TECHNICAL RESEARCH REPORT

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T.R. 96-72

INSTITUTE FOR SYSTEMS RESEARCH

Sponsored by
the National Science Foundation
Engineering Research Center Program,
the University of Maryland,
Harvard University,
and Industry

Submitted to *IEEE Transactions on Semiconductor Manufacturing*

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Abstract

In the semiconductor manufacturing industry, optimization of advanced equipment and process designs must include both manufacturing metrics (such as cycle time, consumables cost, and product quality) and environmental consequences (such as reactant utilization and by-product emission). We have investigated the optimization of rapid thermal chemical vapor deposition (RTCVD) of polysilicon from SiH_4 as a function of process parameters using a physically-based dynamic simulation approach. The simulator captures essential time-dependent behaviors of gas flow, heat transfer, reaction chemistry, and sensor and control systems, and is validated by our experimental data. Significant improvements in SiH_4 utilization (up to 7 x) and process cycle time (up to 3 x) can be achieved by changes in (i) timing for initiating wafer heating relative to starting process gas flow; (ii) process temperature (650 – 750 °C); and (iii) gas flow rate (100 – 1000 sccm). Enhanced gas utilization efficiency and reduced process cycle time provide benefits for both environmental considerations and manufacturing productivity (throughput). Dynamic simulation proves to be a versatile and powerful technique for identifying optimal process parameters and for assessing tradeoffs between various manufacturing and environmental metrics.

1. Introduction

Design for Environment, Safety, and Health (DFESH) is a key technology element in the National Technology Roadmap For Semiconductors. "The strategic intent is to integrate preventive Environment, Safety, and Health (ESH) solutions into process, equipment, and facility engineering" [1]. Environmentally-conscious manufacturing (ECM) requires efficient utilization of materials and energy with minimum waste emission. The rapid advances and ever increasing fabrication capacity in the semiconductor industry places an even greater demand on higher manufacturing efficiency and lower environmental impact. New approaches and new levels of scientific understanding for process design, optimization, and control are needed to achieve such efficient, "green" technologies.

Materials utilization efficiency and process cycle time are two examples of important figures of merit. Higher materials utilization reduces consumables cost as well as waste emission, and is beneficial to both manufacturing and the environment. Shorter process cycle time increases throughput of wafer processing, enhancing manufacturing productivity. Process optimization should be carried out to lead to high materials utilization efficiency, short process cycle time, and improvement in a variety of other manufacturing and environmental metrics.

We have constructed and experimentally validated a physically-based dynamic simulator for rapid thermal chemical vapor deposition (RTCVD) of polysilicon [2] from SiH_4. We have applied the simulator to analyze process parameters and recipes, to identify where significant gains are possible, and to assess where tradeoffs between different manufacturing and environmental metrics. In this paper, we present results for enhancement in materials utilization efficiency and for reduction in process cycle time upon modification of process parameters including temperature, flow rate, and relative timing between pressure ramp and temperature ramp. We have investigated the case of a 2000 Å polysilicon deposition process at 5.0 Torr of 10% SiH_4/Ar gas. By beginning wafer heating at the same time as that for starting gas flow rather than after the process pressure is established, materials utilization efficiency can be increased up to 1.6x while the process cycle time can be reduced by a factor of up to 1.5x. Higher process temperatures (from 650 to 750 °C) result in higher SiH_4 utilization (up to 2.1x) and shorter process cycle time (up to 2.1x), benefiting both the environment and manufacturing. Lower gas flow rate (from 1000 to 100 sccm) enhances the SiH_4 utilization by up to 7x, but increases the process cycle time by 2.7x. Here, tradeoff between the two factors must be balanced based on the overall manufacturing cost and productivity in order to devise an optimal set of gas flow rates.

As these analyses attest, significant gains for environmentally-conscious manufacturing can be expected from process optimization through dynamic simulation. While the physical basis of the simulator and its experimental validation suggest reasonable quantitative accuracy, the results identify clearly where substantial advantage can be expected and can thereby expedite an experimental program to realize such gains. Thus, as shown through the case study of this paper, we will demonstrate that physically-based dynamic simulation is a versatile and powerful tool for process design and optimization for environmentally-conscious manufacturing.

2. Dynamic Simulator Description

2.1. Simulator Structure

The structure of the dynamic simulator used in this paper has been described elsewhere [2] in greater detail. Briefly, the simulator represents the time-dependent behavior of a RTCVD module where our experimental data were collected. The RTCVD module, as schematically shown in Figure 1, consists of a gas handling system, the RTCVD reactor and its pumping system, and a two-stage differentially pumped quadrupole mass spectrometry (QMS) sampling system [3].

The simulator (for the equipment), as illustrated in Figure 2, is constructed using a Windows-based simulation program, VisSim™ (Visual Solutions, Inc.). This allows the user to wire a block-diagram that connects mathematical functionalities to represent a physical model without having to write computer program codes. Each block in such a diagram can represent a constant, a variable, or a mathematical function (such as a summing junction, an integral, or a derivative). An implicit solver can also be used to solve for an unknown parameter, so that tedious analytical solution can be avoided. For better organization, the various computational functions are grouped in compound blocks according to the layout of the physical equipment, with each compound block calculating a specific system parameter such as partial pressure, wafer temperature, surface reaction rate, and film thickness, etc. Hierarchical structure is achieved through multi-level compound block structures, as shown in Figure 2, so that one can immediately identify the role of each group of calculations. In the polysilicon RTCVD simulator used here, there are 8 levels of compound structure and nearly 1200 functional blocks.

2.2. Equipment and Process Models

As shown in Figure 3, the RTCVD simulator synthesizes individual simulator elements to represent **process recipe** (e.g., timing of events, valve status vs. time, lamp power vs. time, overall process timing and conditions), **equipment** (e.g., reactor chamber, pumps, mass flow controller, differential pumping mass spec chambers), **materials process** (e.g., gas flow, partial pressures, heat transfer, surface chemical reaction, film growth), **sensor** (e.g., temperature, total and partial pressures), and **control system** (pressure ramp, temperature ramp, throttle valve position). Physically-based models are used wherever possible so that application of the simulator can be extended to as broad a process parameter as possible. Since the assessment of manufacturing and environmental metrics requires a fairly complete system-level description, reduced-order and empirical/statistical models are used where physics and chemistry either involve high complexity or are poorly known.

For instance, the model for deposition kinetics is based on the current understanding of the physics and chemistry for Si chemical vapor deposition from SiH_4 [4, 5]. The model includes boundary layer transport of SiH_4 molecules to the surface, surface chemisorption of SiH_4, surface decomposition of SiH_x species, thermal desorption of H_2, and the resulting Si deposition. The rate for each of the above processes are calculated in the simulator. The overall deposition kinetics can be transport-limited or surface reaction-limited depending on the process temperature and process pressure [5].

