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Process Sensors, Simulation, and Control to Build in Reliability

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Abstract

Building in reliability is fundamentally difficult because detailed mechanistic origins of reliability failures are not commonly known. Controlled process experiments and sophisticated characterization methods offer hope of revealing mechanisms more broadly. Real-time and in-line sensors present perhaps even more potential in two cases, (1) when their information is correlated with reliability performance, and (2) when used to achieve process control through course correction and/or fault management; the latter has special value in difficult situations where the reliability failure emerges from process integration sensitivities. Integrated modeling and simulation structures provide a vehicle for broad knowledge capture, an enabler of design optimization for reliability and other metrics, and a platform for effective process control.

Perspective

Attacking the challenge of building in reliability has several components. First, and most obvious, is the opportunity to identify the underlying physics and chemistry which controls reliability, i.e., the intrinsic mechanisms. These are quite well understood, and thoroughly studied, in several cases, with electromigration in metal interconnects a prime example. Hot electron effects in MOSFET's are another example, but even more complex. I would suggest that the former is perhaps better understood because it is a physical mechanism, while hot electron reliability issues involve both the chemistry and the physics of defect sites.

Another aspect of elucidating fundamental reliability mechanisms involves the development and application of new techniques for sensing and characterization. In this regard, I have experienced this in the use of picosecond laser techniques to generate and detect ultrasonic waves in thin films; from this, we were able to identify signatures of incipient delamination at interfaces [1] and to assess the completeness of interfacial silicide formation at contact interfaces [2]. Often the reliability detractors in microelectronics involve very complex process sequences and device or interconnect structures where mechanical and mechanical/chemical stability are at the heart of reliability performance. Some of the process sensors discussed below could be useful for process learning and identifying reliability mechanisms as well.

It is often difficult to discern fundamental reliability mechanisms, but technology advance requires increasing ability to deal with reliability consequences anyway. In these situations there may be other ways to build in reliability. Here I will discuss the potential for building in reliability through the use of process sensing and control methodologies. Such necessity may appear particularly in two kinds of cases.

First, in my experience, many reliability problems are consequences not of process but of process integration, where the centering and width of parameter distributions for one process works for or against a synergistic relationship with the next process; these are problems which have to do with not of single process, but with a sequence of processes. A common example is adhesion failure, which results from an unfavorable balance between stress distributions and interfacial adhesion.

Second, equipment performance plays a major role in product reliability, because it is really is not the process but the embodiment of the process in equipment which determines the properties of the materials that we structure into devices which are supposed to be reliable. This is an area that I know very well from activities and technology roadmapping for the equipment industry, which contains the issue of how to develop more reliable equipment. However, there is potentially much more to be accessed, such as using real-time and in-line sensors to achieve early warning as equipment problems develop. This is the path to process control. Such work also requires integrated models and simulations in order to take advantage of early sensor information.

Sensing and control are potentially avenues to build in reliability because early warning of equipment drift is equivalent to early learning that process variations will occur. And process variations, individual or as part of a process integration sequence, are the cause of important reliability failures. In this sense, equipment reliability and control turns into process and product reliability and control.

Fundamental mechanisms and process integration

Let me give an example of the chemical origins for yield and reliability problems in the area of FET gate oxide processing. Advanced, ultraclean, and cluster processing equipment [3] permits much better chemical control of the Si surface in surface cleaning, thermal oxidation, and polySi CVD gate deposition. In fact, the fundamental chemistry of the Si-O system turns out to be capable of modifying an innocuous defect structure (electrically inactive) into an electrically active defect, leading to either a yield or a reliability failure. Solutions are available for this problem once the intrinsic microchemistry of the defect is understood, and if reasonable levels of process control are implemented.

