Session [436] – Modeling and Design of Electronic Materials Processes

Simulation-based design and analysis of advanced CVD reactor systems [436e]

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Abstract

The paper discussed the development of a simulator for the Programmable CVD Reactor system using the modular simulation approach. The design of the Programmable Reactor lends itself very naturally to a modular approach because of the segmented showerhead design - while each segment is a fairly complex component, with individually controllable reactant gas supply and residual gas exhaust, the design of each segment is identical.

Using the modular simulation framework we developed, a new simulation can be constructed relatively easily through the integration of user selected modular components. A key advantage of this approach is that it allows the rapid replacement of individual simulator elements, making it possible to easily assess modeling assumptions and the relative importance of the elements that make up a complete simulation.

We show how simulation gives insight into the operation of this CVD reactor quantifying the relative importance of different precursor transport and reaction mechanisms inside this reactor system. The modular-based approach offers great flexibility to rearrange the segment relative positions in the simulation, which facilitates the study of different reactor design and makes it easy to validate different models and reaction mechanisms. The effects of operating parameters tuning can also be rapidly determined through the simulation.

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1. Introduction

The Programmable CVD Reactor system, a highly controllable CVD system (Choo, Adomaitis, *et. al*, 2003, 2004), is developed at the University of Maryland. An important design feature of the Programmable CVD Reactor is its segmented showerhead design which makes possible true 2-dimensional control of gas phase composition across the wafer surface (as shown in Figure 1). To gain the insight into the operation of this CVD reactor quantifying the relative importance of different precursor transport and reaction mechanisms inside this reactor system, a set of simulation tools is necessary to supplement experimental methods.

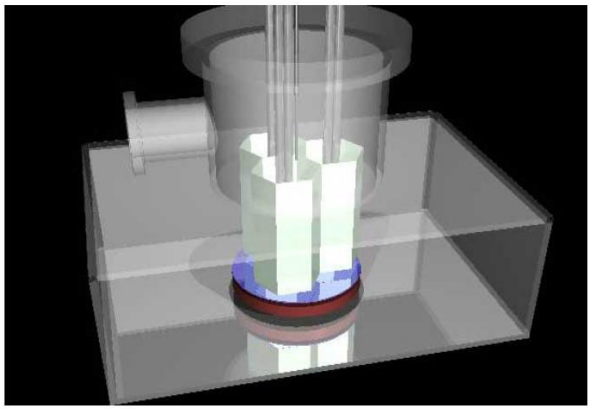


Figure 1. Schematic diagram of the 3-segment prototype Programmable CVD Reactor

Although the simulation will not completely replace the need for experiments, simulators can result in very substantial cost savings in developing new generation of CVD reactor systems and in solving manufacturing problems (Plummer, Deal and Griffin, 2000). Because of the complex geometry structure, conventional CVD simulation tools are no longer appropriate to the newly designed Programmable CVD system. We develop a simulation framework in the form of flexible and reusable modular components for CVD reactor and process simulation. These standalone modules may encapsulate equipment component related information, description of transport phenomena or reaction mechanisms, or contain algorithms for optimizing CVD system designs.

2. Modeling and Simulation

To determine the feed gas flows to the individual segments and to interpret preliminary experimental results, a steady-state one dimensional segment model combined with a well-mixed common exhaust volume model and a model of inter-segment diffusion in the gap region between the wafer and showerhead segments is developed. The geometry of a single segment is depicted in Figure 2. We will introduce the model development along with the construction of individual modules. Instead of developing a complicated simulation program to wrap all modeling equations, we make up several small and simple modules. One of the advantages of this approach is that the redundant work of rewriting similar equations with different variables can be avoided.

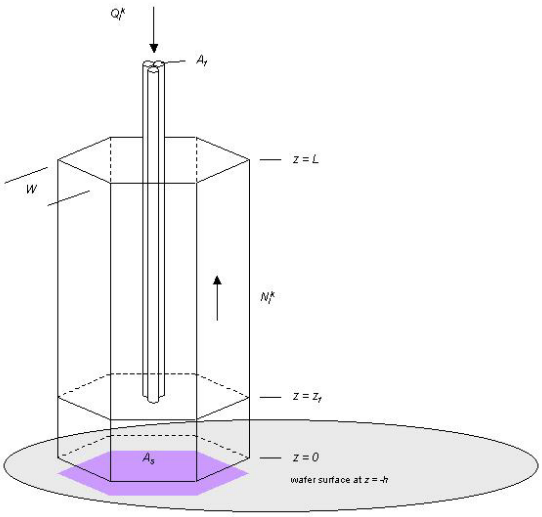


Figure 2. Geometry of single segment

The development of a simulator for this reactor system is based on the modular simulation framework. The design of the Programmable Reactor lends itself very naturally to a modular approach because of the segmented showerhead design – while each segment is a fairly complex component, with individually controllable reactant gas supply and residual gas exhaust, the design of each segment is identical. The module constructions are as follows:

segment module class: This module includes information on describing intra-segment transport, in which the multicomponent gas species transport can be expressed by the Maxwell-Stefan equation:

$$\nabla x_i^k = \sum_{j=1}^{n} \frac{1}{CD_{ij}} (x_i^k N_j^k - x_j^k N_i^k) + \sum_{j=1}^{n} \frac{x_i^k x_j^k}{D_{ij}} \left(\frac{D_j^T}{\rho_j} - \frac{D_i^T}{\rho_i} \right) \nabla \ln T, \quad 0 < z < L$$

with boundary conditions

$$x_i^k(L) = x_i^{exh}$$

In this module, only gas composition x_i^k are defined as variables, all other parameters are known or can be obtained through the interaction with other modules.

gap module class: Three parts contribute to the computation of flux term N_i^k in intra-segment model, i.e.,

$$N_i^k = \sum_n N_i^{k-n} + N_{i,rxn}^k + F_i^k$$

where, F_i^k is a function accounting for the flux change due to feed of species from the segment feeding tube. The changes of inter-segment diffusion flux N_i^{k-n} and species reaction flux $N_{i,rxn}^k$ are determined by the chemical species transport in the gap region between the showerhead and wafer surface. Models developed in this module are used to compute the total flux contribution from gap area to the segmented showerhead. Method *growthrate* included in this class is used to store different reaction models, which can be easily switched on/off to test which reaction mechanism is better fit for the experiments studied.

topmix module class: For the current simulation study, the common exhaust volume is treated as perfectly mixed. The exhaust volume composition x_i^{exh} is computed as the average of the feed compositions to each segment. Therefore, no variables are defined in this class. The parameters x_i^{exh} offer boundary value information for segment class.

chamber module class: The flow rate of gas transport to the chamber is determined by the gap size. The assumption of perfect gas mixing is made within the chamber and the gas composition x_i^{cham} is taken as the average of the feed compositions. This assumption can be validated through the simulation by turn on/off the chamber flux term when computing the inter-segment diffusion flux.

prgcvd module class: This class is developed to handle and facilitate the parameter exchanges between objects of module classes described above, which encapsulates information from user and simplifies the main program. It is also responsible for offering information of different segment pattern designs to each module class. A method called *segdeprate* is developed to output information on each segment deposition rate.

The class diagram in Figure 3 shows the relationship of constructed module classes. The simulation framework developed can be used for n-segment showerhead CVD reactor simulation with desired align patterns, which greatly facilitates the test of different reactor design ideas and saves substantial cost, labor and time of experiments.