A good example of reduced-order model in our simulator is the wafer absorptivity and emissivity calculation. The modeling and measurement of wafer temperature have been the focus of most theoretical studies of rapid thermal processes. The calculation of wafer absorptivity and emissivity is a key element in wafer temperature modeling. The wafer absorptivity is dependent on the heating lamp spectral distribution, the wafer temperature, and the surface layer structure (or film thickness during deposition). The wafer emissivity is dependent on the wafer temperature and the film thickness. Due to the complexity of calculations, a reduced-order model was used in our simulation. We first used a model developed by F.Y. Sorrell et. al [6] to establish a database for the wafer absorptivity and emissivity. Model reduction was then performed by curve-fitting the database against three variables, lamp temperature, wafer temperature, and film thickness. The mathematical expression from the above model reduction process is then incorporated into our simulator to calculate the wafer absorptivity and emissivity as a function of lamp temperature, wafer temperature, and film thickness. During the RTCVD process, these three parameters vary continuously, and the wafer absorptivity, emissivity, and temperature are then calculated at every iteration step of the simulation. Other system properties such as across-wafer uniformity and gas flow dynamics are also very complex, and reduced-order models are being developed.

2.3. Dynamic Simulation of Polysilicon RTCVD

System-level simulation of a deposition process is achieved by integration of individual simulator elements through control implementation as defined by the process recipe. In Figure 3, the three plots on the right hand side for film thickness (top panel), for QMS partial pressure signals of Ar, SiH_4, and H_2 (middle panel), and for wafer temperature and growth rate (bottom panel) illustrate the time-evolution of each parameter during the implementation of a process recipe for polysilicon RTCVD at 5.0 Torr (10% SiH_4/Ar), 650 °C for 35 sec. using 300 sccm flow rate. The simulator first started gas flow and establishes process pressure. This was shown as a partial pressure rise for Ar (top line) and SiH_4 (middle line) in the QMS partial pressure plot. The H_2 partial pressure was 0 since surface reaction was not yet initiated. During this period, the heating lamp was off, the wafer remained at room-temperature (25 °C), the growth rate was 0 (bottom panel), and the film thickness was also 0 (top panel). At ~ 30 sec., the process pressure was reached (both Ar and SiH_4 partial pressures begin to level off). The heating lamp was then turned on. The wafer temperature started to increase as shown in the bottom panel (top line) and the growth rate also rose rapidly (bottom line). The slight temperature overshoot at ~ 38 sec. and the corresponding growth rate oscillation were also clearly observed in simulation. PID (proportional, integral, and derivative) control loops were implemented to regulate the throttle valve position (to keep pressure constant) and the lamp heating power (to keep wafer temperature constant). At this point, the deposition was initiated, H_2 was produced as indicated by the QMS H_2 partial pressure rise (bottom line in middle panel), and film thickness increased over time (top panel). At the end of the 35 sec. deposition process, both gas flow and wafer heating were terminated, and the throttle valve was fully opened to pump down the reactor. This sequence of actions caused the subsequent decreases in wafer temperature, growth rate, and partial pressures for Ar, SiH_4, and H_2. The film thickness also stayed constant thereafter.

Time-dependent behavior of the equipment and process are direct outputs of a simulation. As a consequence, time- and history-dependent manufacturing and environmental figures of merit can be immediately calculated during the simulation. Such metrics of significance include film thickness, quality, process cycle time, materials utilization, power consumption, gas emission, etc..

3. Experimental Validation of Simulator

Validation of the polysilicon RTCVD simulator has been accomplished from three approaches which will be described in detail elsewhere [2]. In brief, the three aspects include the deposition chemical kinetics, the equipment dynamics, and the overall process dynamics.

(1) As discussed in section 2.2, a model describing the chemical kinetics of polysilicon RTCVD was constructed from knowledge and data in the literature [4, 5] and incorporated into the simulator. Subsequently, the temperature-dependence of the deposition rates in various pressure regimes was compared to experimental data [5]. Consistency in both the kinetics-limited and transport-limited regimes suggests that the kinetics model correctly describes the deposition chemistry.

(2) The partial pressures of reactant SiH_4, carrier gas Ar, and product H_2 in the reactor and in the mass spectrometer chambers were simulated as a function of time through the process cycle, and the results were compared to our experimentally measured mass spectrometer sensor signals [3]. Figure 4 shows the comparison of simulated (solid line) and experimental (data points) QMS signals of H_2 during a deposition process using a process recipe of 750 ^{o}C, 5 Torr (10% SiH_4/Ar), for 40 sec.. An increase in flow rate from 200, to 500, and to 1000 sccm caused the H_2 signal measured by QMS to decrease significantly. The simulation was able to quantitatively capture this change in measured H_2 partial pressure, which arises from the competition between H_2 product generation rate and reactor residence time. For each flow rate, the lineshape of the simulated H_2 signal as a function of time was also in excellent agreement with that from the experimental measurement. The small deviation of experimental data from simulation for the 1000 sccm process was due to a malfunction in the

temperature control system during that particular experimental run. The above results suggest that the physical models in our simulator correctly describe the equipment behavior.

(3) The overall process dynamics and system-level description can be reflected in the total film thickness from a deposition process through the implementation of a process recipe and is directly relevant to the issues which will be addressed in this paper. A correlation plot of film thickness from simulation and from experiment is presented in Figure 5 for 27 process recipes. The experimental thickness are Nanometric measurements for polysilicon deposition using 27 different combinations of process time and process temperatures (between 600 and 850 °C). If the simulation results are identical to that from the experiment, all data points should fall on the diagonal line. The data distribution indicates that overall agreement are reasonably good. The simulator tends to slightly overestimate the deposition thickness in the low temperature regime, and it underestimates the thickness in the higher temperature regime. This suggests that the simulator captures the physics and chemistry of the system well to first order over a broad dynamic range, but that some systematic subtleties are not yet represented. The process optimization exercises presented in the next section are limited to film thicknesses under 2000 Å where excellent agreement between simulation and experiment have been established.

4. Process Optimization for Process Cycle Time and for Materials Utilization

Manufacturing is a complex process requiring a large number of variables both for defining the procedure and for evaluating the final outcome. Experimental optimization of equipment and process parameters is extremely costly and time-consuming, and requires a coherent analysis of multiple manufacturing and environmental figures of merit from a large number of combinations of parameters, each defining a single manufacturing process. An experimentally validated dynamic simulator is a powerful tool to facilitate optimization of individual and multiple manufacturing metrics for complex time-dependent behavior. In this section, we will use the above described simulator to investigate the effect of process parameters (temperature, flow, and process timing) on the overall process cycle time and the materials utilization efficiency, which are two important metrics for manufacturing and for the environment.

