ABSTRACT

Smith, Robert Merrill. Real-Time Control of Polysilicon Deposition in Single-Wafer Rapid Thermal Chemical Vapor Deposition Furnaces. (Under the direction of Dr. F. Yates Sorrell)

This thesis describes the development of a real-time control system for depositing polysilicon films on silicon wafers by means of rapid thermal chemical vapor deposition. Results are presented which characterize the ability of the control system to deposit films of an average desired thickness and predict the film’s spatial thickness distribution.

A rapid thermal chemical vapor deposition system was used to individually process wafers. During processing, a mass spectrometer monitored the chemical species present in the exhaust gases to determine the total volume of material deposited. Simultaneously, optical probes resolved the spatial temperature distribution of the wafer. The mass spectrometry and optical temperature data were combined with an Arrhenius equation to model the deposition process. Validation of the model was ex-situ. After processing, film thickness measurements were made on each wafer and compared to the computer model’s predictions.

Experimental results identified hydrogen, a by-product of the deposition reaction, as the metric for determining the total volume of polysilicon deposited. Process recipe control (today’s standard control technique) produced films varying over a range of 280 Å when repeatedly employed to deposit film’s of 900 Å. Application of the real-time control
system produced films varying a maximum of 74 Å when attempting to deposit films of average thickness ranging from 800 to 1200 Å. Modeling results predicted the thickness of the deposited film to within 20 Å at the center of the wafer. Predictions at the wafers edge were off by a maximum of 160 Å.

From the experience gained during this project, the following two recommendations are made to guide future efforts. First, the mass spectrometer’s reaction time to an event occurring in the furnace was found to be one second. Employing an optical sensor could improve control by reducing the time lag of the system. Second, designing the furnace with the necessary optical access so that the sensors can be located outside the vacuum system would greatly facilitate the accuracy and reliability of the system. This would eliminate exposure of the sensors to the high temperatures and corrosive gases present inside the furnace which can adversely affect their performance.
REAL-TIME CONTROL OF POLYSILICON DEPOSITION IN SINGLE-WAFER RAPID THERMAL CHEMICAL VAPOR DEPOSITION FURNACES

by

ROBERT MERRILL SMITH

A dissertation submitted to the Graduate Faculty of North Carolina State University in partial fulfillment of the requirements of the Degree of Doctor of Philosophy

MECHANICAL ENGINEERING

Raleigh 1998

APPROVED BY:

[Signatures of committee members]

Dr. Richard R. Johnson
Chair of Advisory Committee
DEDICATION

The education of an individual requires much more than just the efforts of the student. Long hours of study need to be complemented by a mentor--a teacher with the ability to guide, foster, and enlighten.

As my formal education concludes, I would like to take this opportunity to recognize the three most important teachers in my life. First and foremost, my parents, Merrill and Carole Smith. From my first days in school, they have always provided the support and encouragement vital to ensuring my success. The other significant educator I would like to acknowledge is Dr. Dwight W. Senser. I met Dr. Senser quite by accident and became one of his graduate students shortly after beginning my master’s degree at Purdue University. While at Purdue, Dr. Senser and I became good friends. I often sought his advice always finding it insightful and useful. Tragically, Dr. Senser was murdered on September 9, 1995. Even though I can never personally express my gratitude to him for all that he did for me, I would simply like to say thank you, Dwight.
BIOGRAPHY

In the fall of 1985, I began my collegiate studies at North Carolina State University. Upon completing my bachelor’s degree in mechanical engineering in May of 1990, I began working for The Boeing Company as a systems engineer tasked as part of a team responsible for integrating the design of Space Station Freedom. In August of 1991, I left The Boeing Company to continue my education at Purdue University. While attending Purdue, I studied the thermal sciences and completed a thesis investigating the atomization characteristics of conventional air spray paint guns and the effect atomization has on finish quality. Upon completion of my master’s degree in December of 1993, I began working for Ford Motor Company’s Scientific Research Laboratory researching techniques to improve both spray and dip coating painting processes. I returned to North Carolina State University in January of 1996 to pursue a doctoral degree in mechanical engineering. My doctoral research focused on developing a real-time control system for rapid thermal chemical vapor deposition. In December of 1998, I completed my degree and returned to work in private industry.
ACKNOWLEDGMENTS

During my studies at North Carolina State University, many people and organizations made significant contributions that helped me complete my degree. At this time, I would like to take a moment to acknowledge both the people and organizations who made my work possible.

At the top of the list, I must note the guidance and assistance of my major professor, Dr. F. Yates Sorrell. I have enjoyed working with him right from the start and sincerely appreciate all that he has done for me. Also, I would like to acknowledge the other members of my committee--Dr. Dennis E. Garoutte, Dr. Richard R. Johnson, and Dr. Kevin M. Lyons.

Financial support was provided by the University in the form of a research assistantship. Support was also provided by the University’s Advanced Electronic Materials Processing Center.

Additionally, I would like to thank Dr. John Hauser for the use of his laboratory. Both Kevin Kimberland and John Flanagan provided technical assistance that saved countless hours.

Along with the assistance provided by the University and its faculty and staff, I have had the opportunity to meet and work with many fellow students. Most notably I would like to thank Ji-Dih Hu, Simon Kelly, Nehal Desai, Eric Rying and Brian Timberlake. Their help and friendship has made my time spent here at NC State a truly enjoyable experience.
## TABLE OF CONTENTS

- List of Tables ................................................................. viii  
- List of Figures ............................................................... ix  
- List of Symbols ............................................................... xii

