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UNDERSTANDING AND IMPROVING MATERIALS PROCESSING THROUGH INTERPRETING AND MANIPULATING PREDICTIVE MODELS

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ABSTRACT

Most physically based modeling software accepts input in the form of geometry definition, physical parameters, initial conditions, and boundary conditions; and then, on the basis of solving physical conservation equations, predicts the steady-state or transient behavior of a system or process. There is a growing need to create software tools that can themselves control or manipulate the physically based models in certain ways to enhance the usability of models for equipment design and process optimization. These required tools can be described broadly in the following categories: sensitivity analysis, parameter estimation, inverse problems, dynamic optimization, and real-time control. This paper discusses generally the development and application of such modeling tools, drawing examples from a specific RTP reactor design. These techniques accelerate significantly the optimal design of processes and the concurrent engineering of real-time process-control algorithms.

INTRODUCTION

Sensitivity analysis, which is perhaps most used of the interpretive computation tools, seeks to determine quantitatively the relationship between (possibly uncertain) model parameters and the model predictions. For example, how do predicted deposition rates depend on reaction-rate parameters, or how do wafer temperatures depend on the radiative properties of glass ware? Mathematically, these relationships, or first-order sensitivity coefficients, are expressed as the matrix of partial derivatives of the model's dependent variables with respect to the model's parameters. There is a great deal of mathematical and numerical-analysis literature concerning alternative approaches to sensitivity analysis.

Predictions from physically based models invariably depend on a great many uncertain parameters. These parameters may be physical properties (e.g., thermal conductivities, surface emissivities, or chemical reaction rates) or they may relate to modeling approximations (e.g., material-interface resistances or lumped material properties). Parameter estimation is a formal mathematical procedure, which uses experimentally measured system responses to establish best-fit parameters. Thus, parameter estimation provides the means to "tune" or "calibrate" a model to measured behavior under certain operating conditions. In fact, it is often desirable to develop certain experimental procedures expressly for the purpose of facilitating parameter estimation. Given the results of the parameter estimation, a model can be used with greater confidence to evaluate alternative designs or process modifications. When there are only a few parameters or when the solution depends strongly on a parameter (i.e., a high sensitivity of a measured variable with respect to the parameter), parameter estimation works well. Clearly, there is a relationship between parameter estimation and sensitivity analysis and the computational approaches have much in common.

Inverse analysis is used to establish the boundary conditions or parameter values required to achieve a certain solution. Even though most analysts pose and solve "direct" problems (i.e., fix boundary conditions and parameters, and solve conservation equations for field variables), most designers need the results of inverse problems. That is to say, a process designer knows the desired solution (e.g., wafer temperature), and seeks to design a process to achieve that solution (i.e., to establish the appropriate process parameters and boundary conditions). Because the inverse problem is what really needs to be solved in practical design, analysts have always done de-facto inverse problems. However, the typical approach is to solve direct problems repeatedly in a lengthy and costly iterative process.

Dynamic optimization is related to the inverse problem, but rather than specifying the desired trajectories as specific constraints they are specified as least-squares inequality constraints. For example, instead of requiring exact temperature-time histories at certain points on a wafer (the inverse problem), the problem would be posed by requiring that the wafer follow a specified temperature trajectory within plus or minus 10 degrees and with no more than 5 degrees temperature variation within the wafer. Mathematically, dynamic optimization is derived from optimal control theory.

Both Inverse Problems and Dynamic Optimization provide the equipment designer with powerful capabilities. One important application is to evaluate and understand trajectory feasibility and control authority. For example, consider a nominal CVD reactor design with a maximum heater power of 50 kW and a process that calls for a temperature ramp to process temperature in 20 seconds with a specified maximum temperature gradient within the wafers of 5 degrees. The inverse approaches will determine the power-time histories for the heaters. If the required power exceeds the maximum available for the given design, then the desired trajectory is infeasible. The constraints would either have to be relaxed or a alternative design developed that provided sufficient "control authority." While the inverse problems are not used to design the controller per se, they do provide important information on controllability and process feasibility.