4.1. Description of Process Cycle

The virtual experiment is designed to grow 2000 Å of polysilicon using a 5 Torr process gas which contains 10% SiH_4 in an Ar carrier. The conventional process sequence includes the establishment of process pressure (5.0 Torr) with a constant gas flow rate (e.g., 300 sccm), followed by a heating ramp to the process temperature. The wafer temperature is kept constant at the process temperature (650 - 750 °C) until 2000 Å of polysilicon is deposited on the surface. Gas flow and lamp heating are terminated at the end of the deposition. Figure 6 illustrates the time sequence of the pressure and temperature ramps. In the following discussions, process cycle time is defined as the total time it takes from the initial gas flow until the deposition is finished. Shorter process cycle times are preferred for increased manufacturing throughput (and therefore, productivity). The SiH_4 utilization efficiency (or process conversion yield) is defined as the percentage of SiH_4 molecules that are converted to polysilicon film with respect to the total number of SiH_4 molecules input to the RTCVD reactor over the entire process cycle. A higher conversion yield is preferred to reduce both consumables cost and waste of reactant.

4.2. Process Timing and Process Temperature

If the wafer heating is initiated at an earlier time as illustrated in Figure 6 (such as when the pressure reaches 3.0 Torr instead of after the 5.0 Torr process pressure is established), both the overall SiH_4 utilization efficiency and process cycle time are changed. In Figure 7, the top and bottom panels show the SiH_4 utilization and the process cycle time, respectively, for three process temperatures as a function of the reactor pressure at which the heating is initiated. A pressure of 5.0 Torr at which the heating begins means that the heating lamp is turned on after the 5.0 Torr process pressure is established. A lower pressure means that the heating begins at an earlier time. A pressure of 0 Torr means that the heating is initiated the same time as the gas flow.

As shown in Figure 7 for the 650 °C process, the process cycle time is reduced from 95 sec. to 71 sec. if the heating is started at 0 Torr as compared to at 5 Torr, while the materials utilization efficiency is increased from 14.2% to 18.8%. As the process temperature is increased, the effect of process timing becomes more important. For the 750 °C process, both the process cycle time and the materials utilization efficiency are improved by over 50% for a similar process timing change. The temperature increase itself has an even greater effect, shortening the cycle time by 2x and enhancing the utilization efficiency by 2x as the temperature is increased from 650 °C to 750 °C. A combination of both process timing and temperature changes gives up to 3x improvement on each of the two manufacturing and environmental metrics. In this case, the significant gains in process cycle time and in materials utilization can be achieved simultaneously with a change in process timing or temperature.

In the above process optimization exercise, the issue of materials quality has not been explicitly considered, although the parameters are varied only within the pressure and temperature range where good quality films can be produced. For real manufacturing optimization, the materials quality factors should be included especially if optimizations are performed outside those parameter windows. A simple approach is to put a limit on the allowable input values for temperature and pressure where good quality materials are known to be produced; optimization exercises outside the limit are not allowed, so that a valid set of optimal process parameters can be obtained.

4.3. Process Timing and Gas Flow Rate

Similar virtual experiments are designed as in the above section for growing 2000 Å polysilicon except that here the process temperature is kept constant at 650 °C and the flow rate is varied from 100 to 1000 sccm. In Figure 8, the materials utilization efficiency (top panel) and the process cycle time (bottom panel) at 650 °C are presented as a function of process timing for various mass flow rates. For 100 sccm flow rate, early heating improves the SiH_4 utilization efficiency by as much as 1.7x, and the process cycle time is 1.6x shorter. For higher flow rate, gains in the two metrics are not as significant with earlier wafer heating, but are still as much as 1.13x at 1000 sccm. Therefore, early heating benefits both SiH_4 utilization and process cycle time at all gas flow rates.

For the same heating schedule, changes in the flow rate have a quite different effect on the cycle time compared to the utilization efficiency. For initiating wafer heating after process pressure is established (5 Torr on X-axis), decreasing the flow rate from 1000 sccm to 100 sccm causes 4x higher SiH_4 utilization efficiency, while the process cycle time becomes nearly 2.7x longer. For initiating wafer heating and gas flow at the same time, SiH_4 utilization efficiency is increased from 6.3% to ~ 42%, a gain of nearly 7x. The process cycle time, on the other hand, is again changed from 64 sec. to 96 sec., corresponding to a 50% increase. Because an improvement on the materials utilization is accompanied by a loss in the process throughput upon changing the flow rate, tradeoffs must be made in order to devise the optimal process parameters.

4.4. Simulator Strengths and Limitations

Given the complexity of the process cycle in time, the dynamic simulation offers substantial advantage in enabling the computation of process behavior and manufacturing metrics through rapidly changing and sensitive process parameters. We have demonstrated that a validated dynamic simulator can serve as a design vehicle for identifying, assessing, and understanding possible improvements in manufacturing and environmental figures of merit. Complex system behavior can be described and predicted with reasonable accuracy over a broad dynamic range for various process parameters.

In the two cases described above, process optimization has been limited to the parameter range where the process is known to produce good quality products. For example, 650 - 750 ^{o}C is the most common temperature window for device quality polysilicon deposition, and optimization is performed only within this temperature range. The materials quality must be taken into account if design of an optimal process is needed beyond this temperature regime. At this stage, the simulator does not include a materials quality factor, and further development along this direction is underway. In addition, the simulator does not yet include a methodology to combine individual figures of merit for identifying the optimal point when tradeoffs are needed. Efforts are also being devoted to further improve some of the models in the simulator in order to better describe the experimentally determined equipment and process behavior.

5. Discussion

Environmentally-conscious manufacturing addresses the environmental impact of the interrelated decisions that are made at various stage of product life, from conception to design, raw materials consumption, synthesis, processing, use, recycling, and/or disposal. The ESH section of the National Technology Roadmap For Semiconductors underscores the need for assessment and model development for materials mass balance and energy balance, both on the tool level and for the whole factory. This will allow for identification of risks and improvement in process, tool, and factory design. Optimal equipment and process design includes high product quality and reliability, high materials utilization efficiency, low consumables cost, low cost of ownership, short process cycle time, high throughput, and minimum environmental impact.

