is both to develop and use methods for reliably generating the data necessary for process modeling. The reliability, quality and utility of the generated data must also be demonstrated to the user community. Consequently, the development of process models of wide applicability is essential, as is model validation carried out in reference reactors prototypical of industrial processing equipment. This typically requires the development of reacting flow computer simulations that employ the aforementioned data for input.

Results and Future Plans: Our effort in the area of microcontamination in CVD reactors continued with the most significant numerical/experimental comparisons of particle layer characteristics during silane decomposition to date. The reactor conditions employed were a pressure of 200 torr, a susceptor temperature of 1050 K, and susceptor rotation rates of 500, 750, and 1000 rpm with 0.25 mole percent silane in helium. Particle scattering intensities were measured experimentally via laser light scattering. These intensity profiles were compared with those generated numerically by the semi-empirical NIST microcontamination model. This model contains two empirical parameters relating to thermophoretic force and condensational sticking coefficient. With these parameters properly chosen, the numerical/experimental comparisons were observed to be excellent, as shown in the figure for a rotation rate of 750 rpm. Both intensity profiles are seen to depict very similar narrow particle layers at a height above the susceptor of 4.86 mm. This height was found to decrease with increasing susceptor rotation rate, which is consistent with the thinning of the thermal boundary layer as rotation-induced suction increases. During FY2001, efforts will continue to characterize the particle layer as well as to determine the gas-phase species concentrations in the region of the layer. Finally, a new web site *(http://www.cstl.nist.gov/div836/836.02/cvd/toppage.html)* has been established in order to serve as a comprehensive source of public information on this research effort.

Our work in database compilation for chemical species of importance in semiconductor processing continued. Good results were obtained for bond dissociation energies during the decomposition of fluorinated ethanes. An experimental effort to measure decomposition rates for organometallic CVD precursors was initiated and will continue during FY2001.



Publications:

Davis, R. W. and Moore, E. F., ***"Two Model Problems for Testing Aerosol Dynamics Algorithms for Stagnation-Flow Reactors,"*** Aerosol Science and Technology, 31, pp. 456-462 (1999).

Davis, R. W., Moore, E. F., Maslar, J. E., Burgess, D. R., Kremer, D. M. and Ehrman, S. H., ***"A Numerical/Experimental Investigation of Microcontamination in a Rotating Disk Chemical Vapor Deposition Reactor,"*** Proceedings of the 2000 International Conference on Characterization and Metrology for ULSI Technology, Gaithersburg, MD, American Institute of Physics (in press).