### CHAPTER 1 Introduction .................................................. 1

### CHAPTER 2 Literature Review .......................................... 3  
  2.1 Introduction .............................................................. 3  
  2.2 Mass Spectrometry ....................................................... 3  
  2.3 Temperature Measurement .............................................. 5  
    2.3.1 Acoustical Temperature Measurement ............................ 5  
    2.3.2 Thermal Expansion Temperature Measurement .................. 6  
    2.3.3 Optical Temperature Measurement ................................ 7  
  2.4 Process Modeling ....................................................... 9  
    2.4.1 Film Deposition ..................................................... 9  
    2.4.2 Optics of Thin Films .............................................. 10  
  2.5 Radiative Properties .................................................. 16  
  2.6 Strategies for Controlling Rapid Thermal Processing ............. 18  
    2.6.1 Process Recipe Control .......................................... 19  
    2.6.2 Real-Time Control ................................................. 19  
    2.6.3 Model Based Control ............................................. 20  
  2.7 Summary ................................................................. 22

### CHAPTER 3 Experimental Facility and Procedures ..................... 24  
  3.1 Introduction ............................................................. 24  
  3.2 Rapid Thermal Chemical Vapor Deposition Furnace .................. 24  
  3.3 Sensors ................................................................. 25  
    3.3.1 Gas Analyzer ...................................................... 26  
    3.3.2 Temperature Probes .............................................. 28  
    3.3.3 Pressure Gauges ................................................ 30  
    3.3.4 Rapid Thermal Processing System’s Sensors ..................... 31  
  3.4 Real-Time Data Acquisition System .................................. 31  
    3.4.1 Data Acquisition Software ..................................... 31  
    3.4.2 Data Acquisition Hardware .................................... 32  
    3.4.3 Data Signals ................................................... 32  
  3.5 Silicon Wafer ................................................................ 34  
  3.6 Film Thickness Measurements ......................................... 35  
  3.7 Wafer Processing Procedures ......................................... 37

### CHAPTER 4 Experimental Results ....................................... 40  
  4.1 Introduction ............................................................. 40
4.2 Mass Spectrometer ......................................................... 40
   4.2.1 Response Time .................................................. 40
   4.2.2 Repeatability Experiments .................................... 41
      4.2.2.1 Nitrogen Experiments .................................. 42
      4.2.2.2 Silane Experiments .................................... 45
   4.2.3 Mass Spectrometer Calibration Technique .................... 46
   4.2.4 Polysilicon Experiments ........................................ 48
4.3 Optical Temperature Probes .......................................... 50
4.4 Effect of Temperature on the Deposition Rate of Polysilicon .... 53
4.5 Temperature Measurement, Film Deposition, and the Optical Theory of Thin Films ............................................ 59

CHAPTER 5 Real-Time Control Applications .............................. 62
   5.1 Introduction ......................................................... 62
   5.2 Deposition Process and the Real-Time Control System .......... 62
   5.3 Real-Time Control Experiment .................................... 65
   5.4 Real-Time Control Results ....................................... 67
   5.5 Numerical Predictions ............................................ 69

CHAPTER 6 Conclusions and Recommendations ............................ 74
   6.1 Mass Spectrometer ................................................ 74
   6.2 Optical Temperature Probes ...................................... 75
   6.3 Real-Time Control Strategy ...................................... 76
   6.4 Additional Recommendations .................................... 77

LIST OF REFERENCES .......................................................... 78

APPENDICES ................................................................. 81
Appendix A ........................................................................ 82
   Fortran Program: RTCVD Control .................................. 82
   Fortran Subroutine: Wafer Grid ..................................... 84
   Fortran Subroutine: Labview Data ................................. 88
   Fortran Subroutine: Deposition Process ......................... 92
   Fortran Subroutine: Film Deposition .............................. 99
   Fortran Subroutine: Optics .......................................... 103
   Fortran Subroutine: Output ......................................... 110
Appendix B ........................................................................ 113
   LabVIEW® Program: DAQ.vi ....................................... 113
   LabVIEW® Program: Sensor Calibrate.vi ....................... 118
   LabVIEW® Program: Startup.vi ................................... 123
   LabVIEW® Program: Timer2.vi .................................... 125
Appendix C ........................................................................ 126
   Maple Program: Emissivity ......................................... 126
Appendix D ........................................................................ 130
Matlab Program: Insight.m ...................................................... 130
Matlab Subroutine: Hdrload.m .................................................. 138
Matlab Program: Massspec.m .................................................... 141
Matlab Program: Polysurf.m .................................................... 145
LIST OF TABLES

Table 3.1  Summary of the mass-to-charge ratios monitored by the mass spectrometer during processing. ................................. 33
Table 3.2  Summary of the analog signals acquired during processing. ............... 34
Table 3.3  Wafer Specifications....................................................... 34
Table 3.4  Process conditions employed while depositing polysilicon films. ....... 39
Table 4.1  Variation in the daily electron multiplier voltage setting required to maintain a \( N_2^+ \) signal of \( 2.10 \times 10^{-8} \) A. ............................ 48
LIST OF FIGURES

Figure 2.1 Emissivity of silicon over the range of temperatures and wavelengths of interest for rapid thermal processing (from Satô, 1967). .......................... 9

Figure 2.2 Plane wave incident upon an optically smooth boundary between two homogeneous media of different refractive indices. ......................... 11

Figure 2.3 Graphical representation of the wave vectors describing the incidence of a plane wave on the boundary of a medium with a complex refractive index. ................................. 13

Figure 2.4 Plane wave incident upon the boundary between two semi-infinite, dielectric slabs. ................................................................. 15

Figure 2.5 Plane wave incident upon a multi layer structure composed of a silicon wafer coated with two thin films. .............................. 16

Figure 2.6 Energy balance of infrared radiation incident upon a slab. ............... 18

Figure 3.1 Sketch of the rapid thermal chemical vapor deposition furnace. .......... 25

Figure 3.2 Mass spectrometry system attached to the chemical vapor deposition furnace. .......................................................... 27

Figure 3.3 Location of the pyrometers and custom built optical probe used to resolve the temperature of the wafer during processing. ................. 29

Figure 3.4 Sketch of the custom built optical probe. ........................................ 29

Figure 3.5 Incident angle of light used by the ellipsometer for measuring the thickness of polysilicon films. ......................................................... 36