The first example centers of post-oxidation annealing of already-grown gate oxides. [4] If we have already grown a good thermal oxide and we anneal it at 750C, microscopic defect which were not electrically active can turn active by what behaves as equivalent to an interfacial reaction, in which Si and oxygen combine to form volatile SiO. While the microscopic chemical reaction at the defect site may not be precisely this, the behavior has all the signatures of this kind of reaction. If we add oxygen at a rate which is somewhat larger than the rate

which we expect to form the SiO, we reoxidize the SiO to SiO_2 and we don't produce electrically active defects (as seen in breakdown or hole trapping). At higher annealing temperatures, this microscopic chemistry leads to macroscopic manifestations in the form of lateral voids in the oxide film. There are two messages from this example. First, here's a mechanism that can generate yield or reliability detractors from what is normally an innocuous and benign kind of microscopic defect. And second, if we understand the mechanism, we can avoid the problem. In this case, adding small amounts of oxygen can prevent the decomposition reaction (by more rapid reoxidation). Alternatively, the decomposition reaction can be accelerated to produce readily observed voids which decorate existing defects.

Question: Does that mean that annealing above 750ºC is detrimental?

Answer: That is exactly what it suggests, if the annealing environment is oxygen-deficient. The degradation is not observed in conventional furnace post-oxidation annealing, because these always have a few ppm oxygen present, sufficient for reoxidation. But if the salesman comes to your door and says he can give you better quality, cleaner systems, without any water vapor or oxygen in the system, your response should be not to buy the equipment, or to buy it with a little controlled leak of oxygen into the system. So the advent of ultraclean processing brings with it the responsibility to know what control must be exercised in the process, and to better understand what the fundamental chemistry really implies.

Question: What kinds of defects are initially active and inactive electrically?

Answer: We found that metal atom impurities which penetrate to the interface from Si stacking faults certainly generate electrically active defect sites upon moderate annealing. There may be other origins of these electrical defects, but we have not identified others yet.

Question: What oxide thickness range are we talking about here?

Answer: These experiments were done at range of 200 to 500 Å.

Question: How are the oxide voids generated at higher temperature?

Answer: We believe that the microscopic reaction somehow opens a small crack here in the oxide, permitting some SiO to escape and freeing reaction volume for further decomposition. These voids grow laterally until they're microns across and you can see them readily in an optical microscope. They are all the same size because they all started together as atomic-scale defects.

Question: Why wouldn't you see these problems during silicide annealing?

Answer: Again, most conventional annealing tubes are not sufficiently oxygen-free to cause the problem. Furthermore, at the stage of silicide anneal, the oxide is covered by more material, so that escape of the SiO is more difficult.

The second example is another embodiment of essentially the same chemistry. If we exploit the cleanliness capabilities in a cluster tool, clean the silicon surface completely free of oxide, and then raise the wafer temperature to oxidation conditions in the absence of intentional oxygen, the trace (ppm level) oxygen impurities etch and roughen the Si surface. [5] This roughness leads to low field breakdown and enhanced hole trapping once the thermal oxide has been grown. Again, the solution is to prevent the roughening mechanism, either by introducing low levels of oxygen during temperature ramping or to passivate the Si surface against the etching by intentionally growing an ultrathin oxide layer at lower temperature. Both examples lead to yield and/or reliability problems.

Question (later): In the integrated process, what are the origins of those defects we saw?

Answer: We have done a number of experiments on that, and have identified transition metal impurities which reach the interface as a clear culprit in the generation of electrically active defects and physical voids in the oxide. These were seen as a result of migration through stacking faults to the interface. However, there may be other kinds of such defects which we have not yet identified.

Real-Time and In-Line Sensors

These examples illustrate the kind of science which can be achieved relevant for defect and reliability issues. While such work is certainly very valuable, the challenges of maintaining or improving reliability in concert with the progress of microelectronics technology cannot wait for fundamental insights. This problems increasingly generates interest in the exploitation of process sensors in order to obtain rapid learning and consequent benefits in the context of building in reliability.