Process design optimization is a complex challenge – for manufacturing efficiency and/or for environmental sensitivity – requiring new tools for meaningful analysis. We have demonstrated that dynamic simulation can be a versatile and powerful tool for such process optimization. The consequence of variations in process parameters such as temperature, flow rate, and process timing have been evaluated against two key manufacturing and environmental metrics, namely, process cycle time and materials utilization efficiency. The dynamic simulator allows us to identify where significant improvement is possible and how much can be expected for each manufacturing figure of merit. In addition, the simulation provides quantitative estimates for changes in conflicting manufacturing and environmental metrics, essential for assessing manufacturing tradeoffs.

Simulation exercises as illustrated here will define a range for various process and equipment parameters within which further optimizations can be performed experimentally. In this way, simulation minimizes the number of experiments needed, significantly reducing the cost, time, and resources required to identify and qualify the optimal point for process and equipment design.

Semiconductor manufacturing is a complex process with multiple input parameters and multiple output manufacturing metrics. We have addressed two such manufacturing issues: process cycle time and materials utilization efficiency. Other metrics of significance include product quality, product reliability, equipment cost and flexibility, environmental safety, etc. All these metrics are strongly influenced by equipment and process parameters such as reactor geometry, gas flow, pressure, temperature, ramp rates, process timing, control parameters, and of course by the time-dependent process recipe employed. Identifying the cross correlation between the input parameters and output manufacturing figures of merit is a major task, but is necessary for process optimization. Dynamic simulation, as shown in this paper, provides a new tool and aids significantly for performing this task. In our simulator, the equipment, process, and control system are modeled based on their underlying physics and chemistry, so the effect of equipment design, process parameters, and control implementation can be investigated with respect to the various manufacturing and environmental issues. Issues such as per wafer cost including consumption of materials, energy, and ultra-pure water can be addressed if the models are further extended to the factory level.

In this paper, we discussed the process optimization for polysilicon RTCVD. Other semiconductor manufacturing processes can be investigated in a similar fashion if a working simulator is available. We are currently developing models and integrated simulation modules for other deposition and etch processes. Additional systems of interest include wafer cleaning, lithography, resist formation and removal, metallization, chemical vapor deposition of oxide, nitride, and metal (e.g., tungsten), and chamber cleaning. Some of these systems involves very complex physics and chemistry, so reduced-order model may have to be used in the simulation. A large number of these systems have been extensively investigated experimentally and quite complete databases are available for establishing reduced-order or empirical models. The dynamic simulation approach, as demonstrated in this paper, will be a powerful tool for process and equipment optimization for these systems, and can have a significant impact on the technology development for environmentally-conscious manufacturing.

6. Conclusions

We have investigated the process parameter optimization for rapid thermal chemical vapor deposition (RTCVD) of polysilicon from SiH_4 using dynamic simulation. We have demonstrated that our physically-based dynamic simulator captures essential time-dependent behaviors of gas flow, heat transfer, reaction chemistry, and sensor and control systems. Significant improvements in SiH_4 utilization (up to 7x) and process cycle time (up to 3x) are achieved by optimizing process timing, temperature, and flow rates. Shorter process cycle time increases process throughput and higher gas utilization efficiency reduce consumbles cost and waste emissions, providing benefits for both environmental considerations and manufacturing productivity (throughput). Dynamic simulation provides a powerful and versatile vehicle for optimization of equipment design and process parameters and recipes for manufacturing and environmental metrics.

7. Acknowledgment

We acknowledge with thanks the funding of this research project by the Semiconductor Research Corporation (SRC contract #94-MP-132 and #94-MJ-563) and the National Science Foundation (Grant CDR 8721505). We thank Visual Solutions, Inc. for consultation on VisSim™, and Dr. Laura L. Tedder for fruitful discussions.

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Figure Captions

Figure 1. Schematic representation of RTCVD module including gas handling, RTCVD reactor and pumping, and two-stage differentially pumped mass spectrometer system.

Figure 2. Structure of Windows-based simulator for polySi RTCVD. The top panel is the VisSim™–Window of the RTCVD equipment simulator. In the middle panel is a compound block for calculatiing SiH_4 partial pressure within the RTCVD reactor. The bottom panel illustrates a second level compound block for calculating the SiH_4 partial pressure change induced by surface reactions. The complete RTCVD simulator consists of 8 levels of compound structure and 1200 functional blocks.

Figure 3. VisSim™–Window of the RTCVD simulator. From top to bottom on the left-hand side of the window are the equipment simulator, the process recipe and control simulator, the deposition kinetics simulator, and a display panel for overall process status. The three plots on the right-hand side are simulation outputs for film thickness (top), QMS partial pressure signals (middle), and wafer temperature and growth rate (bottom).

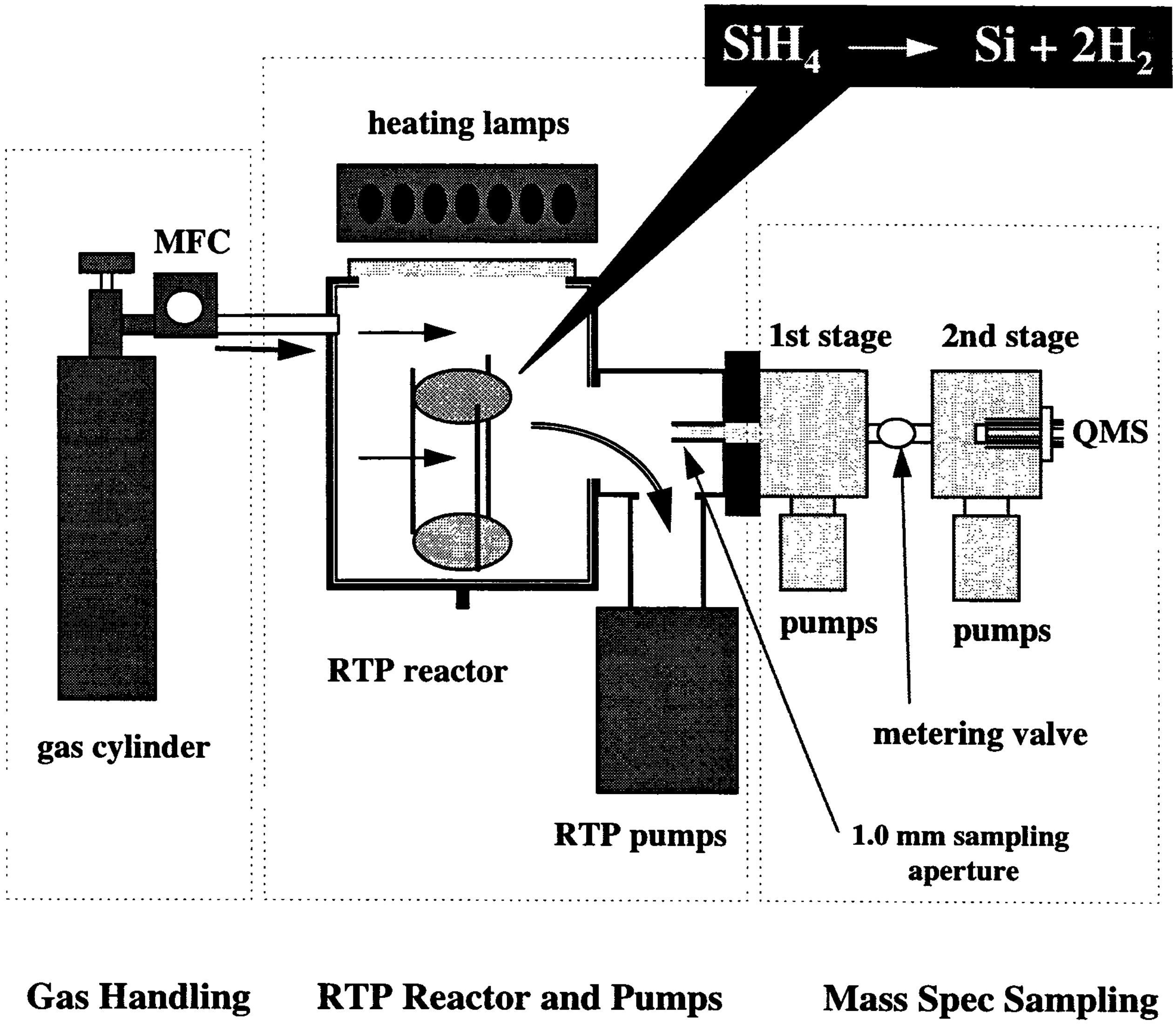
Figure 4. Comparison of H_2 QMS signal during a deposition process for 3 different gas flow rates (200 sccm, 500 sccm, and 1000 sccm). The solid lines are from simulation and the data points are experimental measurements.