Figure 3.6 Location of film thickness measurements made to characterize the thickness and spatial variation of a deposited film. ......................... 37

Figure 4.1 Time lag between an event occurring in the chemical vapor deposition chamber and recognition of that event by the mass spectrometer ($P = 5$ torr, $V_g = 300$ sccm). .................. 41

Figure 4.2 Variability in the signal intensity of nitrogen as measured by the mass spectrometer operating with the electron multiplier turned on ($P = 5$ torr, $V_g = 300$ sccm). ............................................. 43

Figure 4.3 Variability in the signal intensity of nitrogen as measured by the mass spectrometer operating with the electron multiplier turned off ($P = 5$ torr, $V_g = 300$ sccm). ............................................. 44

Figure 4.4 Effect of degassing the mass spectrometer on the measured signal intensity of nitrogen gas ($P = 5$ torr, $V_g = 300$ sccm). ......................... 46
Figure 4.5 Daily variability in the signal intensity of silane gas as measured by the mass spectrometer operating with the electron multiplier turned on ($P = 5$ torr, $\dot{V}_g = 300$ sccm). ................................. 47

Figure 4.6 Correlation between the time integrated $H_2^+$ signal measured by the mass spectrometer and the total volume of polysilicon deposited upon the wafer using process recipe control ($T = 670$ °C, $P = 5$ torr, $\dot{V}_g = 300$ sccm). ................................. 49

Figure 4.7 Variation in the thickness of deposited polysilicon films when employing process recipe control ($T = 670$ °C, $P = 5$ torr, $\dot{V}_g = 300$ sccm). .................................................. 50

Figure 4.8 Histogram of the volume of polysilicon deposited on wafers processed with a dwell time of 35 s ($T = 670$ °C, $P = 5$ torr, $\dot{V}_g = 300$ sccm). ................................. 51

Figure 4.9 Temperature measurements of the pyrometer and optical probe recorded during polysilicon deposition. .................................................. 52

Figure 4.10 Examples of the thermocouple wafer’s temperature profile during calibration of the pyrometer and optical probe. .................................................. 54

Figure 4.11 Repeatability of the thermocouple wafer’s data used to calibrate the pyrometer and optical probes. .................................................. 54

Figure 4.12 The effect of temperature on the volume of polysilicon deposited ($P = 5$ torr, $\dot{V}_g = 300$ sccm, dwell time = 35 s). ................................. 55

Figure 4.13 Plot of the Arrhenius equation relating temperature to the deposition rate of polysilicon. .................................................. 56

Figure 4.14 Profiles of deposited polysilicon films for wafers processed with dwell times varying from 5 to 65 s ($T = 670$ °C, $P = 5$ torr, $\dot{V}_g = 300$ sccm). ................................. 57

Figure 4.15 Mass spectrometer $H_2^+$ data for wafers processed with dwell times varying from 5 to 65 s ($T = 670$ °C, $P = 5$ torr, $\dot{V}_g = 300$ sccm). ....... 58

Figure 4.16 Select spectral, hemispherical emissivity curves for polysilicon deposited on a silicon wafer coated with 1000 Å of silicon dioxide. ....... 61

Figure 4.17 Spectral, blackbody emissive power curves for blackbodies of 875, 1000, and 3000 K. .................................................. 61

Figure 5.1 Throttle valve position and pressure inside the deposition chamber during processing ($P = 5$ torr, $\dot{V}_g = 300$ sccm). .................................................. 63

Figure 5.2 Wafer temperature during processing as measured by the pyrometer ($T = 650$ °C, $\dot{V}_g = 300$ sccm). .................................................. 63

Figure 5.3 $H_2^+$ signal measured by the mass spectrometer during processing. ....... 64
Figure 5.4  Si\(^+\) and N\(_2\)^{+} signals measured by the mass spectrometer during processing. ................................................................. 65

Figure 5.5  Deposition correlations relating the volume of polysilicon deposited to the H\(_2\)^{+} signal used to control processing in real-time (T = 670 °C, P = 5 torr, \(\dot{V}_g = 300\) sccm). ......................................................... 67

Figure 5.6  Real-time control system’s ability to deposit a film of a desired, average thickness (T = 670 °C, P = 5 torr, \(\dot{V}_g = 300\) sccm). ................. 69

Figure 5.7  Ability of the process recipe and real-time control strategies to repeatedly deposit films of the same average thickness. ................. 70

Figure 5.8  A comparison of deposited polysilicon film thickness data with profiles predicted using the real-time control system. ................. 72