The motivation for process sensors is illustrated nicely in a somewhat different case, that of offline characterization and metrology techniques, which we utilize widely during the development cycle and in manufacturing (as indicated in Figure 1). In my role on the Metrology Technology Working Group for the semiconductor industry's National Technology Roadmap [6], I have observed a high degree of interest in achieving early indicators of metrology information from process sensors, since offline measurements are increasingly expensive and increasingly slow in terms of measurement time and in terms of speed of learning.

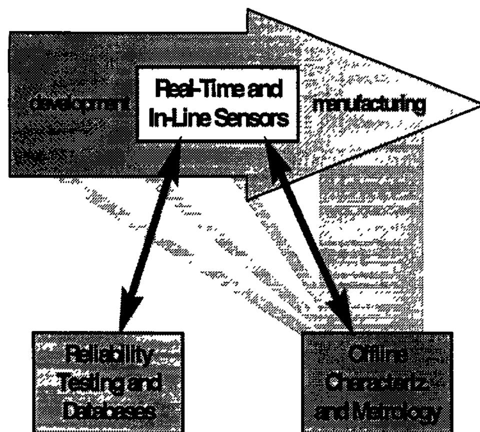

Figure 1. Timing for conventional investment in reliability and characterization learning. If real-time and in-line sensors can provide valid early indicators of reliability and characterization/metrology information, cost of and dependency on conventional measurement and testing approaches may be reduced.

To me this is directly analogous to the problem that we have in reliability. As we built the product, we make a large reliability database by carrying out extensive temperature/humidity tests, stress tests, etc.. But it takes a long time to do such testing at this stage, and having to redo this entire process to requalify a technology for reliability is prohibitive. So what I think we are evolving to is the view that we must look at real time and in line sensors as early warning signals, and use short loop learning to anticipate the reliability consequences of individual process conditions. This is an interesting synergy between what the reliability community needs and what the characterization or metrology community needs.

The reason to do real time and in line sensing is to achieve rapid learning, but this really means early warning as needed to practice process control. Process control means two things. First, it implies the ability to make mid-course corrections during the manufacturing process, either as real-time control or as run-to-run control. Second, it means fault management, so that we know when equipment is deteriorating, and more importantly so that we know what to do and when (e.g., emergency shutdown or early preventive maintenance). Both of these mean that process reproducibility can be improved. And that is critical because a substantial level of reliability qualification will already have been achieved during the early stages of the development cycle (where reliability learning has come from more fundamental scientific work or from a significant experiential base). It turns out that process control - both course correction and fault management - are in themselves major challenges to implement, but this is a hurdle for other manufacturing interests as well.

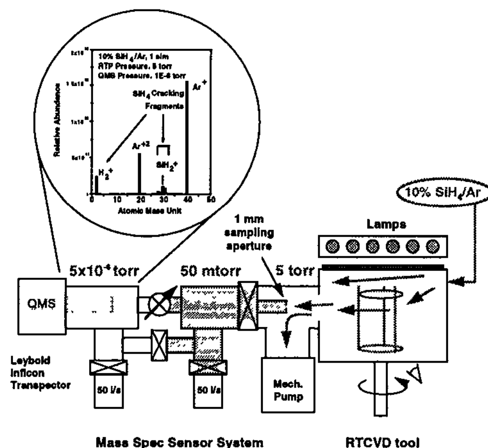

Figure 2. Schematic representation of RTCVD module including gas handling, RTCVD reactor and pumping, and two-stage differentially pumped mass spectrometer system. The fragmentation pattern of measured species is indicated in the inset.