Figure 5. Correlation plot of simulated and experimental film thickness for 27 deposition processes of polySi from SiH_4.

Figure 6. Virtual experiment design for process optimization. The time-sequence of pressure (P) and temperature (T) ramps is schematically represented for a conventional process. Early heating is illustrated as advancing the heating initiation to positions indicated by the dotted line.

Figure 7. Effect of process timing and process temperature on materials utilization efficiency (top panel) and process cycle time (bottom panel).

Figure 8. Effect of process timing and gas flow rate on materials utilization efficiency (top panel) and process cycle time (bottom panel).



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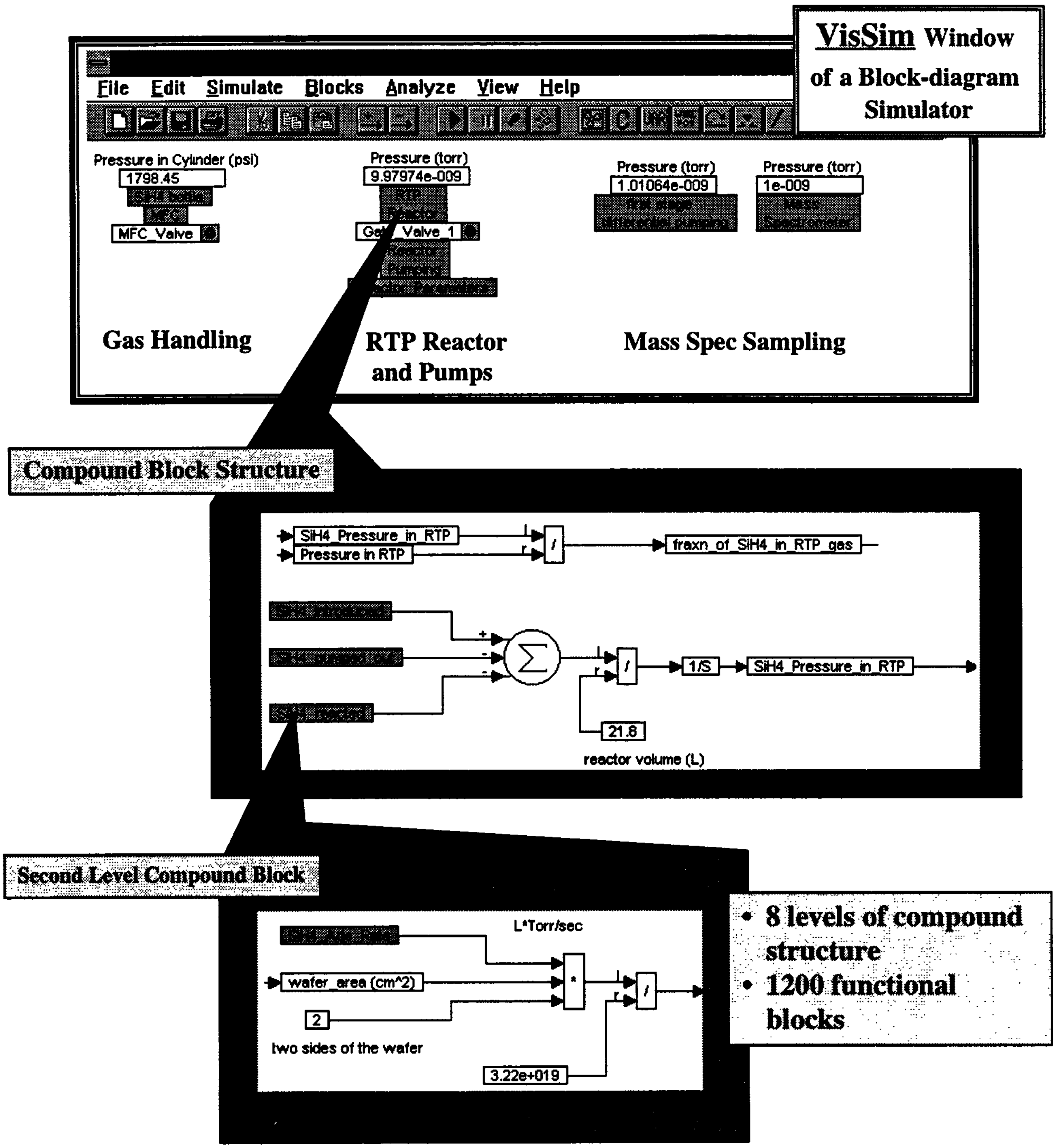