Figure 5.9  Spatial and temporal variation of the wafer’s emissivity during the deposition of polysilicon. ......................................................... 73
# LIST OF SYMBOLS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \vec{a} )</td>
<td>attenuation vector</td>
</tr>
<tr>
<td>A</td>
<td>ampere</td>
</tr>
<tr>
<td>( \AA )</td>
<td>angstrom</td>
</tr>
<tr>
<td>amu</td>
<td>atomic mass unit</td>
</tr>
<tr>
<td>APC</td>
<td>advanced process control</td>
</tr>
<tr>
<td>( \text{Ar}^+ )</td>
<td>argon</td>
</tr>
<tr>
<td>( \text{Ar}^{++} )</td>
<td>argon</td>
</tr>
<tr>
<td>( c )</td>
<td>speed of light</td>
</tr>
<tr>
<td>( c_0 )</td>
<td>speed of light in a vacuum</td>
</tr>
<tr>
<td>C</td>
<td>deposition constant for the Arrhenius equation</td>
</tr>
<tr>
<td>( ^\circ \text{C} )</td>
<td>degrees Celsius</td>
</tr>
<tr>
<td>d</td>
<td>length</td>
</tr>
<tr>
<td>( D_0 )</td>
<td>initial diameter of the wafer</td>
</tr>
<tr>
<td>( \vec{E} )</td>
<td>electric field vector</td>
</tr>
<tr>
<td>( E_a )</td>
<td>activation energy of the Arrhenius equation</td>
</tr>
<tr>
<td>( E_{b\lambda} )</td>
<td>spectral, blackbody emissive power</td>
</tr>
<tr>
<td>( E_\lambda )</td>
<td>spectral emissive power</td>
</tr>
<tr>
<td>( G_\lambda' )</td>
<td>spectral, directional irradiation</td>
</tr>
<tr>
<td>( h )</td>
<td>Planck’s constant</td>
</tr>
<tr>
<td>( \vec{H} )</td>
<td>magnetic field vector</td>
</tr>
<tr>
<td>Hz</td>
<td>hertz</td>
</tr>
<tr>
<td>( \text{H}_2^+ )</td>
<td>hydrogen</td>
</tr>
<tr>
<td>( \text{H}_2\text{O}^+ )</td>
<td>water</td>
</tr>
<tr>
<td>( I_\lambda )</td>
<td>spectral intensity</td>
</tr>
<tr>
<td>( I_{b\lambda} )</td>
<td>spectral, blackbody intensity</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>J</td>
<td>Joule</td>
</tr>
<tr>
<td>k</td>
<td>Boltzmann’s constant</td>
</tr>
<tr>
<td>k₀</td>
<td>vacuum wave number</td>
</tr>
<tr>
<td>ℎ</td>
<td>wave vector</td>
</tr>
<tr>
<td>ℎₖ</td>
<td>complex wave vector</td>
</tr>
<tr>
<td>K</td>
<td>degrees Kelvin</td>
</tr>
<tr>
<td>m</td>
<td>meter</td>
</tr>
<tr>
<td>M</td>
<td>matrix</td>
</tr>
<tr>
<td>n</td>
<td>refractive index</td>
</tr>
<tr>
<td>nₖ</td>
<td>complex refractive index</td>
</tr>
<tr>
<td>N₂⁺</td>
<td>nitrogen</td>
</tr>
<tr>
<td>P</td>
<td>pressure</td>
</tr>
<tr>
<td>r²</td>
<td>coefficient of linear correlation</td>
</tr>
<tr>
<td>r</td>
<td>spatial position vector</td>
</tr>
<tr>
<td>Rₜ</td>
<td>universal gas constant</td>
</tr>
<tr>
<td>RTCVD</td>
<td>rapid thermal chemical vapor deposition</td>
</tr>
<tr>
<td>RTP</td>
<td>rapid thermal processing</td>
</tr>
<tr>
<td>s</td>
<td>second</td>
</tr>
<tr>
<td>ᵃᵢ</td>
<td>direction vector pointing toward the surface</td>
</tr>
<tr>
<td>ᵃₒ</td>
<td>direction vector pointing away from the surface</td>
</tr>
<tr>
<td>sccm</td>
<td>standard cubic centimeters per minute</td>
</tr>
<tr>
<td>Si⁺</td>
<td>silicon</td>
</tr>
<tr>
<td>SiH⁺</td>
<td>cracking pattern of silane</td>
</tr>
<tr>
<td>SiH₂⁺</td>
<td>cracking pattern of silane</td>
</tr>
<tr>
<td>SiH₃⁺</td>
<td>cracking pattern of silane</td>
</tr>
<tr>
<td>SiH₄⁺</td>
<td>silane</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>-----------------</td>
<td>--------------------------------------------------</td>
</tr>
<tr>
<td>Si$_2$H$_6$</td>
<td>disilane</td>
</tr>
<tr>
<td>[$\cdot$Si(NH$_2$)$_3$]</td>
<td>triaminosilane radical</td>
</tr>
<tr>
<td>SPC</td>
<td>statistical process control</td>
</tr>
<tr>
<td>$T$</td>
<td>temperature</td>
</tr>
<tr>
<td>$T_f$</td>
<td>final temperature of the wafer</td>
</tr>
<tr>
<td>$T_0$</td>
<td>initial temperature of the wafer</td>
</tr>
<tr>
<td>$u$</td>
<td>film deposition rate of the Arrhenius equation</td>
</tr>
<tr>
<td>$V$</td>
<td>volts</td>
</tr>
<tr>
<td>$V_g$</td>
<td>volume flow rate of gas</td>
</tr>
<tr>
<td>W</td>
<td>Watt</td>
</tr>
<tr>
<td>$Y$</td>
<td>coefficient used for calculating reflectance</td>
</tr>
<tr>
<td>$\alpha'_{\lambda}$</td>
<td>spectral, directional absorptivity</td>
</tr>
<tr>
<td>$\alpha_{th}$</td>
<td>thermal expansion coefficient</td>
</tr>
<tr>
<td>$\beta$</td>
<td>coefficient used for calculating reflectance</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>angle</td>
</tr>
<tr>
<td>$\delta$</td>
<td>change in the wafer’s diameter</td>
</tr>
<tr>
<td>$\varepsilon_{\lambda}$</td>
<td>spectral, hemispherical emissivity</td>
</tr>
<tr>
<td>$\varepsilon'_{\lambda}$</td>
<td>spectral, directional emissivity</td>
</tr>
<tr>
<td>$\theta$</td>
<td>angle</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>wavelength</td>
</tr>
<tr>
<td>$\vartheta$</td>
<td>coordinate system axis</td>
</tr>
<tr>
<td>$\rho'_{\lambda}$</td>
<td>spectral, directional-hemispherical reflectivity</td>
</tr>
<tr>
<td>$\rho'<em>{\lambda, \pi}$ and $\rho'</em>{\lambda, \sigma}$</td>
<td>spectral, directional-hemispherical reflection coefficients</td>
</tr>
<tr>
<td>$\tau'<em>{\lambda, \pi}$ and $\tau'</em>{\lambda, \sigma}$</td>
<td>spectral, directional-hemispherical transmission coefficients</td>
</tr>
<tr>
<td>$\phi$</td>
<td>angle</td>
</tr>
<tr>
<td>$\psi$</td>
<td>angle</td>
</tr>
<tr>
<td>$\omega$</td>
<td>frequency</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>Ω</td>
<td>ohms</td>
</tr>
</tbody>
</table>
CHAPTER 1 INTRODUCTION

In the manufacturing of semiconductor devices, the ability to produce a thin film of uniform thickness across the entire surface of a wafer is a critical step. Factors such as the diameter of the wafer and the dimension of circuits to be created on the wafer set the tolerance for film uniformity. In addition to wafer diameter and circuit dimensions, dopant profiles must also be considered when selecting a thin film processing technique. Existing dopant profiles can easily be destroyed or damaged by molecular diffusion if the temperature of the wafer is elevated too high or for too long a period of time. The ideal thin film deposition technique would be capable of quickly producing a uniform thin film across the entire surface of the wafer while raising the temperature of the wafer as little as possible.