While nearly all physically based modeling is run "open loop," nearly all processing equipment is run under "closed loop" process control. There is a great need to develop the software tools that permit driving the physically based models under closed-loop control, and thus enable the concurrent engineering of equipment design and control algorithms. We seek to run the physically based simulations under the control of the very same process-control software that would be loaded into the actual hardware controllers. Certain dependent variables in the model become the "sensors" (e.g., the temperature of an element on a wafer) and boundary conditions in the model become the "actuators" (e.g., the power or temperature of heater elements), which are controlled by the process-control software. With well defined communication interfaces, the controller software and the physical model could be running simultaneously on different computer platforms -- the physical model replaces the actual hardware. There is little doubt that equipment-development times would be shortened considerably when the controller design is developed and evaluated on a validated physical simulation during the equipment design and development effort.

Rapid-Thermal Processing Examples

CVC Products, Inc. is developing a new rapid-thermal-processing (RTP) reactor for application to several processing steps in silicon-semiconductor fabrication, including contact silicide formation, dielectric deposition, and source-drain anneal. This new product development, which is an extension of the approach taken by Texas Instruments in the Microelectronics Manufacturing Science and Technology (MMST) program,¹ is being done with a great deal of guidance from modeling and simulation. We draw examples from this modeling and design work to illustrate ways that models are manipulated to resolve specific reactor-design and process-optimization issues.

Figure 1 shows the main features of a lamp-heated RTP reactor.² The lower portion, called the lamp housing, consists of several rings of independently controlled tungsten-halogen lamp bulbs. The radiation partitions that separate the lamp rings limit "cross-talk" between lamp zones and regions on the wafer. One important use of the models is to assist design of the lamp house, including lamp placement and partition geometry. The lamp housing is separated from the reaction chamber by a thick quartz window. The silicon wafer itself sits just above the window. Process gases issue downward from a showerhead manifold at the top of the reactor and exhaust through the annular space outside the showerhead (the inlet and exhaust channels are not fully represented in the figure). Design of the showerhead, the showerhead-to-wafer spacing, and

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exhaust ducting, are among critical design considerations that affect the desired radial uniformity on the wafer.

RTP is a relatively new technology that is designed to minimize the time a wafer is held at elevated temperature, and thus minimize thermally induced damage to existing structures on the wafer. In operation, an RTP system ramps the wafer up to processing temperature in as little time as a few seconds, holds the processing temperature for a few seconds to a few minutes, and then ramps the temperature down as quickly as possible. Throughout the ramps and processing cycle, the temperature differences across the wafer must be limited to a few degrees -- a difficult design and control challenge.

We develop and apply a number of different models to represent various aspects of the RTP system, and thus assist the design process. Figure 1 represents a two-dimensional finite-element thermal model³ that considers the radiative and conductive transport throughout the system. Its primary use is to characterize the coupling between the lamp housing and the wafer, including thermal-radiation transmission through, and adsorption in, the window as well as the reflective properties of the wafer and showerhead. In this paper we discuss manipulating the thermal model in two ways. First is in development of sensor-to-actuator response surfaces that form the basis for concurrent design of the reactor geometry and the real-time control system. Secondly, we establish software links that permit the model to be run under feedback control, thus providing a means to test the effectiveness of alternative design options and control strategies.

Figure 1. Model of a rapid-thermal-processing (RTP) reactor

A second thermal model, called the RTP-specific model,⁴ lacks the generality of the finite-element model, but runs quickly on a workstation computer. It has a more sophisticated treatment of the spectral (wavelength-dependent) radiation transport in the system, but a less general treatment of the thermal conduction in the reactor housing. We use this model to illustrate the formulation and use of inverse analysis, which establishes important information about design feasibility and system controllability.