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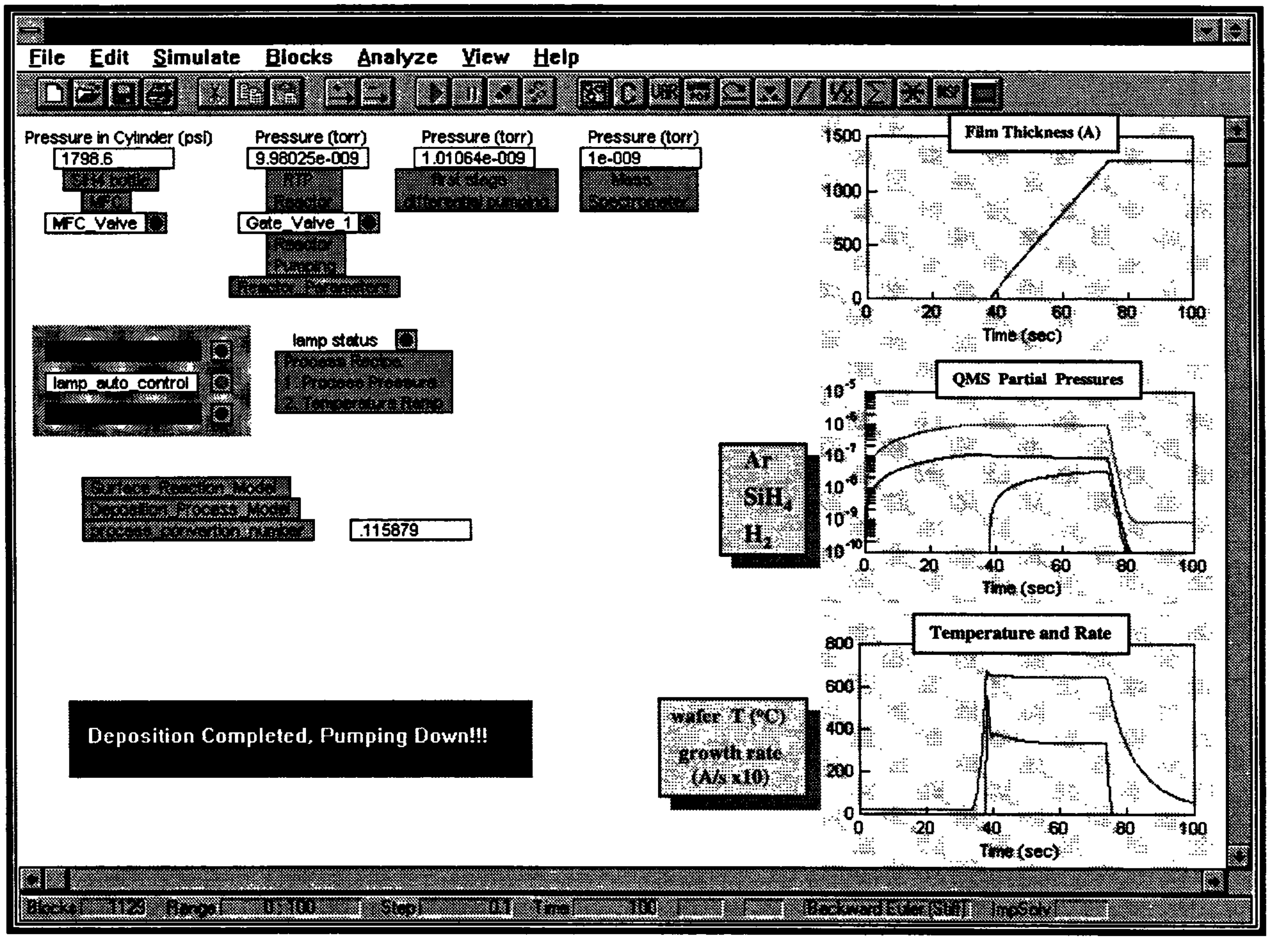

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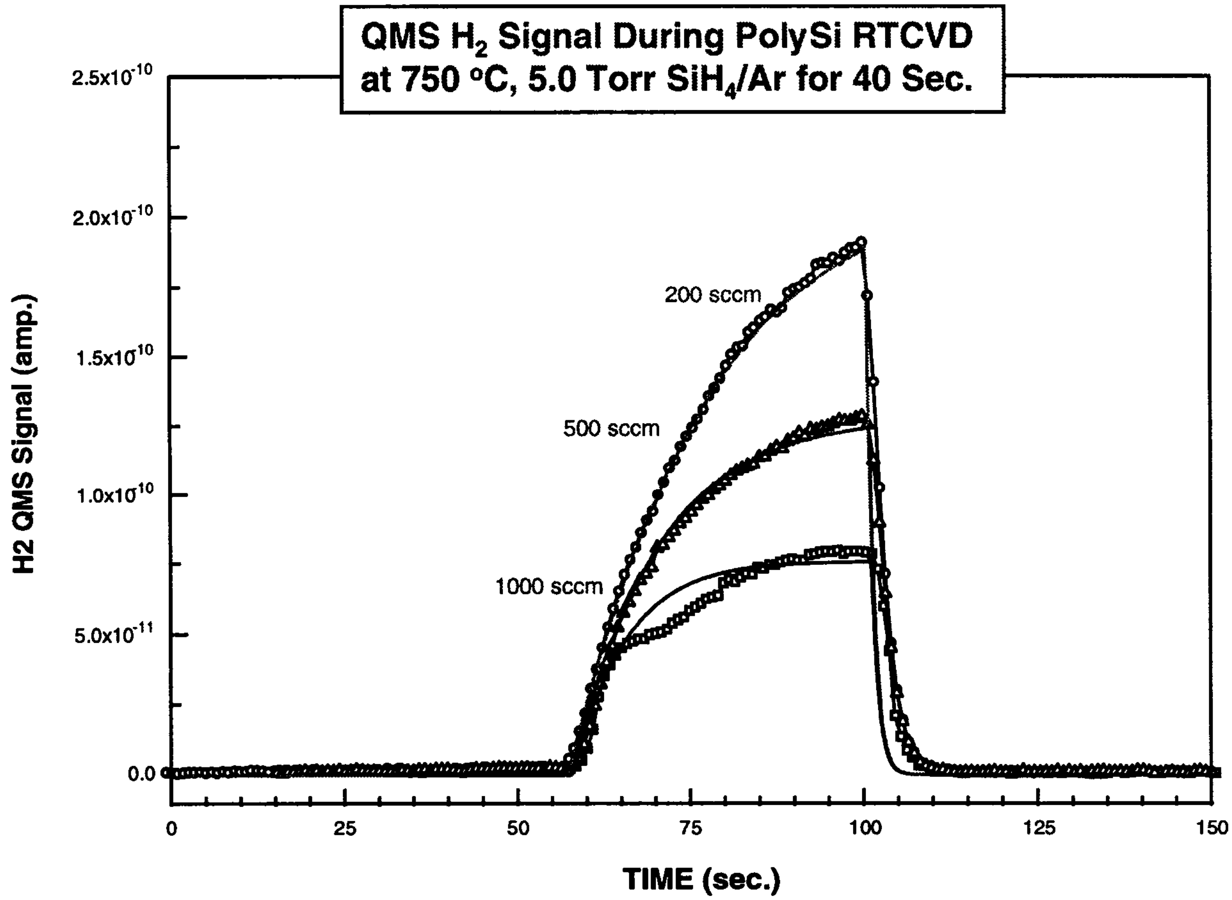