One process that shows considerable promise for producing high quality thin films is rapid thermal chemical vapor deposition (RTCVD). This processing technique has been demonstrated in the laboratory to produce very thin, high quality films while elevating the temperature of the wafer for only a short period of time, leaving any existing dopant profiles intact. However, current rapid thermal processing (RTP) tools lack adequate thermal control capability to meet future processing tolerances. Today’s control strategies are based upon process recipes and statistical process control (SPC). In practice, the tool is operated according to a process recipe which is derived from past experience. After processing, measurements are made on each wafer to determine the thickness of the deposited films. Statistical analysis is then conducted to determine if the tool has been operating within acceptable limits or if corrective action must be taken to alter its performance. This type of control strategy is reactive by nature, and it does not provide information on the best course of action to take for correcting a problem. As such, process recipe control is not expected to be viable in the future when fewer numbers of identical wafers are processed and smaller devices are constructed, each requiring greater control.

A proactive control system is needed if rapid thermal chemical vapor deposition is to be a viable manufacturing technique in the future. Ideally, any new control system would
provide better thermal control as well as a detailed analysis of the state of the deposition process. This type of control has been defined in The National Technology Roadmap for Semiconductors (Semiconductor Industry Association 1994 and 1997) as advanced process control (APC).

The goal of this work is to develop an integrated system incorporating multiple sensors monitoring key process parameters with a data acquisition system. A computer model of the deposition process is also integrated to create an advanced process control system. Specific objectives include the following. First, outfit a rapid thermal chemical vapor deposition chamber with the sensors necessary to monitor all vital process parameters. Second, develop a data acquisition system capable of acquiring all of the essential process data in real-time. Finally, develop a computational model capable of simulating the deposition process and predicting the thickness profile of the deposited film.

The remainder of this thesis is organized as follows. Chapter two reviews the literature relevant to this research project. The experimental equipment and processing procedures developed for this project are detailed in chapter three. In chapter four, experimental results are presented that characterize the two sensors crucial to the development of the real-time control system. The first sensor, a mass spectrometer, was used to monitor the chemical species present in the exhaust gases from which the rate of the deposition reaction could be determined. Concurrently, optical probes monitored infrared emissions from the wafer to determine its spatial temperature distribution. Once the performance of the mass spectrometer and optical probes have been defined, data are presented in chapter five that defines the ability of the integrated control system (sensor, data acquisition system, and computer model) to deposit a polysilicon film of a desired thickness by means of rapid thermal chemical vapor deposition. In chapter six, the thesis is concluded with a summary of the major findings and recommendations of how the real-time control system might be improved.
CHAPTER 2 LITERATURE REVIEW

2.1 Introduction

Rapid thermal chemical vapor deposition is a thin film deposition technique used in the manufacturing of semiconductor devices. Rapid thermal processing of thin films provides specific benefits over other processing techniques. For example, wafers can be processed quickly (typically less than 60 s per wafer) which preserves existing dopant profiles. The process is generally employed at the beginning of the device manufacturing sequence to deposit high quality, defect free, uniformly thick films, such as insulating oxides or polysilicon, from which gate devices can be constructed.

While rapid thermal chemical vapor deposition is able to achieve the thermal control needed to meet current manufacturing requirements, larger diameter wafers and future circuit designs utilizing shallower junctions will require more precise temperature control. Development of noninvasive, nondestructive sensing techniques capable of generating real-time data from which control decisions can be made during processing is essential to develop the full potential of this manufacturing technique. The remainder of this chapter focuses on reviewing sensors and analytical models which will be combined and integrated into a real-time control system for rapid thermal chemical vapor deposition.

2.2 Mass Spectrometry

Mass spectrometry has been widely used as a gas analysis tool for leak detection in ultra high vacuum systems. However, increasing competition and escalating production costs have renewed interest in mass spectrometry and has lead to several studies investigating the use of the instrument as a real-time diagnostic sensor.

One such study is the work of Buckley (1993) who investigated the use of quadrupole mass spectrometry as a fault detection tool for identifying contaminates within vacuum systems. Müller (1993) also studied the use of a quadrupole mass spectrometer as a process control instrument for the sputtering deposition process. In his study, Müller found that quadrupole mass spectrometry could be used to accurately monitor impurity
levels of chemical species such as oxygen and water, which are released from the walls of the chamber during processing.

Rubloff et al. (1996) took the application of quadrupole mass spectrometry one step further investigating the use of the instrument as a real-time chemical sensor for monitoring the deposition of polysilicon in a rapid thermal chemical vapor deposition furnace. In his study, Rubloff located the mass spectrometer downstream of the deposition furnace in the exhaust gas line in order to monitor the products of the deposition reaction. To reduce the pressure of the exhaust gases (~5 torr) to a pressure where the mass spectrometer could operate (<10^{-4} torr), a two stage differentially pumped vacuum system was used. During processing, a mixture of silane and argon gas, 10% silane and 90% argon by volume, was pumped through the system. Results indicated that the quantity of hydrogen generated, a by-product of the deposition reaction (Eq. 2.1), is directly proportional to the total polysilicon deposited.

\[ SiH_4(g) \rightarrow Si(s) + 2H_2(g) \] (2.1)

In a similar study, Greve et al. (1996) investigated the use of quadrupole mass spectrometry as the primary sensor of a multivariable, real-time control system for depositing silicon nitride films by means of plasma enhanced chemical vapor deposition (PECVD). During processing, Greve used the mass spectrometer to monitor the concentrations of molecular hydrogen (amu 2) and ammonia (amu 16) present in the exhaust gases. Additionally, the direct current bias of the electrode was also monitored. This data were then input into a control algorithm which optimized the flow rates of silane and ammonia as well as determined the power setting for the next time step. Using this approach, Greve found that the multivariable control strategy, based partially upon the data collected by the mass spectrometer, improved the reproducibility of the process relative process recipe control, the most widely practiced control strategy used today.