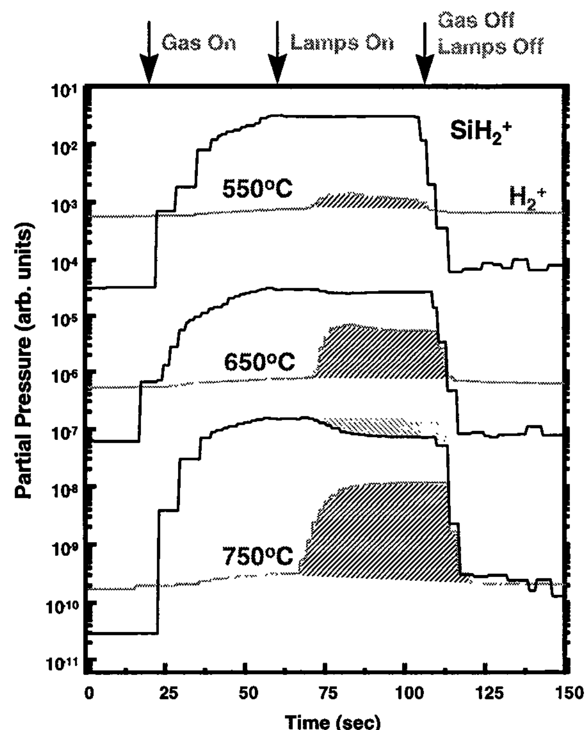

Figure 3. Mass spec signals as a function of time through the RTCVD process cycle. The behavior of reactants (e.g., SiH_4) indicates equipment functionality and process conditions, while the signals associated with product generation (H_2) adds direct information about reaction conditions on the wafer.

We have recently been applying in-situ, real-time, downstream mass spectrometry to achieve chemical information about equipment, process, and wafer conditions in semiconductor processes. [7,8] The arrangement is indicated in Fig. 2. Multi-stage differential pumping is required to achieve fast response times in the short process cycles encountered in rapid thermal chemical vapor deposition (RTCVD) or plasma processes.

An example is depicted in Fig. 3, which displays real-time mass spec signals from an RTCVD polySi process at 5 torr using 10% SiH_4 in Ar. Spectral components indicate reactant SiH_4, inert Ar carrier, and reaction product H_2 behavior through the complete process cycle. Gas flow operation (valves, flow controllers, etc.) are monitored by the time-dependence of Ar and SiH_4 signals, while wafer heating is observed through the reaction product H_2 (from $SiH_4 \Longrightarrow Si + 2H_2\uparrow$), thus sensing the performance of various equipment elements. Process reactant and product concentrations are directly indicated, from which process and wafer state conditions may be inferred. The generation of H_2 reaction product is accompanied by depletion of the SiH_4 reactant, providing two quantitative indicators of reaction rate at the wafer surface.

By appropriate integration of reaction product signals, mass spec sensing can provide real-time metrology for deposition thickness or etch depth. In this case, product signals are integrated through the reaction process. An example is depicted in Fig. 4, in which the H_2 product signal (like that in Fig. 3) was integrated through the process cycle. A well-defined, monotonic relationship is observed between this mass spec sensor signal - obtained in real-time and processed as an in-line measurement - and subsequent off-line determinations of actual film thickness (Nanometrics). Thus the mass spec sensor may be used for rapid determination of film thickness and thereby to drive run-to-run control. With sufficient data processing speed, this may also permit real-time endpointing and control.

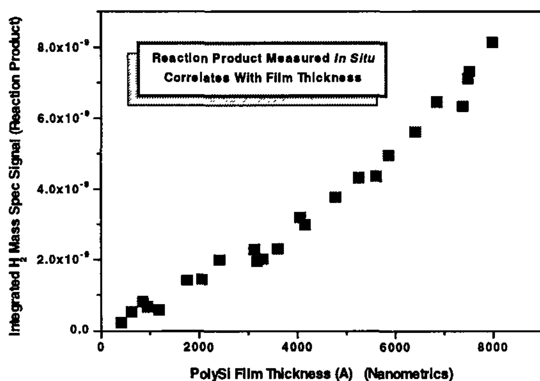

Figure 4. Integrated reaction product signal (H_2) from mass spec sensing vs. Actual polySi film thickness measured ex-situ after the process was completed and the wafer was removed.

The time-dependent chemical signatures from the process are also extremely useful for identifying equipment and process faults, as indicated in Fig. 5. Here the equipment control systems misbehaved when the pressure regime was changed, but the fault was immediately seen by the real-time mass spec sensing system.

