Dynamic Simulation and Optimization of Cu CVD Unit Process for Environmentally Benign Manufacturing

Soon Cho, Wei Lei, Adam Melvin, and Gary W. Rubloff

***Abstract*—Environmentally benign semiconductor manufacturing requires methodologies which enable cooptimization of multiple objectives, namely environmental metrics (e.g., precursor utilization efficiency, energy consumption) simultaneously with metrics for manufacturing productivity (e.g., process cycle time) and technology performance (e.g., material or product quality). We used dynamic simulation to investigate this challenge at the unit process level, incorporating essential characteristics of physical and chemical behavior of the equipment, the process, and their dynamics for a prototype system. This enabled the evaluation of multiple metrics as a function of process recipe specifications and equipment design parameters, namely the extraction of process cycle time, reactant utilization, and energy consumption as metrics for a Cu chemical vapor deposition (CVD) unit process as the prototype. Higher temperature and pressure resulted in reduced process cycle time and increased precursor utilization efficiency, producing a "win-win" situation for the manufacturing and environmental metrics. In contrast, variation in precursor flow rate produced a tradeoff situation between these metrics, which could be quantified in different process parameter regimes by the simulation. Energy consumption is dominated by vacuum pump operation, placing a premium on short cycle times. In addition, energy requirements for wafer heating are reduced at higher wafer temperature because the deposition rate of the thermally activated CVD process increases rapidly with temperature, reducing the cycle time and, therefore, the energy used. These results illustrate that dynamic simulation provides a valuable guide in design-for-environment efforts which seek cooptimization of multiple metrics, win-win situations, and quantification of tradeoffs between metrics.**

***Index Terms*—Cu chemical vapor deposition (CVD), design for environment, dynamic simulation, environment safety health.**

I. Introduction

DESIGN FOR environment (DFE) is becoming a key component in the semiconductor industry in efforts to integrate and proliferate environment, safety, and health (ESH) improvements in semiconductor technology and manufacturing. DFE plays a special role in the ESH section of the International Technology Roadmap for Semiconductors (ITRS) [1], as it provides the conceptual, design, and analytical framework which can best enable specific advances in ESH areas such as chemical, materials and equipment management, resource conservation, workplace protection, and climate change mitigation. The challenge is to build ESH improvements into the way products are manufactured, while still maintaining desirable product characteristics such as competitive price, performance, and quality [1]–[4].

However, successful integration of ESH technologies and manufacturing largely remains a major challenge: While the goals and conceptual framework for DFE are rather well defined, tools and methodologies for implementing DFE in both design and analysis are distinctly limited. Such methodologies must enable not only the identification and assessment of ESH impacts at an early stage of technology development, but also the simultaneous evaluation of metrics for manufacturing productivity (e.g., process cycle time) and technology performance (e.g., material or product quality) to achieve cooptimized designs which respect the realities of a highly competitive industry. On the other hand, suitable DFE approaches of this type promise to stimulate innovation through cooptimization of those "hard constraints" together with various ESH goals [1], [5], [6].

As part of the NSF/SRC Engineering Research Center for Environmentally Benign Semiconductor Manufacturing at the University of Arizona, we have been developing modeling and simulation approaches to enable such evaluation and cooptimization techniques. Interconnect technology poses major ESH challenges because numerous new chemicals, materials, and processes are being introduced along with the industry's evolution to 300-mm manufacturing. Integrated assessment of ESH impacts of those new chemicals, materials, processes, and subsequent byproducts is a critical task at hand, and the ITRS calls for development of a common methodology to determine the lowest ESH impact of those materials and processes as early as possible [1], [6]–[10].

Assessment and integration of multiple ESH impact metrics can be done at several levels of the manufacturing hierarchy (e.g., unit process, infrastructure, subfactory, factory, and global levels). Here we concentrate on developing such methodology for the unit process level. Even at this level, manufacturing is a complex process requiring a large number of variables, both for defining the procedure (process recipe) and for evaluating metrics associated with the outcome. Optimizing such a manufacturing process requires a coherent analysis of multiple

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technology, manufacturing, and ESH figures of merit from numerous combinations of parameters, and clearly, optimization through experimentation becomes a costly and time-consuming venue. In our past and present research, we have demonstrated that a dynamic simulator based on understanding of equipment physics and reaction chemistry can represent complex systems behavior with reasonable accuracy. Once such a simulator is constructed, it can be readily exploited to investigate and compare results from numerous combinations of multiple system design and/or process recipe parameters. Hence, our goal has been to utilize dynamic simulation as a tool to identify areas of opportunities for optimizing multiple technology, manufacturing, and ESH impact metrics with complex time-dependent behaviors [11]–[13].

In this article, we applied our dynamic simulation approach to investigate a prototypical copper chemical vapor deposition (Cu CVD) unit process, which is representative of the new materials and processes being introduced in advanced interconnect technology, along with the 300-mm equipment generation [1], [14], [15]. We have built physically based models for the process and equipment incorporating the essential dynamics occurring through the process cycle. Virtual experiments were carried out on the simulator to generate time-integrated metrics for manufacturing and ESH, in particular reactant (precursor) utilization, process cycle time, and energy consumption. Integrated assessment of the metrics as a function of various key process parameters reveals opportunities for cooptimization. These studies also show tradeoff situations where benefit to one metric is accompanied by degradation of another metric (e.g., process cycle time versus reactant utilization), from which cost–benefit analysis can be made. These relatively simple examples demonstrate the key role of simulation in exploring integrated ESH metrics and the reality that such approaches provide benefit not only to ESH goals, but to optimization of manufacturing productivity and technology performance as well.

II. Modeling and Simulation

A. Overall Simulator Structure

The overall structure of the Cu CVD simulator combines various individual simulator elements to represent the overall system-level behavior of the process and equipment, as illustrated in Fig. 1. For instance, the process recipe determines the sequence of actions initiated in the equipment simulator as a function of time. In turn, the equipment simulator sets up the conditions by which the process physics and chemistry occur on the wafer, as reflected by the process simulator. Some of the process information is used to drive the equipment control system on the one hand, and on the other, various manufacturing and ESH metrics are extracted from evaluation of the process simulator results as a function of time. In particular, the process simulator is also used to extract metrics of interest for integrated assessment of manufacturing and ESH impact of the process, particularly with regard to metrics which are integrated over time through the process cycle, as discussed further in Section III. The integrated simulator includes five specific components as depicted in Fig. 1.

1) The **process recipe** component dictates the various sequencing of events, such as valve status, gas flow conditions, reactor pressure set points, and substrate heater power, all as a function of time or conditional relations through the process cycle.

2) The **equipment simulator** component computes the time-dependent behavior of the physical equipment in response to state changes imposed by the process recipe component. This component, thus, determines pressure, temperature, and flow rate conditions as a function of system design parameters (e.g., chamber volume, heat transfer systems, vacuum, and gas flow characteristics) and the time-dependence executed by the process recipe.

3) The **process simulator** component contains a chemistry model which prescribes the reaction rate at any point in time through the process cycle as a function of current values of process conditions, including wafer temperature, partial pressures of reactants, and products, etc. These reaction rates in turn determine the instantaneous rates for deposition on the wafer, generation of reaction products, and consumption of reactants through the process cycle.

4) The **control system** component modifies input parameters (e.g., throttle valve setting, heater power) to maintain constant process conditions during portions of the process cycle where regulatory controllers assume this function in real systems. In the virtual tool, this can also execute real-time end point control (whether or not such is available in actual equipment), facilitating the determination of metrics such as precursor consumption as a function of design parameters for the same thickness of material deposited on the wafer.

5) The **manufacturing and ESH simulator** carries out calculations of key metrics, typically integrated through the entire process cycle. Metrics such as process cycle time and reactant consumption clearly depend not only on nominal process parameters and time, but also on the details of ramp-up and ramp-down sequences to establish and recover from the nominal process state, during which conditions change dynamically.