Continuing the work of Greve, Knight et al. (1997) changed the chemical species monitored by the mass spectrometer from hydrogen and ammonia to disilane \((Si_2H_6, \text{amu})\)
60) and triaminosilane radical ([\(\text{Si(NH}_2\text{)}_3\)], amu 76). This was done for two reasons. First, by controlling the concentration levels of disilane and triaminosilane radical, the quality of the deposited film could be improved. Second, the signal levels of both disilane and triaminosilane radical were significantly lower than hydrogen or ammonia. By employing a more sensitive mass spectrometer than previously used by Greve, Knight was able to monitor these species. Like Greve before, Knight also found the real-time control strategy improved the reproducibility of the process relative to process recipe based control.

2.3 Temperature Measurement

Rapid thermal chemical vapor deposition is a semiconductor manufacturing technique requiring accurate temperature control across the entire surface of the wafer to within a few degrees Celsius in order to deposit a uniformly thick film. Ideally, any temperature probe designed for use with this process would gather data without effecting the temperature uniformity of the wafer. Several types of temperature probes have been developed and applied to the process. Examples include those of the acoustic type, those based on thermal expansion, and optical techniques. Both the acoustic and thermal expansion techniques have been shown to make accurate measurements. However, they are limited to making spatially averaged temperature measurements and require equipment to be placed inside the furnace. Optical probes provide the capability to make non-intrusive, localized temperature measurements from which the spatial temperature distribution of the wafer can be predicted.

2.3.1 Acoustical Temperature Measurement

Acoustical temperature measurements of silicon wafers have been made by passing acoustical waves through the wafer during processing and measuring the time required for the wave to travel between two points. To do this, the quartz rods which support the wafer were used as emitters and receivers for the sound waves. The virtues of this technique included: 1) insensitivity to the surface properties (optical and metrological) of the wafer,
2), the measurements were not effected by the reactive gases in the chamber, and 3) the technique did not require any special wafer preparation.

Using acoustical temperature measurements, Degertekin et al. (1993) was able to measure wafer temperatures ranging from 20 to 1000 °C during processing with a resolution of ±1 °C. By employing several quartz rods to support the wafer, Degertekin acquired several temperature readings simultaneously from which a map of the wafer’s temperature distribution was generated. The limitations of this technique were that it only measured the spatially averaged temperature of the wafer between the emitter and receiver, additional measurements required placing addition equipment inside the furnace.

2.3.2 Thermal Expansion Temperature Measurement

Peuse and Rosekrans (1993) have also developed a technique for measuring temperature during processing that does not require any special calibration procedures or depend upon the surface properties of the wafer. The technique is based upon the concept of thermal expansion. As the wafer is heated, it expands in direct proportion to the temperature dependent thermal expansion coefficient of silicon. Measurements of the wafer’s diameter are made during processing by an optical micrometer. Measuring the initial temperature and diameter of the wafer prior to processing, Eq. 2.2 can then be used to calculate the temperature of the wafer during processing, where \( \delta \) is the change in the wafer’s diameter, \( D_0 \) is the initial diameter of the wafer, \( T_0 \) is the initial temperature of the wafer, \( T_f \) is the final temperature of the wafer, and \( \alpha_{th}(T) \) is the temperature dependent thermal expansion coefficient of silicon.

\[
\delta = D_0 \exp \left\{ \int_{T_0}^{T_f} \alpha_{th}(T) - D_0 \right\}
\]  

The laser micrometer used by Peuse and Rosekrans had a resolution of 0.25 μm. For a 200 mm diameter wafer, the resolution of the optical micrometer translates into a temperature resolution of 0.3 °C. Upon completion of their study, Peuse and Rosekrans reported that while the technique can be used to make accurate, diametrically averaged temperature measurements, the complexity of the equipment required to obtain those
measurements with a resolution less than one-half a degree Celsius greatly exceeded initial expectations.

2.3.3 Optical Temperature Measurement

Optical temperature probes commonly termed pyrometers or radiation thermometers infer temperature by measuring the infrared radiation an object emits. In practice, pyrometers frequently only monitor a single wavelength or narrow band of wavelengths. Assuming the emissivity of the object does not vary appreciably over the wavelengths monitored, the temperature of the object can be computed from emission measurements, Öztürk et al. (1991) and Sorrell and Gyurcsik (1993).