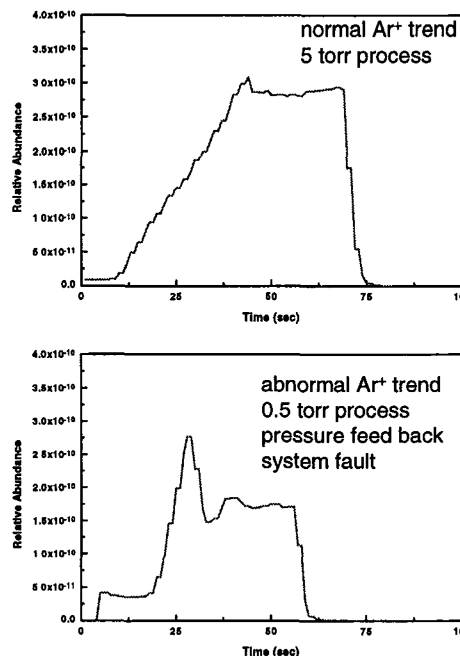

Figure 5. Real-time mass spec signal for Ar carrier through RTCVD polySi process cycle. At 5 torr, pressure control system operated correctly, but at 0.5 torr was unstable. This equipment malfunction is readily detected, permitting appropriate fault management.

Thus, these sensing techniques provide a wealth of information, about equipment behavior, process conditions, and wafer state conditions. And this information is clearly valuable for process control. In turn, rapid identification of process conditions should strongly influence the ability to achieve high degrees of process reproducibility, of major benefit for reliability.

These chemical sensing methods also promise value for elucidating the chemical fundamentals of the process, and hopefully also, a better basis for understanding reliability mechanisms in the beginning. For example, similar methods have been applied to oxide RTCVD from SiH_4/N_2O mixtures, revealing that the process is in fact a two-step sequence in which Si deposition from SiH_4 (as in polySi RTCVD) is followed by oxidation from N_2O, with virtually no water-related reaction products.

Integrated Dynamic Simulation

In fact, these sensing techniques are valuable for early identification of process problems, but in order to be useful for control, course correction, and fault management they require a set of models. We have implemented an integrated modeling platform in the form of dynamic simulation [9,10], which provides the basis for understanding, control, and optimization of the time-dependent process behavior. And this need would exist independent of the kind of sensors in use - mass spectrometry, optical emission, rf power, etc.

An example of dynamic simulation for RTCVD polySi process from SiH_4 is indicated in Fig. 6, which is an actual screen display showing the simulator front end. The simulator is built upon VisSim™ platform [11] operating

under Windows, which provides graphical capability for interconnecting mathematical entities to represent the time-dependent behavior of real systems and exploits a variety of simulation algorithms to execute the simulation. The dynamic simulator depicted in Fig. 6 includes ~1200 functional mathematical elements in a hierarchical structure 8 levels deep, representing the RTCVD equipment, the polySi process, the mass spec sensor system and response, and pressure and temperature systems on the equipment. The simulator generates representations of the time-dependent behavior of the wafer temperature, polySi growth rate and integrated film thickness, as well as signals for the various components measured in the quadrupole mass spec (QMS). Numerous other time-dependent parameters are calculated, though not displayed here, such as reactant and carrier gas partial pressures.