The integrated dynamic simulator is constructed using a Windows-based simulation engine, VisSim from Visual Solutions, Inc. This software allows users to wire a block-diagram that connects mathematical functionalities to represent a physical model without having to write complicated computer codes. An example of the user interface is shown in Fig. 2, along with annotations describing some of the features. 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). Dynamic updating of system parameters is achieved through the built-in iterative computation carried out by the VisSim engine, so that time evolution of the system can be seen in real time or in graphical form. An implicit solver can also be used to solve for an unknown parameter, along with numerous other features. 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 specific subsystem parameters such as partial pressure, wafer temperature, surface reaction rate, film thickness, etc. In this way, a hierarchical structure is

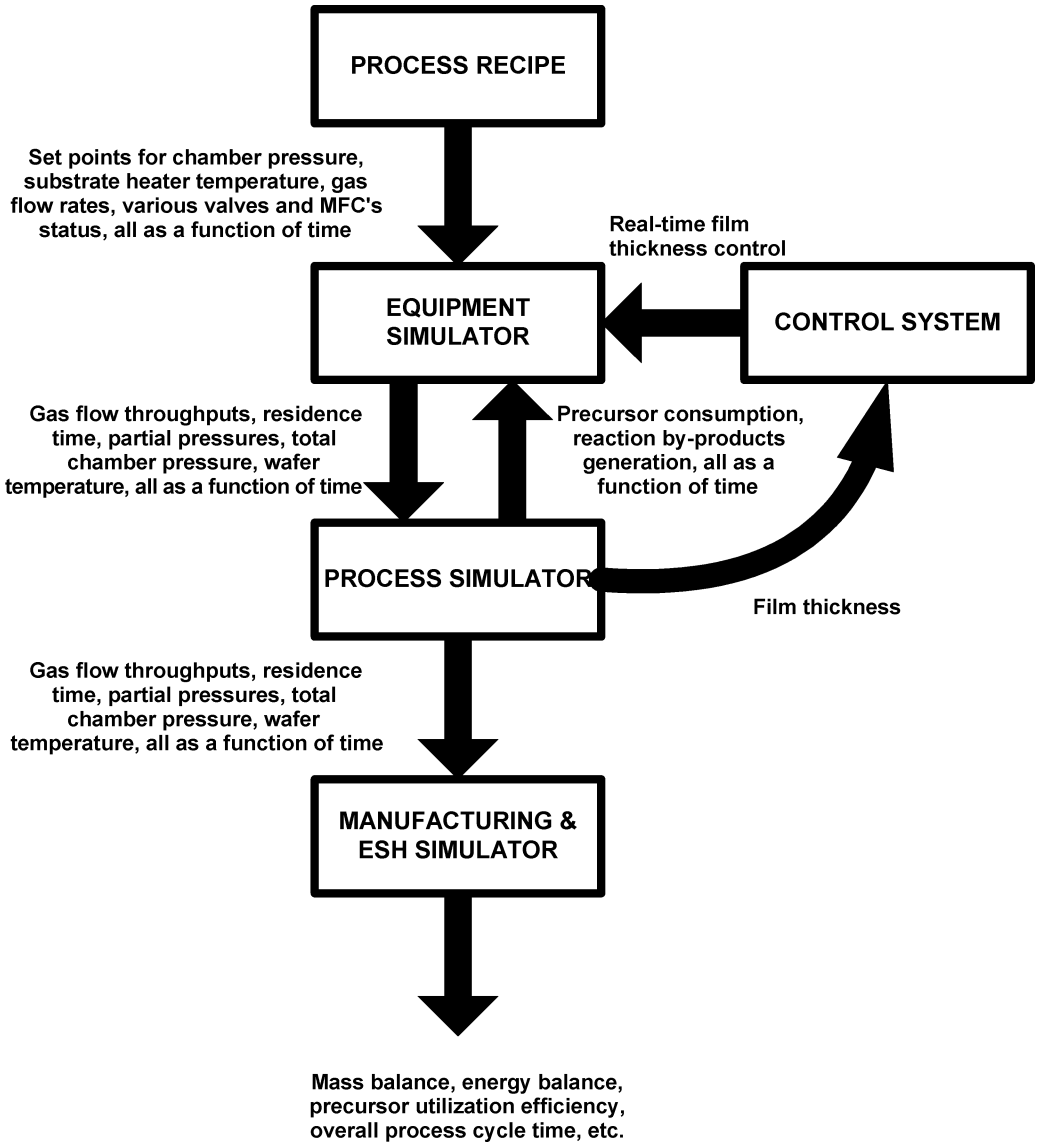

Fig. 1. Block diagram of the integrated Cu CVD simulator structure. The simulator can be thought of being composed of five components: 1) process recipe; 2) equipment simulator; 3) process simulator; 4) control system for terminating the process when desired film thickness is reached on the wafer; and 5) manufacturing and ESH simulator to compute key metrics. Dynamic information flow among the various components is indicated by the arrows.

achieved through such multilevel compound block structures, so that one can immediately identify the role of each group of calculations. In the blanket Cu CVD simulator used here, there are five levels of compound block structure and nearly 1000 individual functional blocks.

While the essence of the dynamic simulation model constructed using VisSim is the mathematical representation of physics, chemistry, dynamic functionality, and metrics computation, the value of the model is substantially enhanced by its visual interface and an array of usability features for both system design and analysis. As shown in Fig. 2, appropriate plotting blocks placed at the highest level of hierarchy (i.e., the topmost user interface level) reveal the progress of a simulated process in real time, while the pop-up dialogue blocks let users input/change the process recipe as well as various other settings related to the virtual process tool configuration (e.g., reactor size, process pump speed), desired simulation mode (e.g., fixed temperature mode or ramping temperature mode), etc., all in real time. Such enhanced interactions between the simulator and its human user have not only added value to our research, but also opened doors to possible use of such simulators for educational/training purposes in both the academics and industry [11], [16], [17].

B. Equipment and Process Modeling

A schematic representation of the virtual Cu CVD equipment and process module is shown in Fig. 3, consisting of a simplified version of the gas delivery system, the blanket Cu CVD reactor, its pumping system, and a control system to terminate the process at the target film thickness. Precursors are delivered to the reactor together with carrier gas and the gas flow is regulated by a set of mass flow controllers. The virtual process chamber,

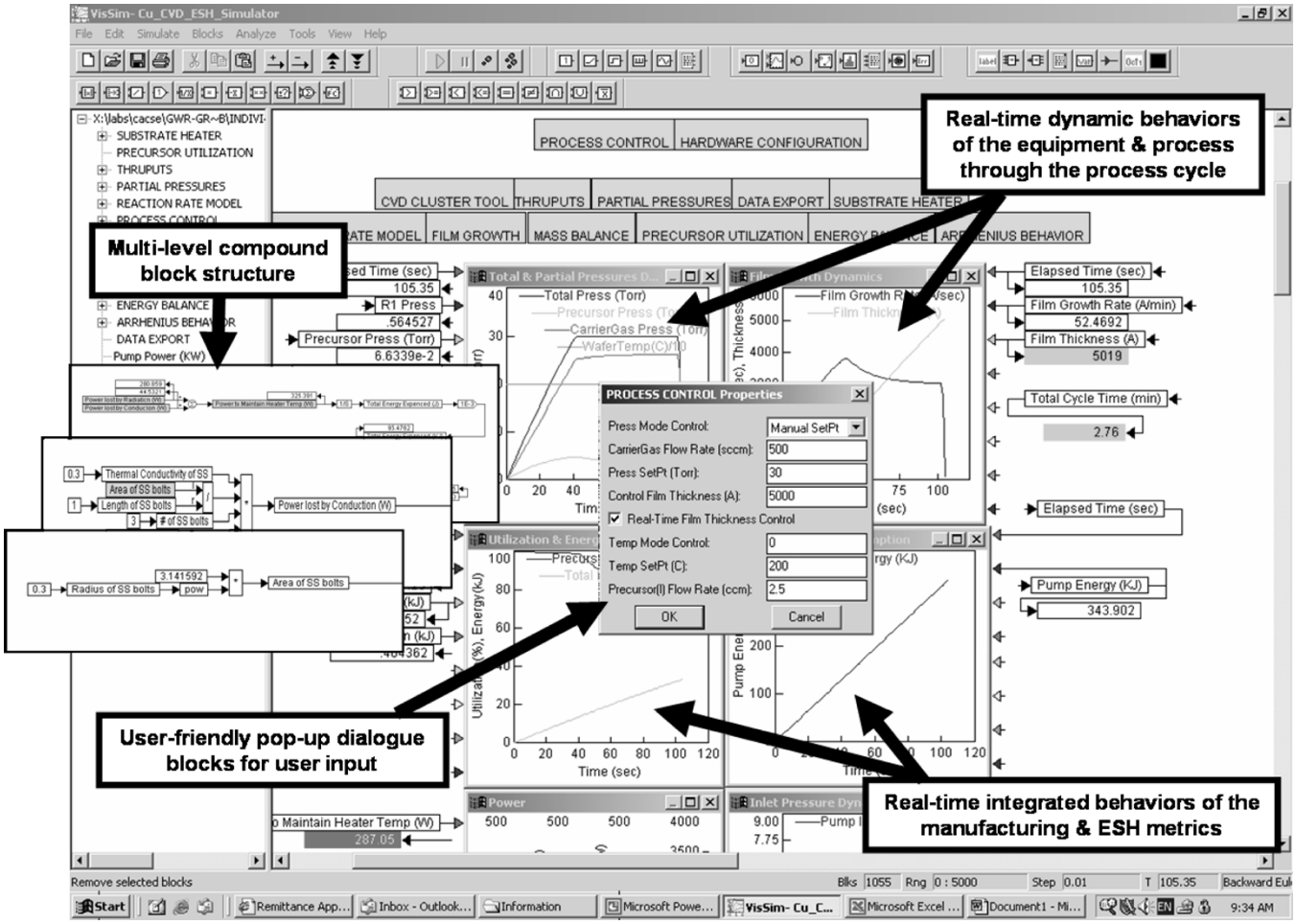

Fig. 2. Computer screenshot of the VisSim-based simulator for Cu CVD unit process. This view shows the highest level of the multilevel compound block structure, where users normally interact with the simulator to 1) monitor the progress of the simulated process cycle via various real-time generated plots, as well as to 2) change various settings related to the process recipe and equipment configuration via pop-up dialogue blocks.

its pressure control system, and the resistive substrate heating mechanism are all designed for blanket Cu CVD in a relatively high pressure range (i.e., 10 –100 torr). During process, pressure in the chamber is stabilized at the desired set point by the downstream low-conductance throttle valve (0.07–24 L/s) coupled to a capacitance diaphragm gauge. Gases are exhausted by a pumping system that includes a roots blower pump backed up by a mechanical rotary pump. In our model, proportional, integral, and derivative control loops were implemented to perform chamber pressure regulation. A virtual control system monitors in real time the thickness of Cu film deposited on the wafer and terminates the process when the target film thickness is reached. Such real-time film thickness monitoring and control technology has been reported in the past for other interconnect metallization processes and can be realized using *in situ* sensors such as mass spectrometry [18]. For our purposes here, this is valuable in ensuring that experiments using different process recipes and/or system designs all deliver the same result on the wafer, so that manufacturing and ESH metrics can be derived for the same product output condition.