Planck’s law defines the spectral emissive power distribution of a blackbody surrounded by a transparent medium with a constant refractive index, see Eq. 2.3 where $E_{b\lambda}(T, \lambda)$ is the spectral blackbody emissive power, $T$ is absolute temperature, $\lambda$ is wavelength, $h$ is Planck’s constant, $c_0$ is the speed of light in a vacuum, $n$ is the refractive index, and $k$ is Boltzmann’s constant.

$$E_{b\lambda}(T, \lambda) = \frac{2\pi hc_0^2}{n^2\lambda^5 \left[e^{hc_0/n\lambda kT} - 1\right]} \tag{2.3}$$

A blackbody is an idealized body that emits the maximum possible energy at each wavelength. All real bodies emit less energy than a blackbody at the same temperature. For an opaque surface, the ratio of the actual spectral emissive power of the surface divided by the spectral emissive power of a black surface at the same temperature is defined as the spectral, hemispherical emissivity, Eq. 2.4. Assuming the emissivity of the surface in question is known, then Eq. 2.3 and Eq. 2.4 can be used to calculate its temperature, Modest (1993).

$$\varepsilon_{\lambda}(T, \lambda) \equiv \frac{E_{\lambda}(T, \lambda)}{E_{b\lambda}(T, \lambda)} \tag{2.4}$$
In practice, calculating the temperature of a silicon wafer during rapid thermal chemical vapor deposition is much more difficult than simply solving Planck’s law. Other factors which affect the emissivity of the wafer in both predictable and unpredictable ways can complicate the process. One such factor is surface roughness. Changes in the surface roughness of the wafer produce unpredictable variations in emissivity. Tight tolerances must be maintained on the surface finish of each wafer to avoid this problem. Silicon also exhibits temperature and wavelength dependent emissivity which can be problematic under certain operating conditions (Öztürk, 1991). Furthermore, the emissivity of a wafer can be altered by a deposited film. Optical models derived from Maxwell’s macroscopic theory of electromagnetic radiation are commonly used to predict emissivity changes resulting from thin film deposition. Finally, additional problems can also be encountered if little consideration is given to temperature measurement during the design of a deposition furnace. Poorly designed systems can result in stray radiation originating from the wafer, the lamp bank, or reflections off the chamber walls skewing the measurements of pyrometers (DeWitt, 1997). Ideally, only radiation emitted from the particular measurement location of interest on the wafer would be measured by the pyrometer.

As mentioned above, silicon exhibits temperature and wavelength dependent emissivity. Satô (1967) conducted a classic study which investigated the emissivity of silicon over a wide range of temperatures and wavelengths. The portion of Satô’s work which covers the range of temperatures and wavelengths of interest in rapid thermal processing is plotted in Fig. 2.1. Polysilicon deposition generally occurs from 600 to 750 °C. Over this range of temperatures, Satô found the emissivity of silicon to be independent of temperature. However, below 600 °C, the emissivity of silicon can vary appreciably, adding to the difficulty of resolving the temperature of the wafer while it is being heated to the target processing temperature. Further inspection of Fig. 2.1 also reveals that from 2 to 15 μm the emissivity of silicon is independent of wavelength. In light of these results, careful selection of the wavelength or wavelengths monitored by the pyrometers can eliminate the need to factor the variables temperature or wavelength into temperature calculations.
Figure 2.1 Emissivity of silicon over the range of temperatures and wavelengths of interest for rapid thermal processing (from Satō, 1967).

2.4 Process Modeling

During rapid thermal processing, several events are occurring simultaneously. For example, radiative heating of the wafer occurs in conjunction with film deposition and changes in the optical properties of the wafer. Developing a control system for rapid thermal processing will require accurate temperature control of the wafer throughout the entire deposition process. Both the kinetic theory of gases and the optical theory of thin films will be used in the control system to account for changes in the optical properties of the wafer which in turn effect temperature measurements. The basics of both the kinetic theory of gases and the optical theory of thin films are described below.

2.4.1 Film Deposition

Rapid thermal chemical vapor deposition is characterized by the formation of a thin film upon a substrate by means of a temperature driven surface chemical reaction. During processing, thermal radiation is used to raise the temperature of the wafer. Above the
minimum reaction temperature, a chemical reaction occurs producing deposition. Experimental observations have shown that the rate of deposition is directly proportional to the temperature of the wafer.

A theoretical explanation for thermally driven deposition is given by the kinetic theory of gases which states that in any system a distribution of kinetic energy exists. Molecules with kinetic energy greater than the minimum or activation energy are capable of reacting. Increasing the temperature of the system increases the kinetic energy of the molecules resulting in a faster reaction rate. Mathematically a thermal deposition reaction can be modeled by the Arrhenius equation, Eq. 2.5, where \( u \) is the rate of deposition, \( E_a \) the activation energy, \( T \) the absolute temperature of the substrate, \( C \) a proportionality constant, and \( R_u \) the universal gas constant (Brady and Humiston, 1982).

\[
u = C e^{E_a/(R_uT)}\]  

(2.5)

2.4.2 Optics of Thin Films

Optical temperature probes operate upon the principle that the temperature of an object is proportional to its infrared emissions and emissivity. In the case of rapid thermal chemical vapor deposition, the emissivity of the wafer varies with the thickness of the deposited film. The constantly varying emissivity of the wafer highlights the difficulty of making accurate temperature measurements using infrared optics during chemical vapor deposition. Changes in the emissivity of the wafer can be predicted using Maxwell’s classical theory of electromagnetic radiation. Beginning with Maxwell’s equations, the Fresnel equations are derived for two cases. In the first, a plane wave propagating through a non-absorbing medium is incident upon an absorbing medium. The derivation is then extended to the more general case of a plane wave incident upon a multi film structure on a semi-infinite medium.

The following discussion is intended to introduce the reader to the optical theory of thin films and draw attention to its applications in regards to the current research. As such, a thorough development of all the mathematics involved is beyond the scope of this work.
A complete mathematical development of the subject matter can be found by referencing either Stone (1963) or Hecht (1987).

To begin, consider a monochromatic wave of light incident upon an optically smooth boundary between two media of different refractive indices. As the electromagnetic wave crosses the interface, part of the incident wave will be reflected while the remainder will be transmitted into the second medium. This situation is depicted graphically in Fig. 2.2. Mathematically this phenomenon is described by Maxwell’s equations (Eqs. 2.6) where $E$ represents the electric field, $H$ the magnetic field, $n_c$ the complex refractive index, and $k_0$, the vacuum wave number, equals the frequency of the field divided by the speed of light, $k_0 = \frac{\omega}{c}$.

