Mechanical Engineering S.M. Thesis Proposal:

DSMC Simulation of Chemical Vapor Deposition with Simple Chemistry Models

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The goal of this work is to develop an improved method to predict deposition profiles in chemical vapor deposition (CVD) processes. CVD is a manufacturing process that chemically deposits high quality thin films and is widely used in the semi-conductor industry as well as other industries. We are interested in an operating regime of the process in which the feature size is of the order of the molecular mean free path; as a result the classical continuum description is unable to capture the transport processes of interest.

In this thesis we will use a stochastic molecular Monte Carlo method (DSMC) to model the transport processes in the gaseous phase at the feature scale. Traditionally, a constant sticking coefficient is used to assign a probability that an interaction with the substrate will result in deposition and growth of the surface. In actual calculations sticking coefficients are calibrated using experimental data to fit known profiles with minimal reaction chemistry modeling. We propose to improve the standard DSMC modeling of substrate growth by incorporating a chemical model into the vapor-wall interaction that will eliminate the empirically fit sticking coefficients. It is hoped that this new approach will not only give more accurate results but also make the prediction of growth rate of many more types of CVD possible. A tentative schedule of the work is attached.

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	Time (week)	End Date	Jan (1)	Feb (2)	Mar (3)	Apr (4)	May (5)	Jun (6)	Jul (7)	Aug (8)
Preliminary Litrature Study+ Define problem+Praposal writeup	5	2/5/2002								
Study and Develop Chemical Reaction Model	6	3/19/2002								
Survay of Available DSMC and Chemical Models	3	4/9/2002								
Find or Develop code that will simulate arbitrary walls	4	5/7/2002								
Combine Different Model in Full CVD Model	2	5/21/2002								
Verficiation of Full CVD Model	2	6/4/2002								
Debug & Optimize (Parrallelize if Requried)	2	6/18/2002								
Find Previous Restuls to compare with CVD	1	6/25/2002								
Run Models	2	7/9/2002								
Compare reustls with previous Experiments and Predictions	2	7/23/2002								
Final writeup of the theisis	4	8/20/2002								