A third model considers chemically reacting flow in the reaction chamber between the showerhead and the wafer. This finite-volume model⁵ facilitates design of the reaction chamber geometry so as to provide uniform deposition on the wafer. For this class of reaction chamber, i.e., gas issuing from showerhead onto wafer, the design goal is to achieve an "ideal stagnation flow," which assures process uniformity.¹ Given a reactor-geometry design that achieves the stagnation flow, the two-dimensional reacting-flow simulation can be reduced to a one-dimensional simulation via mathematical transformation.⁶ We use such a reduced model here to illustrate a sensitivity analysis of the reaction chemistry for a silicon-dioxide deposition process.

OPTIMIZATION AND RESPONSE SURFACES

The concept of a "response surface" is central to our discussion of design optimization and process controllability. The illustration here concerns the design of the RTP lamp housing. Using process-control terminology, we represent the relationship between lamp power and wafer temperature as a steady-state "gain matrix," which is the partial-derivative matrix defined by

$k_{ij} = \partial T_i / \partial P_j$. Computationally we approximate the gain matrix by its discrete analog as $k_{ij} \equiv \delta T_i / \delta P_j$, where δT_i denotes a change in temperature at point i on the wafer caused by a perturbation δP_j of lamp zone j .⁷ This evaluation of k_{ij} is accomplished by the following procedure: determine the steady solution for a given wafer temperature, perturb the power in one lamp zone by a small amount (e.g., 1%), solve for the steady solution with one lamp zone perturbed, and evaluate the temperature response at each point on the wafer. This procedure is repeated for each lamp zone, thus determining each column of the gain matrix.

Figure 2. Power levels required for optimized temperature profiles at 500, 700, 900, and 1100 °C.

Figure 3. Wafer temperature variation from set point for a 5-zone lamp design optimized at 500, 700, 900, and 1100 °C.

One use of the gain matrix is to assist in determining the appropriate lamp powers required to maintain a certain wafer temperature. The typical application of a finite-element analysis calls for specifying the lamp powers (i.e., the boundary conditions), and then solving the discrete analog of the energy-conservation equation for the temperatures throughout the system, including the wafer. However, the analyst and designer really wants to specify the wafer temperature and determine the required lamp powers -- an inverse problem. Using the finite-element software in the normal way to solve the inverse problem leads to a laborious and lengthy trial-and-error procedure. Using the gain matrix as the iteration matrix for a modified Newton iteration automates and accelerates the procedure.

At steady-state operation we desire the wafer to be held fixed at a certain processing temperature T_{set} , with the radial temperature variation minimized and within a certain tolerance. Following the approach of Norman,⁷ we seek a reactor design and lamp-power settings P that minimize the root-mean-square difference between the actual wafer temperature and the set point,

$$\min_P \int_0^R (T_{wafer}(r; P) - T_{set})^2 dr. \text{ The optimal powers are determined iteratively utilizing the gain}$$

matrix discussed earlier. For given powers and their associated temperature profile, corrections to the powers are predicted by solving the linear least squares problem,

$$\min_{\Delta P} \|K \Delta P - (T_{wafer} - T_{set})\|_2, \text{ where } K = [k_{i,j}] \text{ is the } i \times j \text{ gain matrix, } \Delta P \text{ is a vector of updates to the } j \text{ lamp powers, and } T_{wafer} - T_{set} \text{ is a vector of temperature deviations sampled at } i \text{ radial}$$

locations. On each iteration, the lamp powers are updated to $P + \Delta P$. This iteration is continued to convergence.

Figures 2 and 3 illustrate a typical set of results, with Fig. 2 showing the optimized lamp powers for four different wafer set points, and Fig. 3 showing the associated wafer temperature profiles. These results indicate that the optimized temperature uniformity degrades with temperature, i.e., the worst temperature uniformity occurs at the highest operating temperature. The relative importance of the outer lamp zone increases significantly with temperature, owing to the relatively higher radiative losses from the outer regions of the wafer to the cold reactor walls at high temperature.