A salient feature of the simulator is that it allows modification of the key parameters for equipment configuration (e.g., chamber volume, throttle valve conductance range, process pump speed). This enables virtual experiments to be conducted as a function of varying equipment configurations, opening doors to study the effects of changes in hardware configurations on manufacturing and ESH metrics of interest.

Physically based models are used wherever possible so that application of the simulator can be extended to as broad a process parameter range as possible. Furthermore, interactions between physical phenomena are especially important in capturing and simulating system-level dynamics. Since the assessment of manufacturing and ESH metrics requires a fairly complete system-level description, reduced-order and empirical models are used where physics and chemistry either involve high complexity or are poorly known.

For instance, consider the dynamic interactions and modeling required to account for wafer temperature and heat transfer mechanisms. Our model recognizes that the wafer radiates heat outward during the CVD process in an amount which depends not only on the instantaneous surface temperature, but also on the wafer emissivity at that time in the process cycle [19]. Since the Si substrate and Cu have different emissivity values, the emissivity of the wafer changes as Cu is deposited—i.e., the emissivity changes dynamically through the process cycle. Thus, a reduced-order model was constructed to estimate the

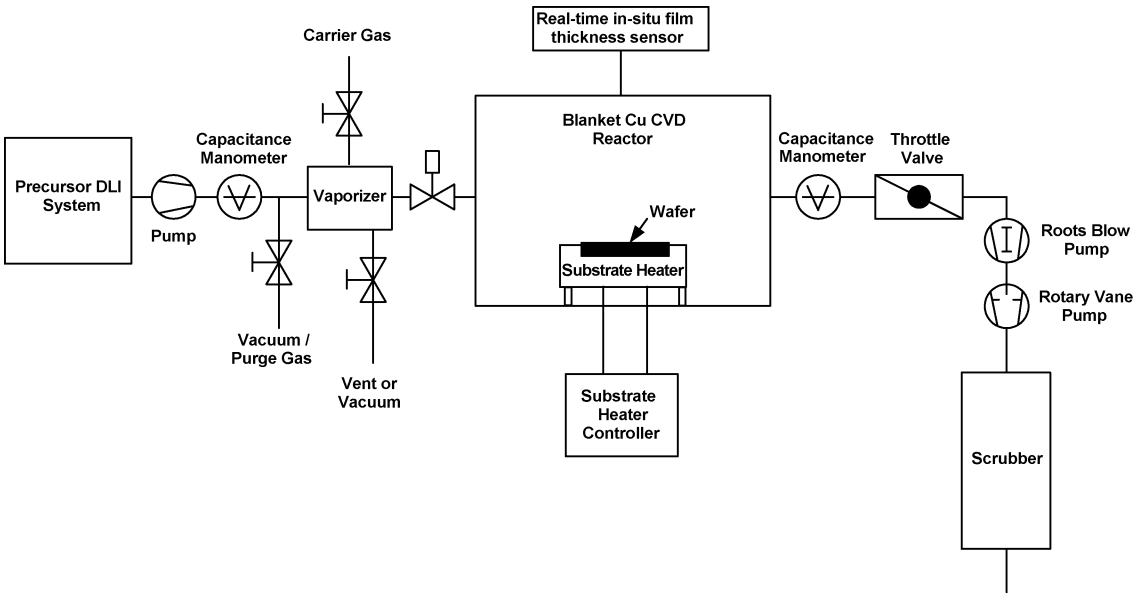

Fig. 3. Schematic diagram of the virtual Cu CVD process system, comprising gas delivery system, blanket Cu CVD reactor, pumping system, and control systems for film thickness and substrate heater temperature.

effective emissivity as a function of Cu film thickness: We assumed the effective wafer emissivity to be a linear function of Cu film thickness, beginning with that for a bare Si wafer and linearly changing to that for bulk Cu at a thickness on the order of the optical absorption depth at infrared wavelengths.

The model for the deposition kinetics is based on current empirical understanding of the physics and chemistry for Cu CVD from Cu(hfac)(tmvs) [14], [15], [20]–[24], a precursor widely available in the industry as CupraSelect from Schumacher [23]. This precursor is liquid at room temperature and is known to deposit pure Cu films at temperatures below 200 °C without the need for adding reducing agents [14], [15], [20]–[24]. Our model includes macroscopic gas transport determined by equipment design and dynamics, boundary layer transport above the wafer surface, deposition of Cu films by pyrolysis on the heated wafer surface, and exhaust of reaction products as well as unreacted precursor gases by the macroscopic equipment. While details of the exact chemistry are not fully understood, the overall deposition reaction can be represented as two precursor molecules decomposing on the hot wafer surface to deposit one Cu atom on the surface and generate byproduct molecules in the gas phase by the following chemical reaction [14], [15], [21], [22]:

$$2\mathrm{Cu}^{I}(\mathrm{hfac})(\mathrm{tmvs}) \rightarrow \mathrm{Cu}^{0} + \mathrm{Cu}^{II}(\mathrm{hfac})_2 + 2(\mathrm{tmvs})$$

where tmvs stands for trimethylvinylsilane $(\mathrm{C_5H_{12}Si})$, and hfac stands for hexafluoroacetylacetonate dehydrate $(\mathrm{C_3HF_6O_2})$. A reduced-order chemical reaction model has been constructed in our Cu CVD simulator from various empirical data available, for example, using transport and surface reaction rate coefficients and activation energy for surface reaction [20]–[22]. From this model, the simulator computes the rate of each chemical process step (e.g., gas phase transport rate for the growth species, surface reaction rate, and the overall deposition rate) at each time step in the simulation, based on the time-dependent parameters (temperature, partial pressures) through the process cycle.

The overall process behavior depends on the pressure–temperature regime encountered, a consequence of the relative rates of gas transport (determined mainly by macroscopic equipment dynamics) and surface chemical reaction (determined primarily by wafer temperature as well as reactant partial pressure). This behavior is exemplified in the Arrhenius plot in Fig. 4(a), which clearly reflects the expected result, namely equipment-determined transport-limited behavior at higher temperatures (left side) and surface-determined kinetics-limited behavior at lower temperatures (right side). This plot was obtained by fixing all process and system parameters (10-torr total pressure, 1.0-ccm precursor flow, 200-sccm carrier gas flow) and scanning the wafer temperature. The counterpart of this behavior is shown in Fig. 4(b), where the parameters were fixed (temperature 200 °C, 1.0-ccm precursor flow, 200-sccm carrier gas flow) and the total pressure was varied by changes in throttle valve setting; As expected, growth rate increases with pressure when pressure is low, but as the pressure is increased kinetics becomes rate-determining and pressure changes no longer influence deposition rate. Taken together, these results show the steady-state behavior of the simulation to be as expected, so that we may expect the simulator to deliver meaningful process metrics as conditions are varied during the dynamic process cycle.