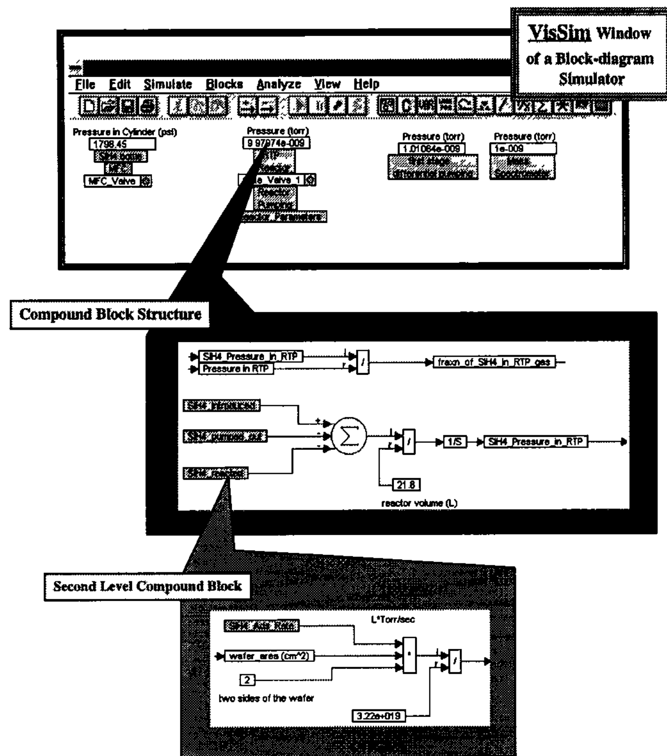

Figure 6. Structure of Windows-based simulator for polySi RTCVD. The top panel is the VisSim™–Window of the RTCVD equipment simulator. In the middle panel is a compound block for calculatiing SiH_4 partial pressure within the RTCVD reactor. The bottom panel illustrates a second level compound block for 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.

The simulation results reveal important aspects seen experimentally, including the evolution of the H_2 product species, the depletion of SiH_4 reactant, and the changes in partial pressures, wafer temperature, and polySi film thickness through the process cycle. It is interesting to note the small overshoot in wafer temperature, which leads to a profound overshoot in growth rate associated with the thermal activatation of the reaction. Also, the cooling of the wafer is considerably slower than the heat-up, a limitation for total process cycle time.

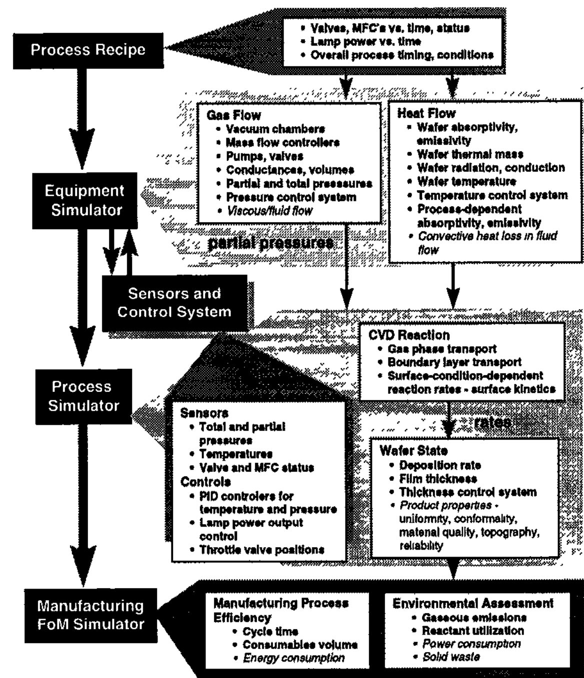

Figure 7. VisSim™–Window of the RTCVD simulator. From top to bottom on the left-hand side of the window are the equipment simulator, the process recipe and control simulator, the deposition kinetics simulator, and a display panel for overall process status. The three plots on the right-hand side are simulation outputs for film thickness (top), QMS partial pressure signals (middle), and wafer temperature and growth rate (bottom).

The physical and chemical phenomena captured in the simulator are reflected in the schematic of Fig. 7. (Aspects in progress but not yet included are represented in italics in the figure.) The process recipe includes lamp power input, valve and flow controller conditions, nominal pressure and temperature, and timing (here, the pressure at which lamp heating is initiated). The various elements determining gas flow are basically conductances and volumes, treated as for molecular flow (viscous flow corrections will be added); the simulator also represents the pressure control system behavior, comprised of a capacitance manometer measurement driving the throttle valve between reactor and pump. Heat flow elements include lamp power for radiative heating, wafer emissivity/absorptivity as a function of changing film structure (as polySi thickness increases), wafer thermal mass, conductive heat loss, and the behavior of the pyrometer-controlled lamp heating system. The CVD reaction is includes gas transport associated with reactor partial pressure and boundary layer, surface kinetics determined by H_2 product desorption, and coverage-dependent reaction probability for SiH_4 impingement on the H-covered surface. The simulator also represents the way product generation and reactant depletion modify reactor total pressure, changing the manometer reading and throttle valve position as part of the pressure control system.