A second important use of the gain-matrix information is in assessing the system controllability.⁸ Figure 4 shows "gain profiles" associated with the center lamp zone for wafer temperatures of 500, 700, 900, and 1100 °C. These gain profiles represent a column of the gain matrix, illustrating the radial variation in wafer-temperature response for a power perturbation of each lamp zone, i.e., $k_i(r) = \delta T(r) / \delta P_i$. Clearly, the center lamp zone has the largest effect on the center regions of the wafer, although the influence of the center lamp is felt to a lesser extent all the way to the wafer edge. Information such as this led Cho and Kailath⁸ to suggest the use of radiation baffles to limit the range of influence of each lamp zone and thus enhance the system controllability.

Figure 4. Change in gain profiles with respect to the center lamp zone for various wafer temperatures.

Figures 5a and 5b show gain profiles for a 5-zone lamp design, where the design parameter is the length of the radiation partitions that separate each lamp zone. The gain profiles show how each lamp zone affects the wafer-temperature distribution. The reason for the increase in the magnitude of the gain from the center zone (zone 1) outward to the third zone is that the maximum power of the zones increase with zone diameter. This trend of gain increasing with zone power does not hold for the outer two zones. These zones have diameters greater than that of the wafer, resulting in a much lower heating efficiency than the inner zones.

Figure 5a. Comparison of gain profiles (zones 1-3) for two alternative radiation-partition designs.

Figure 5b. Comparison of gain profiles (zones 4-5) for two alternative radiation-partition designs.

For good controllability, each lamp zone should strongly influence one area of the wafer and diminish radially from that region. However, when the energy from the zones is too directed, wafer-temperature uniformity can suffer. Figure 5a shows that an increase in the partition length helped to limit the region of influence of the lamp zones on the wafer. A problem that remains, however, is that both zone 4 and zone 5 (the two outer lamp zones) have their greatest influence at the wafer edge. This essentially removes one degree of freedom from the system, which could cause difficulties in developing a stable controller strategy.

PROCESS CONTROL

The ability to link "high-order" nonlinear physically based numerical models with feedback process-control algorithms provides a powerful capability for advanced equipment design. A communication link between the simulation and the controller creates a "virtual environment" that allows concurrent engineering of both the hardware and controller.

We have developed two methods to run large-scale simulations under closed-loop feedback control. The first method is to write the control algorithm as a subroutine, which is called from the physical simulation software. This method is facilitated by the AutoCode feature of the MATRIXx software, which automatically generates a C (or FORTRAN) source code representation of the control algorithm.* The second communication method allows both the finite-element code and the control-development code (MATRIXx) to run as independent processes using UNIX system calls (sockets) to pass data between them. This approach requires communication I/O filters to be written for each code. The advantage of this approach is that the independent processes can run on different computing platforms (e.g., a CRAY and a SUN workstation) and the full power of the controller-development software is available for interactive modifications and evaluation.

Most real-time process-control algorithms run according to a clock that samples the sensors and updates actuator commands at a certain frequency. For an RTP system a 20 Hz clock is typical. Linking the physical simulation to the controller thus requires that the simulation can be interrupted at this frequency, provide sensor information (e.g., wafer temperature), and accept new settings for the actuators (e.g., lamp powers). Accommodations for this procedure must be made to the numerical time-stepping and error-control algorithms.

Our approach for controller development involves system identification, controller design, and closed-loop simulation. Traditionally, system identification is done using actual hardware; however, this forces the hardware design and the controller design to be done serially. Using a finite-element model of the RTP design, we run system identification tests to generate actuator-to-sensor response surfaces. Figure 6 shows a step input for the RTP lamp-zone powers and Fig. 7 shows the temperature response predicted at several radial positions on the wafer. This data is used to develop certain types of controller designs, such as Linear Quadratic Gaussian (LQG). The finite-element model is then linked with the new controller for closed-loop simulations. The closed-loop simulations provide critical information about the hardware and controller design, including the controller stability and robustness. A significant feature of the evaluating the controller in simulation is that the simulation is not limited to information from the sensors. As shown in Fig. 9, the model provides temperature data not only at the sensor locations but over the entire wafer and support (and entire reactor).

* MATRIXx and AutoCode are trademark product names of Integrated Systems, Inc.(ISI), Santa Clara, CA.

Figure 6. Step input to lamp zone powers for numerical system identification.