C. Dynamic Simulation for the Process Cycle

With the modeling elements described above, the key goal of the simulator is to represent the dynamics involved in the process cycle, from which system-level manufacturing and ESH metrics can be extracted as a function of equipment design and process recipe. Table I describes the range of process conditions investigated with our simulations, based on available information on industry process conditions [20], [22], [24]. As an example of such a process recipe, the virtual experiment illustrated in Fig. 5 is designed to deposit 5000 Å of pure Cu film

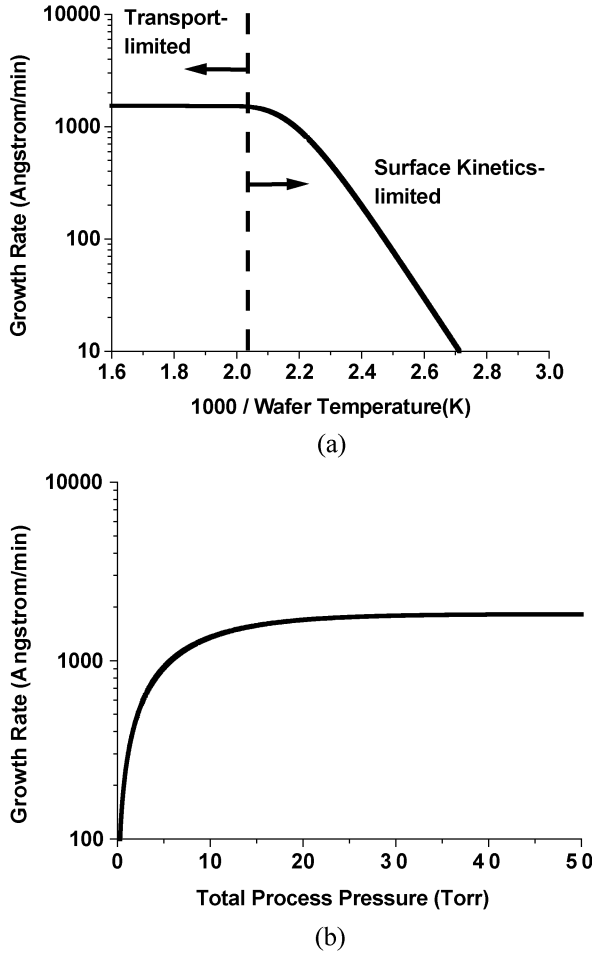

Fig. 4. (a) Arrhenius behavior of the simulated Cu CVD unit process at fixed total pressure (10 torr) and flow rates (1.0-ccm precursor and 200-sccm carrier gas). Depending on the process temperature and pressure, the overall deposition kinetics, represented by the effective rate of reaction, can be either transport-limited or surface reaction-limited. (b) Pressure dependence of the overall growth rate at fixed temperature (200 °C) and flow rates (1.0-ccm precursor and 200-sccm carrier gas).

TABLE I
RANGE OF PROCESS CONDITIONS USED FOR THE VIRTUAL Cu CVD UNIT PROCESS SIMULATION, WHICH WAS DECIDED UPON BY TAKING INTO CONSIDERATION AVAILABLE INFORMATION ON INDUSTRY PROCESS CONDITIONS [20], [22], [24]

Process Parameter	Value
Total Pressure	5 Torr – 50 Torr
Precursor (liquid) Flow Rate	0.5 ccm – 2.5 ccm
Carrier Gas Flow Rate	100 sccm – 500 sccm
Substrate Heater Temperature	150°C – 250°C
Target Film Thickness	5000 Å

on a 200 °C wafer using a 10-torr process gas which contains 2.5 ccm of Cu(hfac)(tmvs) precursor mixed with 500 sccm of carrier gas (Ar or He). The process recipe can be described by the following three stages:

1) **Ramp-up (chamber fill)**, during which the precursor and carrier gas at constant flow rates are introduced into the process chamber to establish the process pressure set point;

2) **Nominal–raw process**, during which the process chamber has reached the desired pressure set point, and process conditions remain essentially constant for the duration of the deposition;

3) **Ramp-down (pump-down)**, during which the deposition process is terminated, and reactant and residual gases within the chamber are pumped away, reducing pressure from its nominal process value down to a negligible value (1×10^{-2} torr, as used in our simulator) as fast as possible, including opening the throttle valve fully.

The real-time end point function in the simulator assures that the virtual process is terminated at the same Cu film thickness for every run, independent of equipment and process conditions chosen. For our investigations, we maintained a constant substrate temperature during the process and during wafer exchange, since thermal time constants for substrate heating as employed in this moderate wafer temperature range would be incompatible with the wafer throughput.

The importance of process dynamics is apparent in the three-stage description of the process. While conditions remain essentially constant during the nominal process stage, the ramp-up and ramp-down stages influence systems-level metrics, including process cycle time per wafer and reactant utilization, and these features necessitate simulation approaches which explicitly address dynamics.

The dynamic simulation generates a clear picture of the time-dependent behavior of equipment, process, and wafer state, as shown in Fig. 5. Furthermore, to convey a more realistic impression of the process, we often execute the simulation in real time, meaning that the observed changes in variables (e.g., pressure, thickness) are updated by the simulator at the actual rate they would occur (rather than as fast as the computer can calculate them). As seen in Fig. 5(a), the total pressure and carrier gas pressure behave simply, increasing linearly in time at a rate determined by the carrier gas inlet flow rate and then stabilizing when the target pressure is achieved and the regulatory total pressure controller begins operation. In contrast, the partial pressures of precursor and byproducts exhibit a quite different, more complex behavior during the ramp-up stage and into the nominal process stage. This is because a notable fraction of the precursor undergoes deposition reaction on the already hot wafer surface, reducing its partial pressure within the chamber (manifested by the decreasing slope in the nominal process stage). At the same time, the reaction generates reaction byproduct species (manifested by the increasing slope), with partial pressure increasing slowly at first as the byproduct partial pressure begins at zero and takes some time (reactor residence time) to achieve a steady-state value during the nominal process stage. Once the nominal process conditions are reached, steady-state overcomes these transient behaviors during the nominal process stage.

The wafer state and system-level metrics depicted in Fig. 5(b) are simulator outputs corresponding to the process cycle in Fig. 5(a). The *instantaneous* precursor utilization efficiency (which contributes to one of our ESH metrics when integrated through the process cycle) is near 100% during the chamber fill period. This is because the throttle valve is nearly closed during the ramp-up stage, so the precursor let into the chamber reacts readily on the hot wafer surface with virtually infinite residence time. This situation persists until the chamber reaches

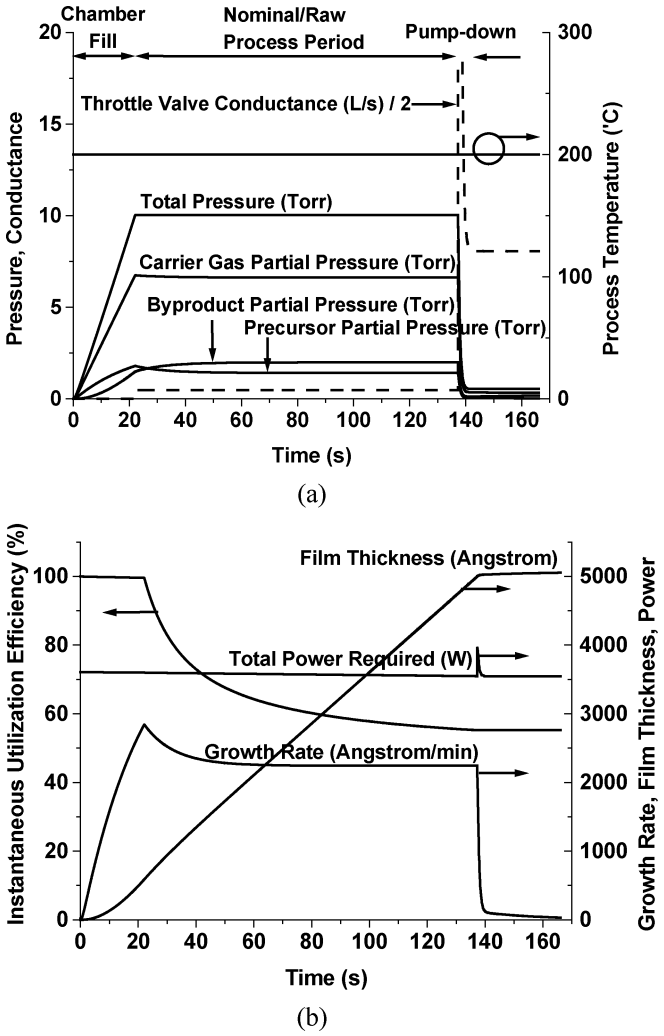

Fig. 5. (a) Dynamic process and equipment behavior through the process cycle for Cu CVD process at total pressure 10 torr, process temperature 200 °C, precursor flow rate 2.5 ccm, and carrier gas flow rate 500 sccm. (b) The resulting dynamics for different process-related variables.

the nominal process pressure. Then the throttle valve opens up to control the total pressure, the effective pumping speed increases, and the residence time decreases, so the instantaneous utilization drops significantly to a value that depends on the residence time of the precursor. The growth rate in Fig. 5(b) shows corresponding complexity in its time-dependence. Growth rate increases quickly as precursor partial pressure increases, then drops as increasing portions of byproduct contribute to the total pressure, and as the fixed total pressure is maintained, the precursor concentration and, thus, growth rate decreases somewhat. In turn, these features of the growth rate dynamics can be seen, although more subtly, in the film thickness curve in Fig. 5(b). Finally, except for a rapid transient at the end of the process cycle, the electrical power required is essentially constant throughout the process, as might be expected given the constant temperature of the wafer substrate heater and the fact that the pumps work continuously; these considerations are dealt with in more detail below.