Process Optimization

We have exploited this dynamic simulator capability to investigate the optimization of process recipe and equipment design for manufacturing and environmental figures-of-merit. This approach presents the opportunity to identify regimes of significant potential improvement, which can then be explored experimentally with higher efficiency. An example is given in Fig. 8, which shows the variation of SiH_4 reactant utilization and process cycle time as a function of nominal process temperature and process timing for the RTCVD polySi process. In this case, the dynamic simulator was employed to study the growth of a 2000A film, determine how much SiH_4 was used not only at temperature but through the entire process, and the time required from initial gas inlet to process termination (other definitions of process cycle time could be employed). The process recipe involves increasing pressure to a given point (conventionally 5 torr), then initiating lamp heating of the wafer. Here the process timing given on the abscissa is the pressure at which lamp heating is initiated.

The results in Fig. 8 demonstrate clearly that advantages can be achieved by earlier initiation of wafer heating than conventionally practiced. By turning wafer heating when gas inlet is initiated rather than waiting until 5 torr is reached, SiH_4 utilization can be increased and process cycle time decreased substantively, especially at higher nominal reaction temperature. Higher temperature (750°C cf. 650°C) improves both figures-of-merit, benefitting manufacturing (lower consumables cost and cycle time) and also environmental impact (reduced materials consumption). PolySi material quality should not suffer significantly over this temperature range, but further work is needed to quantify this aspect of manufacturing value. We have also recognized through these simulations that other process changes generate more complex returns: reduced flow rate also enhances SiH_4 utilization, but lengthens process cycle time, thereby involving tradeoffs between different figures-of-merit. Such situations suggest more complex process recipes which further optimize these tradeoffs, but issues of process controllability then enter the picture. In any case, by integrating elements which reflect dynamic behavior at the system level, these simulation capabilities promise substantial advantage for engineering design in CVD systems.

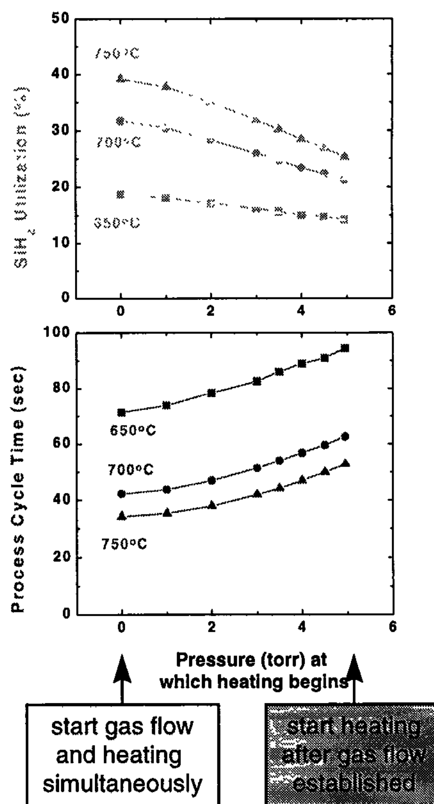

Figure 8. Effect of process timing and process temperature on materials utilization efficiency (top panel) and process cycle time (bottom panel) as a function of process recipe timing, i.e., the point at which lamp heating of the wafer begins.