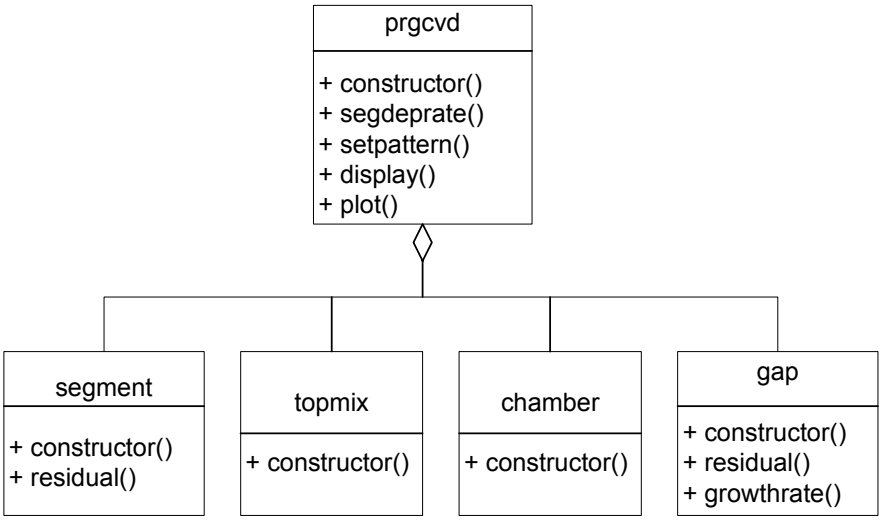
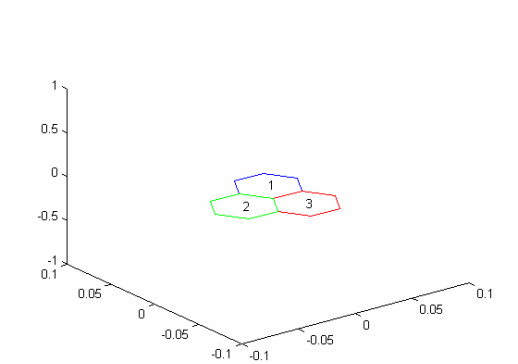
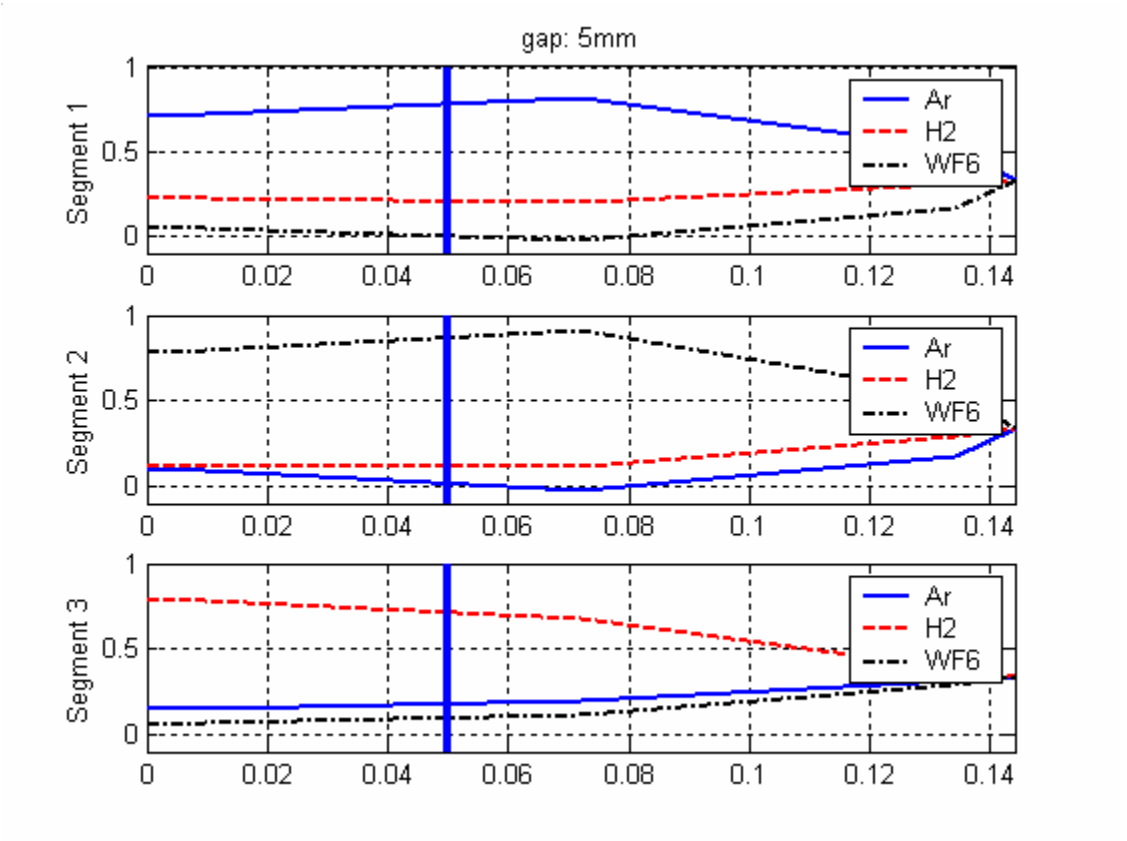


Figure 3. Class diagram of module classes

Figure 4 illustrates simulation results of 3-segment prototype reactor design with a pattern of triangular alignment of segment center. Gas composition profiles are plotted for each segment: Ar fed segment (top), WF_6 fed segment (middle), and H2 fed segment (bottom). The vertical axis marked the bottom of segment at z=0; the vertical line marked the feed tube bundle outlet location. Z is the direction along segment height.



(a)



(b)

Figure 4. (a) segment align pattern; (b) gas composition profiles in each segment

3. Conclusions

The Programmable CVD Reactor system is a new approach to spatially controllable system. This reactor concept incorporates a number of novel design features, and a three-segment prototype reactor has been constructed based on this design.

Using the proposed design framework, a new simulation can be constructed relatively easily through the integration of user selected modular components. A key advantage of this

approach is that it allows the rapid replacement of individual simulator elements, making it possible to easily assess modeling assumptions and the relative importance of the elements that make up a complete simulation.

The modular-based approach offers greatly flexibility of rearrange the segment relative positions in the simulation, which facilitates the study of different reactor design and makes it easy to validate different models and reaction mechanisms.

The effects of operating parameters tuning can be rapidly determined through the simulation, which saves time and effort of researchers and gives instructive guidance for operation condition and system improvements.

References:

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