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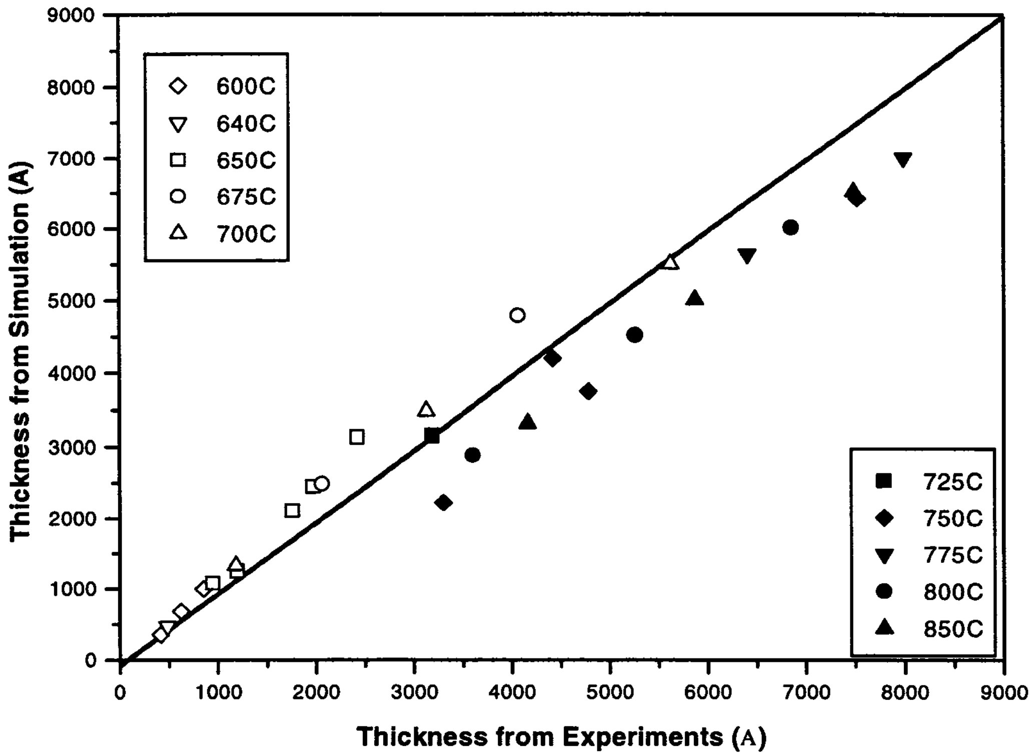

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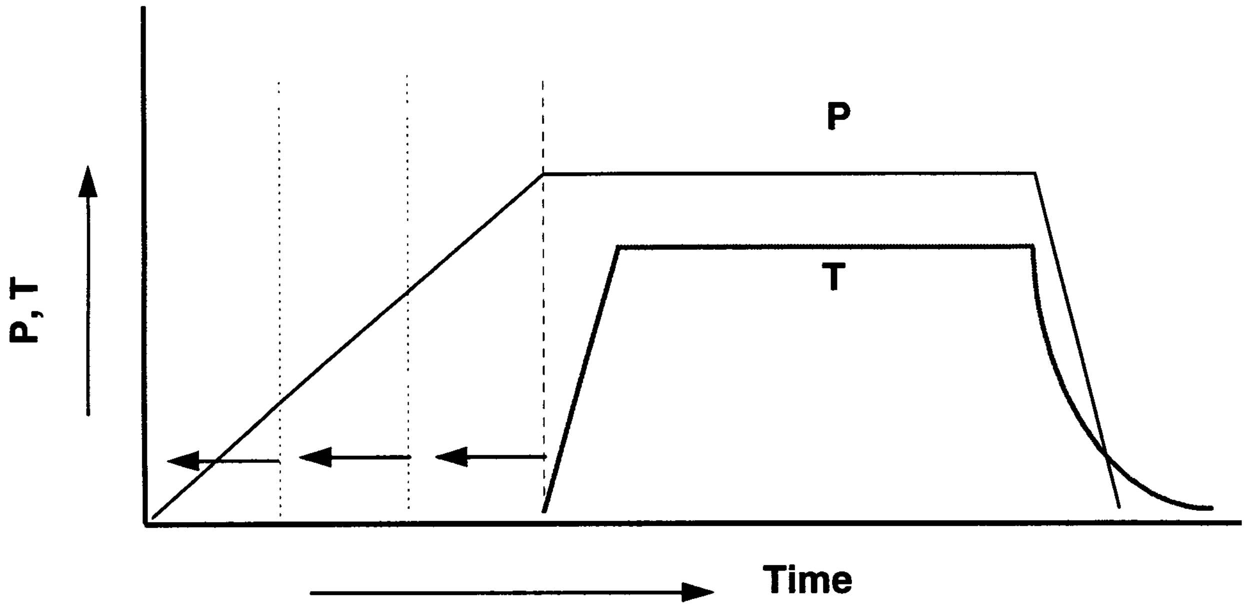