These dynamic phenomena are the direct outputs of the physically based modeling and simulation, reflecting real behavior of the process and equipment through the process cycle. As this example suggests, the relative duration of the chamber fill period with respect to the entire process cycle, as well as the detailed dynamics occurring within the period, have significant influence on the manufacturing and ESH metrics of interest (e.g., overall precursor utilization efficiency). Manufacturing and ESH metrics are determined from time-integration over the *entire* process cycle, thus depending to a greater or lesser extent on the detailed time-dependent behaviors within each stage of the process cycle. The dynamic simulation methodology facilitates evaluation of transient as well as nominal steady state process behavior, thus enabling both a more complete assessment of system-level metrics and a deeper understanding of complex system dynamics.

III. Integrated Assessment for Manufacturing and ESH

As an extremely competitive industry rooted in cutting-edge technologies for materials, devices, circuits, and manufacturing, meeting the challenge of environmentally benign manufacturing requires the recognition that technology performance and manufacturing productivity cannot be compromised. This suggests two approaches. The conservative approach is to attempt to optimize ESH within the limited bounds and context of conventional approaches to technology evolution and manufacturing productivity, improving ESH performance for existing technology and—more importantly—developing manufacturable ESH-friendly technologies for the future. A more proactive approach is to develop powerful methodologies and tools for design and optimization which can be exploited to cooptimize multiple metrics at a higher level of integration. Such approaches represent decision support strategies with benefit not only to ESH in concert with technology and manufacturing pressures, but even for addressing conflicting postures between technology and manufacturing metrics independent of their ESH consequences. We believe that physically based modeling and simulation hierarchies provide a powerful means to such ends. The work presented here is intended as an example for the case of a prototypical unit process and a limited set of manufacturing and ESH metrics.

A. Metrics of Interest

In general, such approaches should address three sets of metrics—technology performance, manufacturing productivity, and ESH, all of which are consequences of equipment and process design as well as detailed process recipes. Technology performance metrics relate directly to specifications of the semiconductor product and can be recognized as, for example, transistor speed, device density, device power efficiency, product reliability, etc. Manufacturing productivity metrics depend on how equipment is employed to produce the technology products and to the capital and operating costs associated with factory equipment and operations, leading to metrics such as cost-of-ownership (COO), overall equipment effectiveness, yield, wafer throughput, process cycle time, etc. Environmental impact metrics relate to materials and energy consumption as well as byproduct generation (i.e., mass and energy balance), and so they are reflected in metrics such as reactant–precursor

utilization efficiency, hazardous byproducts and waste generation–emission, energy consumption, water usage, etc. Of the three sets of metrics, technology performance is most difficult to relate to detailed equipment and process design, requiring either a set of technology computer aided design tools or the adoption of empirical rather than physics-based models. For demonstration purposes here, we, therefore, restrict our attention to manufacturing and ESH metrics, specifically *process cycle time*, *reactant–precursor utilization efficiency*, and *energy consumption*. Reactant–precursor utilization efficiency and energy consumption have direct ESH impacts as well as significant cost consequences for manufacturing productivity, while process cycle time plays a critical role in manufacturing productivity and competitiveness.

In this article, **process cycle time** is defined as the nominal–raw process time plus process overhead times for ramp-up, ramp-down, and other activities, as illustrated in Fig. 5. Nominal–raw process time is the period during which deposition occurs on the wafer at the nominal process pressure. Total overhead time includes three components: 1) ramp-up (chamber filling) time for achieving process pressure; 2) ramp-down (pump-down) time after the process is complete; and 3) other overhead times, e.g., the time it takes to load–unload the wafer into the process chamber (assumed to be 50 s in our simulator) and the time it takes to stabilize the wafer surface temperature prior to each deposition process (assumed to be 10 s in our simulator). Of course, at the unit process level minimal process cycle time is a strong manufacturing productivity driver.

Reactant–precursor utilization efficiency (or process conversion rate) is a direct manifestation of the unit process mass balance through the process cycle, and is defined as the percentage of the precursor Cu(hfac)(tmvs) molecules that are converted to a deposited Cu thin film with respect to the total number of precursor molecules introduced into the CVD process chamber over the duration of entire unit process cycle. High utilization efficiency is desired for both manufacturing and ESH considerations in order to reduce consumables cost (especially for expensive, high purity, and proprietary precursor chemicals) and to reduce materials waste. The ESH impact of materials waste has important secondary impacts as well—upstream in terms of the environmental costs incurred in precursor manufacturing, and downstream in terms of recovery, abatement, and disposal of the wasted precursor.

Energy consumption is here defined as the total amount of energy expended within the unit process to deposit a nominal thickness (e.g., 5000 Å) of the Cu thin film on the wafer. Normalization with respect to film thickness deposited enables us to compare different processes and equipment designs as employed to achieve the same product as output. This normalized energy consumption has both manufacturing and ESH impact, because energy costs are significant to COO and manufacturing productivity, and because energy consumption has global environmental (and political) consequences.

The goal of our simulation and optimization studies is to seek trends which minimize process cycle time and energy consumption while maximizing reactant–precursor utilization efficiency as a function of process and equipment parameters (e.g., temperature, pressure, flow rate, chamber volume, pump speed). As already mentioned, this is only a subset of integrated metrics chosen for our Cu CVD example, and considerations for other metrics (e.g., material quality) are discussed later.

B. Mass Balance: Process Cycle Time and Precursor Utilization Efficiency

Here we consider metrics which relate to mass balance, a major focus for environmental consequences. In particular, we have utilized the simulator to investigate how two specific metrics, **process cycle time** and **precursor utilization efficiency**, vary as a function of *process temperature*, *pressure*, and *flow* rates. Process cycle time is a critical manufacturing metric, determining wafer throughput in the CVD tool. Precursor utilization efficiency relates directly to mass balance, indicating how much material is needed to create the product (here a Cu thin film on the wafer), and it is also relevant to manufacturing in that there is significant cost associated with high purity precursors. By exploring specific combinations of the process parameters, we identify situations in which both metrics can be improved (which we call "win-win" situations), and we find other situations in which improvement in one metric comes only at the cost of degradation of the other (which are designated as tradeoff situations).

Win-Win Example: A win-win situation between manufacturing and ESH metrics arises when we consider process cycle time and precursor utilization efficiency as a function of process temperature and pressure with all other conditions fixed (e.g., fixed flow rates). A total of 50 single-wafer virtual deposition processes were carried out to see the effect of varying process temperature and pressure under otherwise fixed condition. The process temperature was varied between 150 °C and 250 °C, while the pressure was varied between 5 and 40 torr, all under fixed flow rates of 1.0-ccm precursor and 200-sccm carrier gas.

As shown in Fig. 6(a), higher temperature and higher pressure each result in shorter cycle time. The benefit of moving process parameters in these directions (i.e., the sensitivity) is greatest in regions of higher temperature ($>$200 °C) and higher pressure ($>$20 torr), which is mainly the transport-limited regime on the Arrhenius curve in Fig. 4(a), where the overall reaction rate (i.e., deposition rate) is the highest. Clearly, higher rates translate to shorter process cycle time. While the detailed response depends on the relative values on temperature and pressure, both in the Arrhenius rates and process cycle time, one would normally anticipate from typical Arrhenius behavior that increased temperature and increased pressure will reduce cycle time.

Higher temperature and higher pressure also produce increased utilization efficiency, as shown in Fig. 6(b), but the underlying reasons are somewhat more subtle. As indicated above, higher temperature and pressure both increase the reaction rate on the surface, enhancing precursor utilization. In addition, since these experiments maintain constant flow rate, increasing pressure is accomplished by reducing the effective pumping speed of the system by closing the throttle valve aperture. In turn, this increases residence time of gases in the reactor, allowing on average more impingement events for each precursor molecule before it is pumped away. Thus, the increase in pressure at constant flow rate provides a second means to increase utilization efficiency.

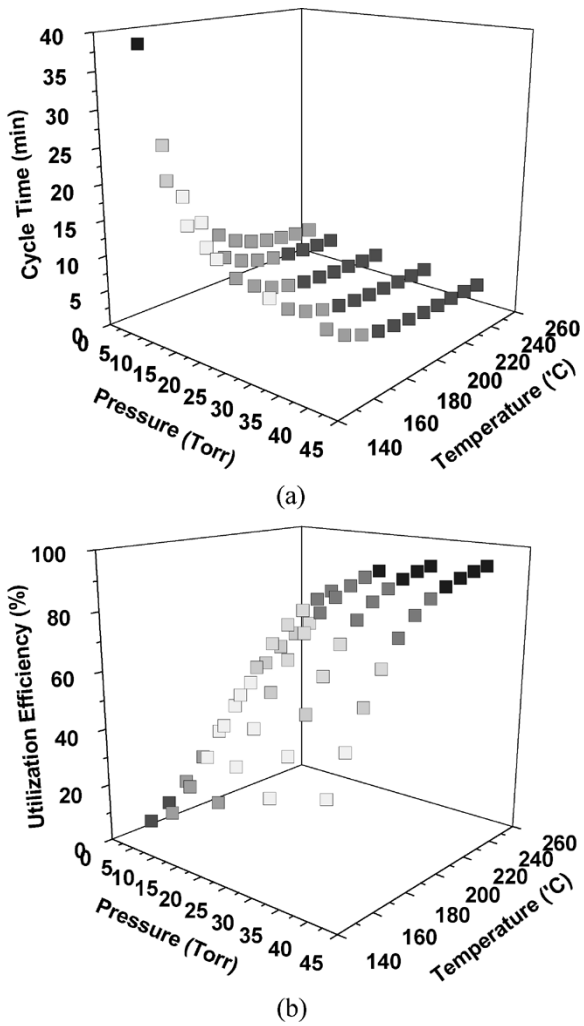

Fig. 6. Simulation results for process cycle time and utilization efficiency at fixed flow rates. Total process pressure and temperature were varied between 5 and 40 torr, and $150\ ^{\circ}\mathrm{C} - 250\ ^{\circ}\mathrm{C}$ respectively, under fixed flow rates condition (1.0-ccm precursor and 200-sccm carrier gas). (a) High process temperature and high pressure conditions were found to result in minimum process cycle time, and (b) high temperature and high pressure conditions also produced maximum precursor utilization efficiency. Hence, cooptimization for cycle time (a manufacturing metric) and utilization efficiency (both manufacturing and ESH metric) is possible at higher temperatures and pressures.