Figure 7. Temperature response to lamp power step input computed at three radial positions on the wafer.

Evaluating the number and location of temperature sensors provides an illustration of the capability to engineer concurrently an important aspect of reactor development. Figure 9 shows wafer temperature profiles for two sets of sensor locations. Clearly, the temperature uniformity degrades as the five sensors are spread over a 10 cm. radius to a 12.7 cm. radius, even though the temperature at the sensor locations is nearly perfect in both cases. Thus the model provides valuable information that the process sensors are unable to see. The information is used in sensor design and placement, as well as potentially real-time model-based sensor interpretation in the control algorithm.

Figure 8. Predicted temperature profile along wafer and wafer-support.

Figure 9. Wafer temperature profiles for two different temperature-sensor configurations (five sensors per profile).

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INVERSE ANALYSIS

We illustrate further the application of inverse analysis using an RTP-specific model.⁴ This model, which considers the dynamic response of the RTP system, has less geometric complexity than the finite-element model, but has far more sophistication in its ability to treat wavelength (spectral) dependencies in the radiation transport. Shown schematically in Fig. 10, this model consists of two essential mathematical parts. Transient one-dimensional (radial) energy-balance equations are solved for the wafer (including support structure) and the window. Radially dependent convective and radiative fluxes impinge on both surfaces of the window and wafer. Moreover, both the window and wafer can reflect, transmit, and absorb thermal radiation, depending on their temperature and the wavelength of the radiation. The window and wafer energy balances are represented mathematically as parabolic partial differential equations, with time and radius as the independent variables and temperature as the dependent variable. The model considers spectral radiation exchange between all surfaces in the reactor, including internal reflections within partially transmitting media. The reactor geometry is specified by a radiation view-factor matrix that represents the geometrical relationship between all surfaces.

Figure 10. Schematic of the RTP-specific reactor model

Numerically, the governing energy conservation equations are discretized using a finite-difference approach. The coupled system is solved computationally via a method-of-lines approach using DASSL⁹ as the underlying numerical software.

Here we illustrate the modification of the model to solve a dynamic inverse problem. We specify the transient trajectory of the wafer temperature, and solve for the lamp power trajectories required to meet the desired wafer trajectory. The approach we take converts the parabolic initial-boundary value problem into a differential-algebraic problem.

In this four-lamp-zone reactor, we specify the desired temperature trajectories at four points on the wafer. In addition to the residual equation resulting from the energy balance at each point on the wafer, the specified trajectory introduces a new residual equation, $F_i = T_i - T_{\text{set}}(t)$. Since there are now two residual equations at four points on the wafer (the energy-equation residual and the trajectory constraint), the problem would be over specified unless new dependent variables were introduced. Here we introduce the lamp powers as the needed dependent variables. Thus rather than specifying the lamp powers as parameters or boundary conditions (the direct problem), we solve for their values as a function of time (the inverse problem).

The direct problem can be solved without difficulty by a variety of methods, including the method-of-lines. The inverse problem, however, can cause great difficulty for traditional computational methods. One problem is that most ordinary-differential-equation software requires problem specification in the "standard form," where each residual equation must contain the time derivative of a dependent variable. The trajectory constraint equations do not fit that form. The algorithms that underpin the DASSL software can handle the problem specification and the solution, but there are computational difficulties when trajectories are infeasible, as discussed later.

Figure 11 shows the results of an inverse simulation and illustrates some potential uses for the analysis. The specified wafer trajectory is shown as a heavy line, and the required lamp powers are shown as a function of time. As expected the lamp powers increase initially to drive the wafer temperature up according to the trajectory. Perhaps surprisingly, however, after peaking at about 5 seconds, the lamp powers decrease even though the wafer temperature continues to increase. This behavior is caused by the fact that the silicon-wafer infra-red transmissivity changes rapidly around 600 °C from relatively high transmission to essentially opaque.¹⁰ Thus, because the radiation is coupled more effectively to heat the wafer, the lamps must reduce power to maintain the wafer trajectory.