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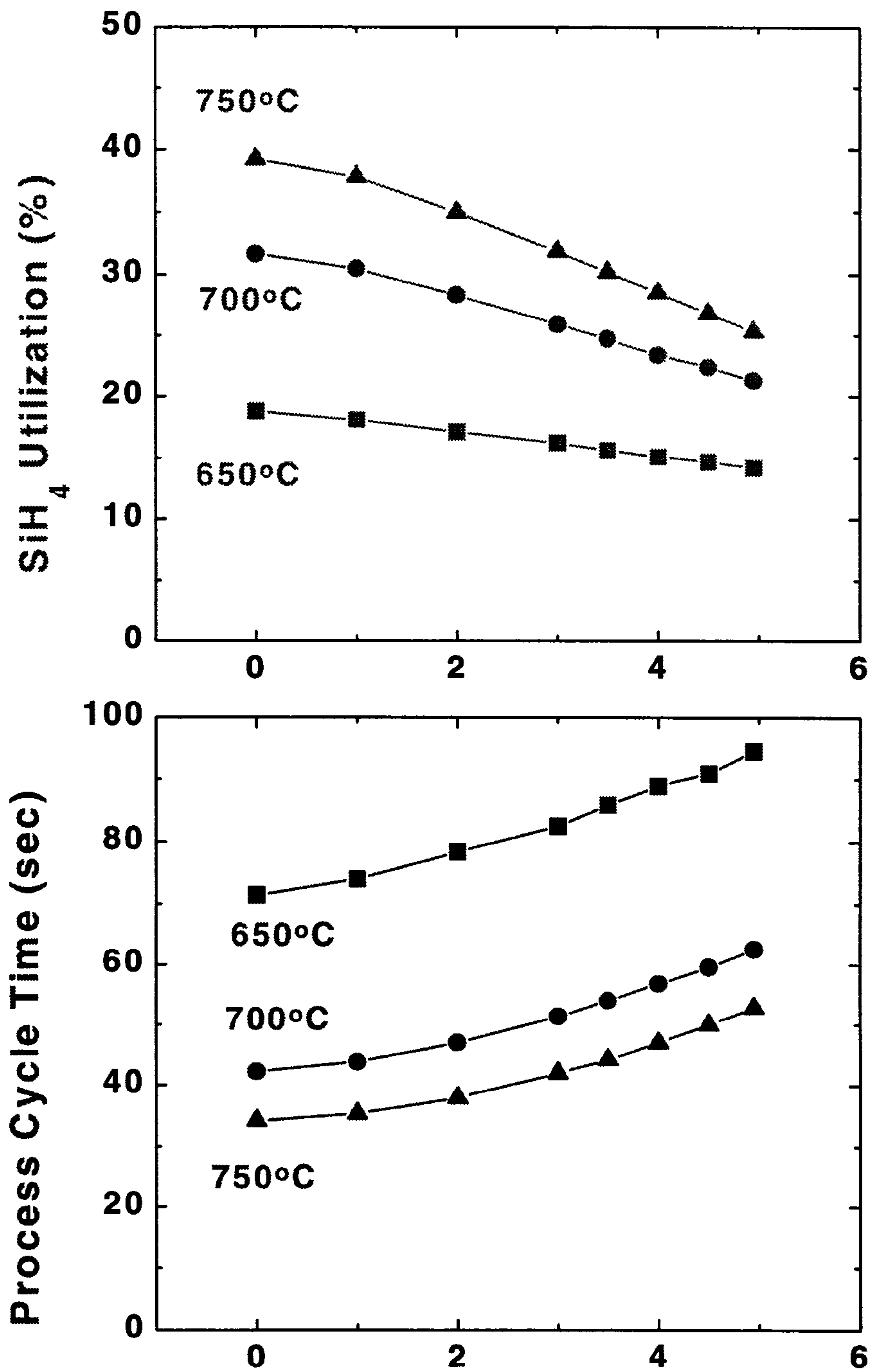

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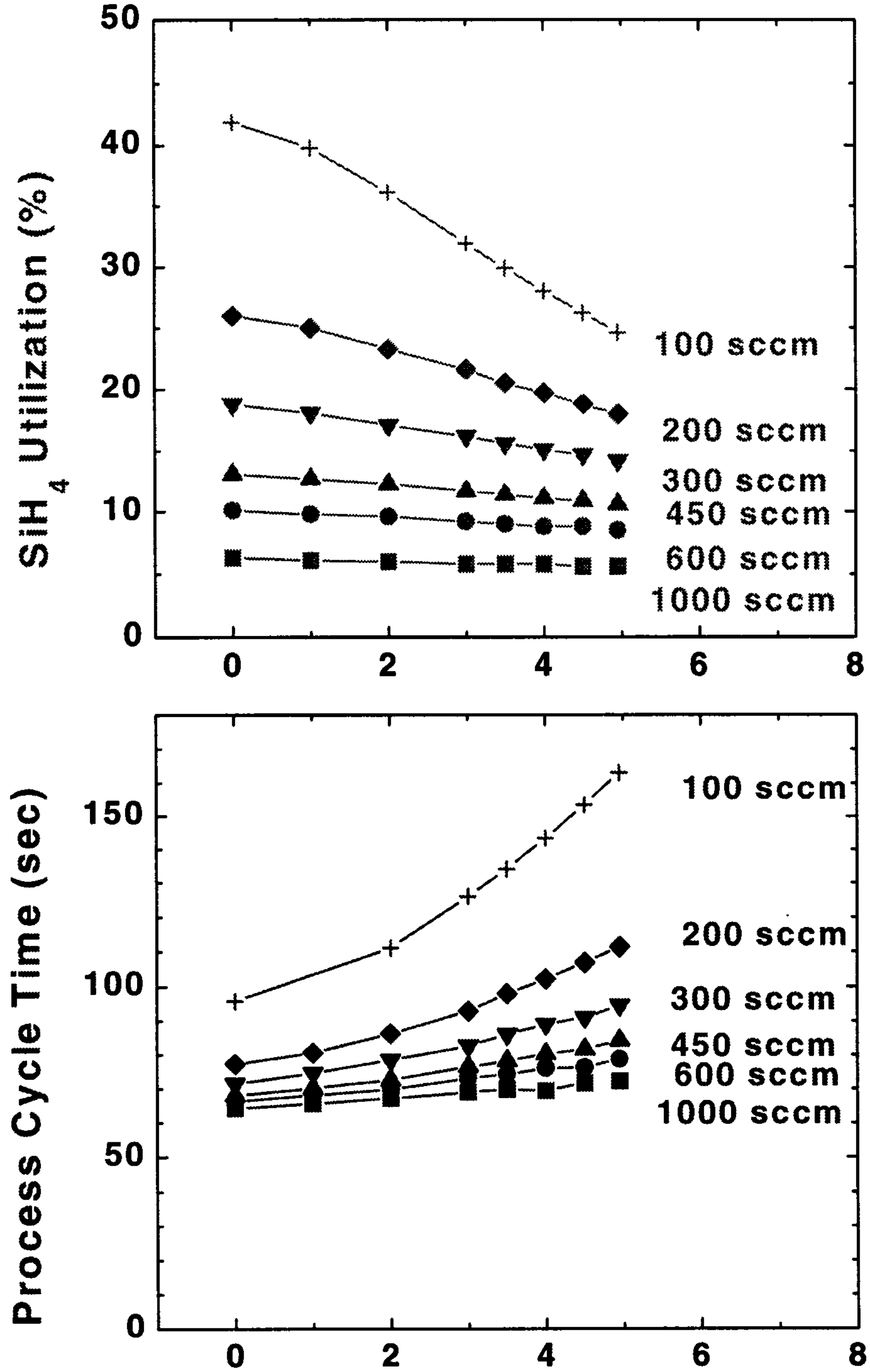

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