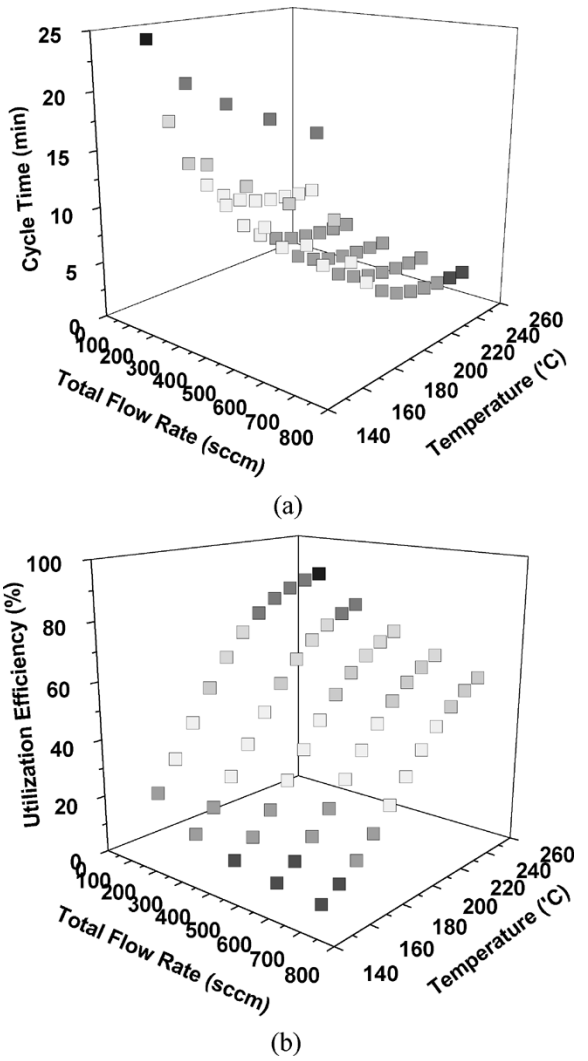

Fig. 7. Simulation results for process cycle time and utilization efficiency at a fixed pressure. Total gas flow rate and process temperature were varied between 141 and 707 sccm, and 150 °C and 250 °C, respectively, under a fixed total pressure (10 torr) and flow ratio (1 ccm of precursor in liquid phase per every 200 sccm of carrier gas). (a) Minimum process cycle time is achieved at high temperature and *high* total flow rate condition, while (b) precursor utilization efficiency is maximized at high temperature and *low* total flow rate conditions. Hence, a tradeoff situation exists between cycle time (a manufacturing metric) and utilization efficiency (both manufacturing and ESH metrics) in the case of total flow rate variation.

This example demonstrates that a win–win situation exists, at high temperature and pressure regime, between cycle time (a manufacturing metric) and utilization efficiency (both a manufacturing and an ESH metric) as a function of the two key process parameters for Cu CVD. Quantitatively, within the range of temperature and pressure variations considered here, appropriate process optimization can deliver up to $10\times$ and $13\times$ improvement of cycle time and utilization efficiency respectively.

When situations are win-win as shown in the foregoing example, directions for process optimization are clear. However, under other circumstances—and, one should assume, the general case—process modifications will improve some metrics and degrade others, i.e., a tradeoff situation. In these common cases, simulation provides a powerful vehicle for assessing the relative sensitivity of multiple metrics to specific changes in process parameters and recipes. Tradeoff analysis is a central theme of systems engineering, requiring modeling and simulation as the starting point for optimization methods to deal with the complexity of tradeoff situations.

Tradeoff Example: An example of a tradeoff situation arises when we compare the same two metrics, process cycle time, and precursor utilization efficiency as a function of process temperature and total gas flow rate, with all other conditions fixed (e.g., fixed pressure). A total of 50 single-wafer virtual deposition processes were carried out to see the effect of varying process temperature and flow rate under otherwise fixed conditions. As in the preceding set of experiments, the process temperature was varied between 150 °C and 250 °C, while the total flow rate was varied between 141 and 707 sccm, all under fixed total pressure of 10 torr. To maintain chemical process situations constant while the total gas flow rate was varied, the ratio

between the precursor and carrier gas remained fixed at 1 ccm of liquid phase precursor per 200 sccm of carrier gas. Simulation results shown in Fig. 7(a) reveal that shorter cycle time is achieved at higher temperature and higher flow rate. Clearly, higher temperature provides for higher reaction rate on surface and, therefore, shorter cycle time. Consistent with arguments above, higher flow rate at constant pressure means shorter residence time of molecules in the reactor, so that a larger fraction of the nearly constant number of molecules present in the reactor at any time are precursor species able to contribute to deposition, rather than the reaction byproducts. Thus, higher flow rate achieves the target deposition thickness more rapidly.

However, as shown in Fig. 7(b), maximizing utilization efficiency requires *lower* flow rates as well as higher temperatures. Consistent with the arguments above, lower flow rates mean longer residence times and more efficient conversion of precursor species to actual deposition of these species on the wafer. Thus, one is forced to choose between 1) *higher* flow rates for manufacturing benefit in shorter cycle time and 2) *lower* flow rates for higher precursor utilization efficiency, with benefit to ESH materials consumption and to manufacturing cost reduction.

This leads to several important observations. First, this particular example illustrates that tradeoff situations are common not only when one is trying to optimize ESH performance with the context of manufacturing productivity metrics. Even if one only wanted to optimize manufacturing productivity in this situation, one would have to choose between 1) higher flow rate for improved (shorter) cycle time and 2) lower flow rate for reducing materials costs. Thus, it is *not simply a question of ESH versus manufacturing*, but of how to deal with tradeoff situations in the context of multiple goals, including manufacturing productivity, ESH, and technology performance metrics.

Second, when multiple metrics and tradeoff situations appear, *the real challenge is to quantify the tradeoff*, i.e., to determine how large a penalty must be paid in one metric to achieve how much benefit in another. Simulation provides a means to achieve this quantification in reasonable detail. In the present example, our simulations show that at 150 °C nearly 4× in utilization efficiency (from 5.8% to 23%) is accompanied by only 1.3× loss in cycle time (from 19.6 to 24.5 min), whereas, at 250 °C only 1.5× improvement in utilization efficiency (from 58.6% to 87.57%) requires nearly 2.5× reduction in cycle time (from 2.9 to 7.2 min). Clearly, the quantitative cost–benefit situation depends significantly on the process parameter regime in which one is operating, as illustrated here for two temperatures for which the tradeoff in cost–benefit ratios is quite different. Within the entire process, parameter range of temperature and flow rate defined for this study, nearly 8.4× cycle time reduction can be achieved, but only at the cost of a 2.5× loss in utilization efficiency.

Finally, while modeling and simulation are essential to integrated assessment of manufacturing, ESH, and technology metrics, one ultimately needs a rational means to quantify a prioritization of the output metrics themselves, i.e., how "important" is cycle time as compared to utilization efficiency? Even if one understands the tradeoff between these metrics at a specific process design point (i.e., sensitivity analysis), ultimately one must express the relative value of the two metrics. This even more difficult challenge, normally expressed in terms of a value or utility function in systems engineering, is described more fully in Section IV.

C. Energy Consumption

Now we turn attention to energy consumption, another crucial focus for environmental impact in semiconductor manufacturing. Energy usage even at the unit process level contains numerous components. Using information from our own laboratory and sources related to equipments in it, we have carried out a rough Pareto analysis of the relative contributions to total energy use in a stand-alone Cu CVD process module, results for which are shown in Fig. 8. Our estimates indicate that the vacuum pumping system dominates (71%) energy consumption, with other significant contributions arising from the radio-frequency power needed to carry out plasma chamber cleaning, the heater power needed to maintain elevated wafer temperature, the direct liquid injection system for Cu precursor introduction, and a computer to control the module. In this section, we consider two of these sources as examples, first the substrate heating because it relates directly to the simulator and discussion of mass balance above, and second the pump package because it is dominant.