Process Control

Run-to-run comparisons of equipment, process, and wafer state behavior indicated by mass spec data suggests run-to-run equipment drifts and trends in statistical reproducibility. The use of mass spec for thickness metrology has been extended to estimating polySi film thicknesses on product wafers after gate poly deposition where *ex-situ* film thickness measurements are impractical. PolySi was deposited onto 13 product wafers without varying the RTCVD process used (650°C wafer temperature, 30 sec deposition time, 5 torr total pressure, 300 sccm 10% SiH_4/Ar). Time-integrated H_2^+ data was used to estimate film thickness, as shown in Figs. 3 and 4. This exercise resulted in detection of a drift in deposited thickness with each subsequent run, but the data shown in Fig. 9 could not be used alone to determine the origin of fault. Time-dependent data of the carrier gas, Ar, provides a measurement of reactant flow throughout the process cycle. As shown in Fig. 9, following the variations in source gas flow indicates the source of the thickness drift fault. In this case, a gas flow system fault, instead of a temperature/lamp power control-loop fault, led to the drift in polySi thickness. Another possible source of thickness variation from run-to-run was a variation in deposition cycle time, but an analysis of the H_2 production throughout each run (Fig. 9) indicates that no apparent variation in deposition cycle width occurred.

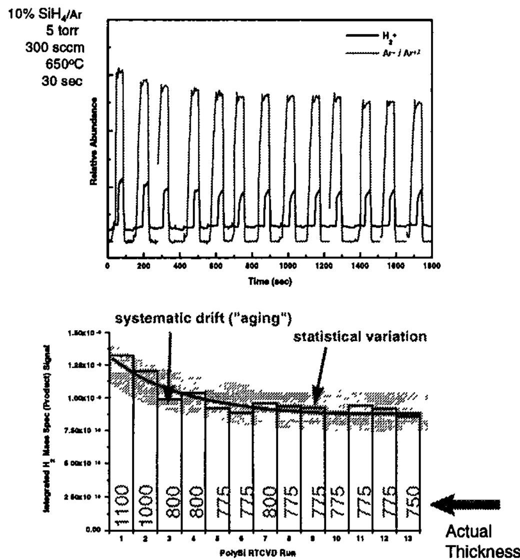

Figure 9. Equipment fault (drift) detection using fault classification (gas flow system fault) through time-dependent mass spec data (top) and using in-situ thickness metrology (time-integrated mass spec data) during polySi RTCVD on device wafers (bottom). Run-to-run estimated thickness values (750-1100Å) are listed in (bottom).

The complete decision-making process for process control, including course correction and fault management, is particularly challenging in the area of fault classification and prognosis. Significantly more sophisticated methodologies will be needed to systematically implement such decisions. Fortunately, these are needed for manufacturing technology in the future, in synergism with the possibility that sensors can enhance the drive to build in reliability. And to the experienced engineer, the sensor signatures themselves already facilitate significant insight into process and equipment performance, with benefit to reliability.

Conclusions

In-situ and real-time sensors provide profound possibilities in terms of early learning for building in reliability. First, chemical sensors reveal fundamental mechanisms in processes, so that reliability failure mode origins may be better distinguished and process windows for integrated sequences understood. Second, sensors convey a crucial basis for early identification of process drift and error, so that process sequences may be controlled to maintain established reliability expectations.

In order to achieve the potential benefits of process sensors, however, three things are required. Models are needed as a platform for interpretation and action; we have approached this using hierarchical, system-level descriptions of time-dependent behavior. Decision tools must then be developed so that one can infer from sensor information the origin of process drift or fault, in order to make the appropriate choice of corrective action. Finally, perhaps most challenging, it will be critical to identify the correlation between sensor information and real reliability consequences, so that the early sensor learning constitutes a genuine ability to predict reliability. For this, substantial effort must be devoted to integrating the two sets of data, to analyzing their correlations adequately, and if possible to continuously refine the representation of these correlations as additional process sensor and reliability data emerges from the factory.

Acknowledgements

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11. VisSim™, available from Visual Solutions, Inc. 487 Groton Road, Westford, MA 01886 (508) 392-0100, flexwire@vissol.com, htttp://www.vissim.com/.