Solution of the inverse problem provides important information about trajectory feasibility and control authority, and thus influences approaches to process-control design. For example, for a desired wafer-temperature ramp, the inverse analysis predicts the required lamp power or cooling capacity. If the required lamp power exceeds that available in a given design, then the trajectory is infeasible, regardless of the controller strategy. Thus, the reactor must be redesigned or a less-aggressive trajectory considered. Inverse analysis also provides information on "control authority," which relates to the ability of the actuators to respond quickly enough. Lamps typically have very fast response times, but resistive heaters or cooling systems may not have the dynamic response needed to accomplish certain trajectories.

Figure 11. Solution of a dynamic inverse problem showing the lamp powers required to achieve a specified wafer-temperature trajectory.

SENSITIVITY ANALYSIS

Sensitivity analysis is used to determine quantitatively the relationship between physical parameters in a problem specification and its solution. Here, we use the chemically reacting fluid flow in the RTP reaction chamber to illustrate sensitivity analysis. The specific example chosen calls for a cool mixture of tetraethyl-ortho-silicate (TEOS) and nitrogen to issue from the showerhead and deposit SiO₂ on a wafer at 900 °C. Figure 12 shows the temperature and gas-phase species fields for TEOS itself and a reactive intermediate species, triethoxysilanol, that is produced by gas-phase decomposition of the TEOS.

The reaction chamber has been designed to achieve a close approximation to an ideal stagnation flow in the region between the showerhead and the wafer. Evidence for this situation is seen in Fig. 12 by the radial independence of the temperature and species fields. For our purposes here, we take advantage of this design to analyze the chemistry further in a "one-dimensional" stagnation-flow setting.¹¹

The formulation and solution of the ideal-stagnation-flow problem, including sensitivity analysis, are discussed elsewhere.^{1, 6, 11, 12} Here, our intent is only to discuss briefly the formulation of the sensitivity-analysis problem and illustrate some results for the TEOS deposition. In the ideal-stagnation-flow form, the governing mass, momentum, energy, and chemical-species

conservation equations form an ordinary-differential-equation boundary-value problem. The boundary conditions are derived from the inlet conditions at the showerhead and the surface-chemistry specifications at the wafer. After finite-difference discretization on a mesh network, the differential equations are represented by a system of nonlinear algebraic equations. In a shorthand notation, we state this algebraic system as $F(\Phi; \alpha) = 0$, where F represents the vector of residual equations (discrete approximations of the conservation equations evaluated at Φ), Φ represents the vector of dependent variables (velocities, temperatures, and species mass fractions at the mesh points), and α represents a vector of parameters that help define the problem. For the illustrations here, the parameters will be the rate constants for the gas-phase and surface reactions.

Formulation of the sensitivity problem begins by differentiating the residual equation with respect to the parameters, yielding

$$\frac{\partial F}{\partial \Phi} \frac{\partial \Phi}{\partial \alpha} + \frac{\partial F}{\partial \alpha} = 0.$$

The matrix $\partial F / \partial \Phi$ is the Jacobian of the original system and $\partial F / \partial \alpha$ is the matrix of partial derivatives of F with respect to the parameters. We think of $\partial F / \partial \alpha$ column by column, each column representing the explicit dependence of the residual vector F on the parameters. There are as many columns as there are parameters, e.g., reactions. The matrix $\partial \Phi / \partial \alpha$ represents the sensitivity coefficients, which are computed easily once the Jacobian matrix and the $\partial F / \partial \alpha$ matrix have been evaluated at the solution Φ . We evaluate the Jacobian and $\partial F / \partial \alpha$ matrices numerically using perturbations of the Φ and α vectors, not by deriving the exact analytic representations. Furthermore, we solve the original boundary-value problem using a numerical method based on a modified Newton algorithm.^{11, 13} Because it is required by the Newton iteration, the Jacobian has already been formed and factored. Thus, each column of the sensitivity-coefficient matrix is computed by back substitution for each column of $\partial F / \partial \alpha$.