Substrate Heating: Following on our investigation above of the consequences of temperature, pressure, and flow changes, we have examined the energy expended for substrate heating to achieve the desired wafer temperature. A set of virtual experiments were conducted by varying temperature (150 °C to 250 °C) at fixed pressure (5 torr) and flow rates (1.0-ccm precursor and 200-sccm carrier gas). The power required to maintain substrate heater at the nominal process temperature and the energy expended per 5000 Å of film deposition are plotted in Fig. 9, recognizing that the process recipe specifies maintaining constant substrate temperature for the wafer through the entire process cycle. Both radiation and conduction are found to be important heat transfer channels in the process temperature regime for Cu CVD. The radiative heat loss is a function primarily of the temperatures and emissivities of the wafer and substrate heater surfaces (which change with deposition) and their surface areas, while the conductive heat loss is a function of the temperature difference between the heated bodies and the surroundings as well as the thermal conductivity and cross-sectional area of solids and gases which connect the two [19]. Radiation proves to be the dominant heat transfer mechanism and is a strong function of temperature ($\propto \mathrm{T}^4$). As illustrated by the total power requirement curve in Fig. 9, maintaining higher process temperature incurs higher power input, from which we might have expected to prefer lower process temperature for reduced energy consumption.

However, when the integrated energy consumption per 5000 Å of film deposition is calculated from the simulation, the opposite conclusion is obtained, as seen in Fig. 9. This result arises from the fact that the deposition rate is a strong—in fact exponential—function of wafer temperature, since the CVD process is thermally activated. As explained above, this shortens the process cycle time and correspondingly the time over which heating power must be integrated to determine

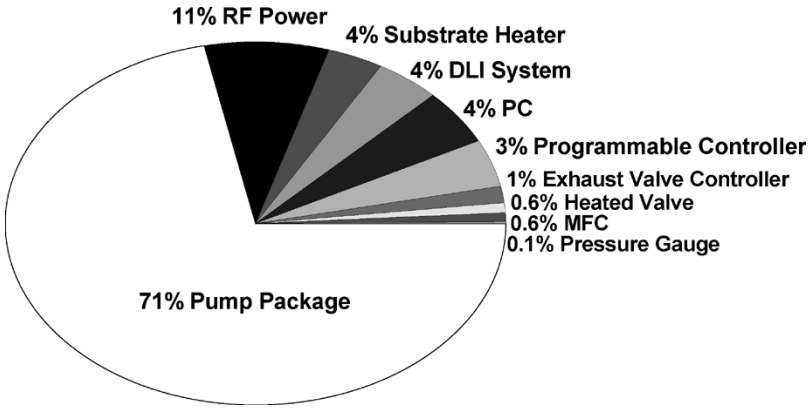

Fig. 8. Pareto analysis of the various sources of energy used in our virtual Cu CVD system. Data from Ulvac Technologies, Inc., Leybold Vacuum, Inc., and MKS Instruments, Inc. Pump package is found to be the biggest source of energy used in Cu CVD.

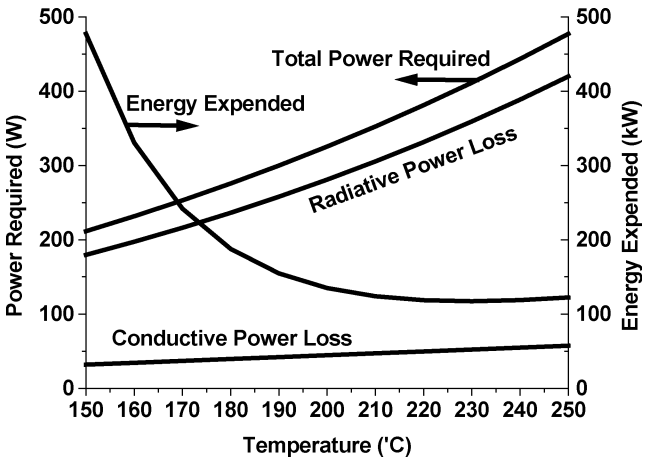

Fig. 9. Power required to maintain the substrate heater at the nominal process temperature and the energy expended per 5000 Å of film deposition are plotted here for a fixed total pressure (5 torr) and flow rates (1.0-ccm precursor and 200-sccm carrier gas). Both radiation and conduction are found to be important heat transfer channels in the process temperature regime for Cu CVD.

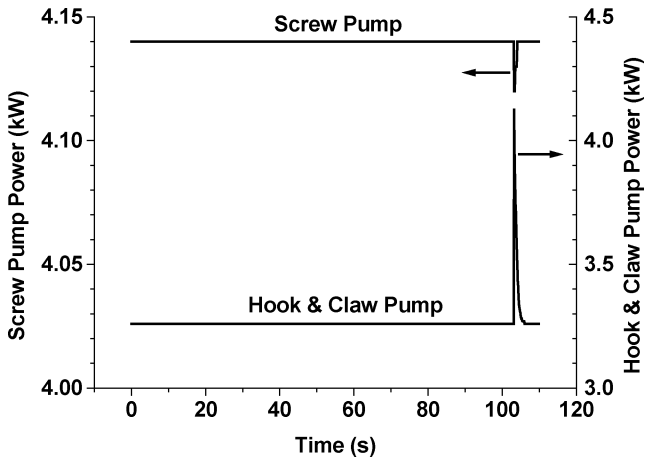

Fig. 10. Dynamic power consumption behavior through the process cycle for two different pump designs, using process conditions of total pressure 20 torr, process temperature 200 °C, precursor flow rate 2.5 ccm, and carrier gas flow rate 500 sccm. Note that the two pump curves relate to different power axes, used so that details of the pump-down transient can be shown. The screw pump design (left axis) exhibits an average power rating during process of 4.14 kW and a dip in power usage during the chamber pump-down period. The hook-and-claw pump design (right axis) requires a significantly lower average power rating during process (3.26 kW) and shows a spike in power usage during the same pump-down transient period. Average power during steady-state pumping at process pressure dominates energy consumption, with pump-down transients contributing negligibly to the total energy consumption through the process cycle.

the total energy consumed per wafer. Thus, the temperature dependence of the energy usage associated with wafer heating is dominated by the cycle time effect, in which the increasing power associated with higher wafer temperature is more than compensated by acceleration of reaction rate and shortening of cycle time at higher temperatures.

Vacuum Pumping System: Several different types of vacuum pumps are candidates for use in Cu CVD, particularly mechanical designs which are referred to as screw and hook-and-claw configurations. Both are dry pumps, as typically required for contamination control purposes in vacuum-based semiconductor manufacturing equipments. Since vacuum pumps involve motors, power consumption is expected to increase during a start-up transient and whenever the pressure upstream of the pump places a high load on the pump. Since these two pump configurations are fundamentally different, their power consumption specifications (for the same nominal pumping speed) are somewhat different, both at low pressure and during pressure transients. By incorporating their power consumption curves in the simulator, we have been able to generate results for power consumption as a function of time through the process cycle, for which results are shown in Fig. 10 (Leybold Vacuum, Inc.). Note that Fig. 10 presents power data on two vertical axes, the screw pump on the left (with average power 4.14 kW) and the hook-and-claw pump on the right (with average power 3.26 kW). During steady-state pumping at process pressure or vacuum, the hook-and-claw pump consumes about 25% less power than that of the screw pump. It is interesting to note that the power transient has a different sign for the two pump designs. However, given the short time required for the pump-down transient ($\sim$104 s in Fig. 10) compared to the process cycle time, the integrated energy associated with the transient is small. Therefore, the steady-state power consumption rating dominates energy consumption through the process cycle, and the hook-and-claw design is favored for minimizing energy consumption (of course, there are other factors relevant in choosing the actual pump design).

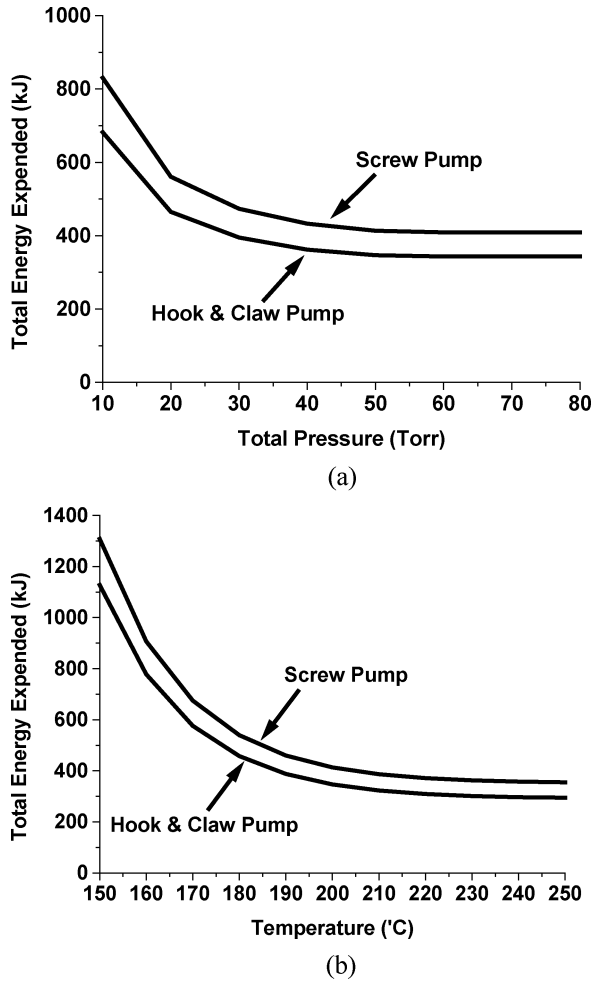

Fig. 11. "Total" energy usage in a Cu CVD unit process as a function of different pump types, (a) process pressure (at fixed temperature of 200 °C and flow rates of 2.5-ccm precursor with 500-sccm carrier gas), and (b) temperature (at a fixed total pressure of 50 torr and flow rates of 2.5-ccm precursor with 500-sccm carrier gas). For both screw and hook-and-claw pumps, the total energy usage is minimized at high temperature and high pressure, which are the conditions for minimum process cycle time. Hence, another "win-win" situation is found between manufacturing (cycle time) and ESH (total energy consumption) in Cu CVD.

Combined Energy Usage: Combining vacuum pump and substrate heater components of energy consumption gives the results in Fig. 11, which show the total energy expended from these two sources as a function of nominal process pressure and temperature for the two pump configurations. For both pump designs, energy consumption is minimized at higher pressures and temperatures. Since pump power is virtually constant through the process cycle (the pump-down transient contributing negligibly to the total energy use), variation of the total energy with pressure and temperature is dominated by the substrate heating component. In turn, the energy requirements for substrate heating are determined by process cycle time, where the extra power required to maintain higher wafer temperature is more than offset by the increased deposition rate (i.e., shorter process cycle time) achieved at higher temperatures. Furthermore, it is easy to identify the energy consumption benefit of the right pump system choice, namely the hook-and-claw design as derived from the pump choices considered in this example.

IV. Discussion

A. Dynamic Simulation for Unit Process Optimization

The simulations utilized here are based on known behavior of physics and chemistry as they operate in a Cu CVD unit process. By explicitly incorporating dynamics, the simulations capture details which are critical to assessment of key metrics such as process cycle time. Construction of such simulation models relies on incorporating known physics of vacuum system behavior, gas flow, and heat transfer. Representation of operative chemistry is more challenging, because the reactions are complex, and often—as here—empirical models are needed within a context of known qualitative behavior, such as the competition between transport and kinetic steps reflected in Arrhenius behavior. For certain, both physical and chemical components of the simulation models are incomplete and imperfect. However, two factors provide confidence for their use in ways which are illustrated in this work. First, numerous aspects of such physics and chemistry have been previously validated in our work on real-time, *in situ* sensors [13]. Second, the purpose of these—and for that matter any—simulation-based studies is to explore qualitative and quantitative behavior relating output metrics to process parameters and recipes. The results indicate systems-level behavior, provide insight into the underlying relationships, and reveal opportunities for optimization that can be subsequently followed up by experiments and/or further development of the models.

B. Other Important Metrics

In this investigation, we have focused on several very important metrics—process cycle time, precursor utilization efficiency, and energy consumption—which reflect impact on both manufacturing productivity and environmental sensitivity. However, these are by no means the only significant factors. At the unit process level, we have not addressed metrics which relate to **material quality**, such as electrical resistivity, microstructure, deposition conformality, reliability and its dependence on stress, thermal history, current density, etc.; such factors can be experimentally evaluated using a number of characterization techniques such as photoluminescence, X-ray diffraction, secondary ion mass spectrometry, scanning electron microscopy, transmission electron microscopy, and X-ray photoemission spectroscopy [25]–[29]. Clearly, material quality is one determinant of process yield and device/product performance, in the domain of **technology performance** metrics outlined earlier. Furthermore, a number of key metrics relate to *process sequences* and *factory-level considerations*, including device and circuit performance, process yield, COO for capital equipment, equipment reliability and maintainability, etc.

This raises the question of how the methodology demonstrated here can be expanded to accommodate a broader spectrum of metrics for cooptimization of manufacturing productivity, technology performance, and ESH benefits. At this stage of computational materials and process science, it would be a major challenge to link the unit process simulation model used here to the resulting material properties. Instead,

one can envision building empirical models from vast amounts of data gathered during process development, and using these as submodels within the framework presented here. Two considerably larger challenges can be identified. One involves integrating sequences of unit process models to assess process yield and device/circuit performance, where yet another character of modeling (e.g., device technology computer aided design) and yield analysis/management methodologies and tools are needed. Another involves deriving from sequences of processes the manufacturing productivity metrics associated with characteristics ranging from COO to the optimization of tool populations, cluster tool configurations, and lot scheduling through the factory [30].

C. Tradeoff Analysis: Utility Functions

Win-win situations for multiple metrics (e.g., cycle time and utilization efficiency) are relatively straightforward to understand, and certainly to optimize. On the other hand, managing and optimizing tradeoff situations are a common and challenging task. In the present work, this was illustrated by the case of flow rate variation: Increasing flow rate improves process cycle time, but degrades precursor utilization efficiency. The dynamic simulations described and exploited here can readily reveal how much cycle time improvement can be obtained per unit degradation of utilization efficiency, and furthermore, this can be assessed in any range of process parameters, providing a versatile sensitivity analysis. Results of the simulation and a sensitivity analysis derived from it are valuable in exploring avenues to process optimization for one or more metrics of importance. However, these results do not address a more fundamental question, which is the quantitative prioritization of multiple metrics: Put simply, how much value is attached to a specific improvement in cycle time versus an improvement in utilization efficiency? Addressing such a question involves both systems engineering and enterprise judgment.

Systems engineering provides a means for representing the prioritization of multiple metrics in requiring the mathematical representation of a utility function or value function in order to execute powerful optimization algorithms. Once relations between process and equipment design parameters as inputs and multiple metrics as outputs are solidified in the form of models or simulations, systematic algorithms for optimization require that these relationships be accompanied by a mathematical representation of a single utility or value function which is to be optimized. In the example treated here, we know that any sensible utility function should seek minimum cycle time and maximum utilization efficiency. Thus, a utility function is expressed in a form such as

$$\text{Utility} = \frac{\alpha}{\text{Cycle Time}} + \beta \times \text{Utilization Efficiency}.$$

With the use of appropriate weighing factors α and β to represent the relative importance of the two metrics, cycle time and utilization efficiency, optimization of the utility function can be carried out.

The difficulty, of course, is to rationally establish such a utility function, determining sensible values for α and β, as well as deciding whether the mathematical form suggested is appropriate. These are difficult judgment calls to be made by the enterprise. The basis for such judgments might be an assessment of enterprise, involving cost, anticipated market and profitability, and/or corporate relationships with the local or global community. Furthermore, translating any such judgment down to the unit process level is necessary if unit process optimization is to be accomplished. These are all difficult challenges, which despite their difficulty, will be made in one form or another. In an important sense, a goal of the present work is to demonstrate the analytical modeling and simulation methodologies that can provide decision support in evaluating multiple metrics, to encourage and assist enterprise decision-makers in their task.

V. Conclusion

Environmentally benign semiconductor manufacturing requires methodologies which enable cooptimization of manufacturing and technology metrics (such as process cycle time and product quality) along with ESH (environmental) metrics (such as precursor utilization efficiency and energy consumption). We have investigated this challenge at the unit process level, with Cu CVD unit process and equipment as our prototype. Physically based dynamic simulation enabled us to take into consideration the process recipe and resulting time-dependent behaviors of vacuum and gas flow, heat transfer, reaction chemistry, equipment components, and control systems.

Higher temperature and pressure result in reduced process cycle time and increased precursor utilization efficiency, producing a win-win situation for the manufacturing and ESH metrics. In contrast, variation in precursor flow rate generates a tradeoff situation between these metrics. At lower temperatures, however, significant gain in utilization efficiency is indicated at lower flow rate, with relatively small cycle time penalty.

Energy consumption associated with substrate–wafer heating is substantially reduced at higher temperature because the deposition rate of the thermally activated CVD process increases faster with temperature than does the heating power required to reach and maintain these temperatures for Cu CVD. The largest source of energy consumption, however, is associated with the vacuum pumping system, and particularly with its steady-state value during process, while transients associated with increased gas load during pump-down contribute negligibly to the overall energy consumption picture.

These results at the unit process level demonstrate that the dynamic modeling and simulation approach 1) provides insights into complex physical–chemical system behavior and quantitative estimates for tradeoff analysis, and 2) reveals win-win situations in which ESH and manufacturing benefits may be achieved together. Accordingly, this simulation approach presents a powerful strategy for integrated assessment of manufacturing and ESH metrics in semiconductor manufacturing processes.

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