Most physical problems have many dependent variables Φ_i and many parameters α_j . The first-order sensitivity matrix $\partial \Phi_i / \partial \alpha_j$ can be very large, containing an overwhelming amount of information. Thus, a challenge in using sensitivity analysis effectively is to develop graphical or other means to extract the important information and present it in an understandable form.

Figure 13 shows the species profiles for the problem defined in Figure 12. The reaction mechanism used in this illustration consists of one reversible gas-phase reaction in which TEOS

Figure 12. Temperature, flow, and species fields in an RTP reaction chamber. Inlet conditions are 500 sccm of N₂ and 161 sccm of TEOS entering at 60 C through a showerhead into a reactor at 1 Torr total pressure. Wafer temperature is 900 C, and the inlet manifold is separated from the wafer by 3 cm.

dissociates to triethoxysilanol $\text{Si}(\text{OH})(\text{OC}_2\text{H}_5)_3$ and ethylene C_2H_4 . The surface reaction mechanism consists of eight reversible reactions. Altogether, there are six gas-phase species. In addition to triethoxysilanol (TES), ethylene, and the nitrogen carrier, ethanol and water are products of the surface reaction. The surface state itself is described in terms of five adsorbed compounds and the deposited SiO_2 .

The objective of the sensitivity analysis is to understand how each of the reactions influences the solution. One such illustration is shown in Fig. 14, where normalized sensitivity coefficients show the influence of four reactions on the gas-phase concentration of triethoxysilanol as a function of position between the wafer and the showerhead. A high positive sensitivity coefficient means that if the rate of a certain reaction is increased, then the affected species concentration is also increased. The triethoxysilanol concentration is sensitive to the gas-phase decomposition reaction in an intuitive way. That is, if the reaction rate increases, the reaction product also increases. The sensitivity is somewhat lower near the inlet where the reaction is already slow due to low temperature. The triethoxysilanol reaches the showerhead due to reaction in the hot zones and subsequent diffusive transport upstream to the showerhead.

The sensitivity analysis also provides some less intuitive insights. Figure 14 shows sensitivity to three surface reactions, none of which involve triethoxysilanol itself. The gas-phase triethoxysilanol is most sensitive to a surface reaction that describes a surface rearrangement and desorbs water. The sensitivity is negative, indicating that if the reaction rate is increased, the triethoxysilanol concentration is reduced. The analysis reveals some long range effects, whereby the concentration everywhere is affected by surface reaction at one boundary. Information such as this is quite valuable in interpreting experimental observations or deciding which reactions merit further research.

Figure 13. Gas-phase mole fractions as a function of height above the wafer for the RTP system described in Fig. 12.

Figure 14. First-order sensitivity coefficients for the concentration of triethoxysilanol (TES) with respect to gas-phase and surface reactions.

CONCLUSIONS

Simulation software is traditionally designed to accept input that describes a particular problem (i.e., geometry, physical properties, and processing conditions), and then to predict the resulting behavior by solving appropriate systems of equations representing fundamental physical laws that describe, for example, heat transport, fluid flow, or chemistry. Traditionally, the analyst has applied modeling following much the same procedure that a process designer uses in the laboratory. That is, describe the process, simulate it, and examine the solution to see if the process meets the product requirements. This procedure is repeated until the process realizes the required product specifications. While simulation is often faster and less expensive than building

and testing the process in the laboratory, the procedure does not take full advantage of the mathematical content locked in the models.

Important hidden information in models can be used effectively to reduce development time and improve materials processes. For example "inverse analysis" and "dynamic optimization" are techniques that permit the analyst to provide the desired results of a processing step as input and solve for the conditions required to achieve the results. Other analysis techniques facilitate the concurrent engineering of processing equipment and the associated feedback control systems -- lengthy processes that are commonly done sequentially.

There is a growing need to create software tools that can themselves control or manipulate the physically based models in certain ways to enhance the usability of models for equipment design and process optimization. Conventional software design often limits the application of physical models to critical manufacturing issues. Developers of new process-simulation models should be cognizant of information hidden in models, and design software to facilitate the manipulation that is required to extract heretofore under-used information.

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