Figure 2.2  Plane wave incident upon an optically smooth boundary between two homogeneous media of different refractive indices.
If the incident wave is assumed to be a plane wave for the purpose of simplifying the mathematics, the wave will propagate through the non-absorbing medium unchanged until it reaches the boundary between the two media. If no restrictions are placed upon the refractive index of the second medium, meaning it may be complex representing an absorbing material, the following two boundary conditions must be satisfied: 1) the components of \( n_c^2 \vec{E} \) or of \( \vec{H} \) in the direction of the vector \( \vec{V} \) must be continuous across the boundary (Eqs. 2.7), and 2) the tangential components, components parallel to the boundary, of the electric and magnetic fields must also be continuous across the boundary (Eqs. 2.8).

\[
\begin{align*}
\n_c^2 (\vec{E}_1 \cdot \vec{V}) &= n_c^2 (\vec{E}_2 \cdot \vec{V}) \\
\vec{H}_1 \cdot \vec{V} &= \vec{H}_2 \cdot \vec{V} \\
\vec{E}_1 \times \vec{V} &= \vec{E}_2 \times \vec{V} \\
\vec{H}_1 \times \vec{V} &= \vec{H}_2 \times \vec{V}
\end{align*}
\]

The general solution of Maxwell’s equations for a plane wave under these conditions is given in Eqs. 2.9 and Eqs. 2.10 where \( \vec{E}_1 \) and \( \vec{H}_1 \) represent the electric and magnetic waves in the first medium while \( \vec{E}_2 \) and \( \vec{H}_2 \) define the electric and magnetic waves in the second medium.

\[
\begin{align*}
\vec{E}_1 &= \vec{E}_t e^{ik_x \cdot r} + \vec{E}_r e^{i(k_x + ia_y) \cdot r} \\
\vec{H}_1 &= \vec{H}_t e^{ik_x \cdot r} + \vec{H}_r e^{i(k_x + ia_y) \cdot r} \\
\vec{E}_2 &= \vec{E}_t e^{i(k_x + ia_y) \cdot r} \\
\vec{H}_2 &= \vec{H}_t e^{i(k_x + ia_y) \cdot r}
\end{align*}
\]
The subscripts $i$, $r$, and $t$ designate the incident, reflected, and transmitted waves, respectively. $E_i$ delineates the amplitude of the incident wave which is assumed to be known. The vectors $\vec{k}$ and $\vec{a}$ are the wave and attenuation vectors, respectively. Both are real and components of the complex wave vector $\vec{k}_c$ where $\vec{k}_c = \vec{k} + i\vec{a}$. The vector $\vec{r}$ defines the spatial position of each wave with respect to the origin of the system, which for simplicity has been located on the boundary between the two media. The relationships between these vectors is shown graphically in Fig. 2.3.

\[
\begin{align*}
E_i + E_r + E_t &= 0 \\
H_i + H_r + H_t &= 0
\end{align*}
\]

(2.11)

\[
\begin{align*}
E_{i\pi} + E_{r\pi} &= E_{i\pi} & E_{i\sigma} + E_{r\sigma} &= E_{i\sigma} \\
H_{i\pi} + H_{r\pi} &= H_{i\pi} & H_{i\sigma} + H_{r\sigma} &= H_{i\sigma} \\
H_{i\pi} &= Y_{1\sigma} E_{i\sigma} & H_{r\pi} &= Y_{1\sigma} E_{r\sigma} & H_{i\pi} &= -Y_{2\sigma} E_{i\sigma} \\
H_{i\sigma} &= Y_{1\pi} E_{i\pi} & H_{r\sigma} &= -Y_{1\pi} E_{r\pi} & H_{i\sigma} &= Y_{2\pi} E_{i\pi}
\end{align*}
\]

(2.12)

Figure 2.3 Graphical representation of the wave vectors describing the incidence of a plane wave on the boundary of a medium with a complex refractive index.

Applying conservation of energy to the boundary conditions, Eqs. 2.11 can be developed which relates components of the electric and magnetic fields across the interface. The components of the magnetic field can then be defined in terms of the electric field as shown in Eqs. 2.12.
where

\[
Y_{1\pi} = \frac{k_0 n_1^2}{k_0} \quad Y_{2\pi} = \frac{k_0 (n_2 + ik_2)^2}{k_0 + ia_i} \\
Y_{1\sigma} = \frac{k_0}{k_0} \quad Y_{2\sigma} = \frac{k_0 + ia_i}{k_0}
\]  

(2.13)

Using Eqs. 2.11, Eqs. 2.12, and Eqs. 2.13, the spectral, directional-hemispherical reflection and transmission coefficients can then be derived as shown in Eqs. 2.14 and Eqs. 2.15 from which the spectral, directional-hemispherical reflectivity, \( \rho'_{\lambda} \), of the boundary can be computed.

\[
\rho'_{\lambda, \pi} = \frac{E_{r\pi}}{E_{i\pi}} = \frac{Y_{1\pi} Y_{2\pi}}{Y_{1\pi} + Y_{2\pi}} \\
\rho'_{\lambda, \sigma} = \frac{E_{r\sigma}}{E_{i\sigma}} = \frac{Y_{1\sigma} Y_{2\sigma}}{Y_{1\sigma} + Y_{2\sigma}}
\]  

(2.14)

\[
\tau'_{\lambda, \pi} = \frac{E_{t\pi}}{E_{i\pi}} = \frac{2Y_{1\pi}}{Y_{1\pi} + Y_{2\pi}} \\
\tau'_{\lambda, \sigma} = \frac{E_{t\sigma}}{E_{i\sigma}} = \frac{2Y_{1\sigma}}{Y_{1\sigma} + Y_{2\sigma}}
\]  

(2.15)

\[
\rho'_{\lambda} = \frac{1}{2} (|\rho'_{\lambda, \pi}|^2 + |\rho'_{\lambda, \sigma}|^2)
\]  

(2.16)

As an example of the equations just developed, consider the situation shown in Fig. 2.4 for two semi-infinite, dielectric slabs. From Snell’s law, the angle at which light is transmitted in the second medium, \( \phi \), can be related to the incident angle, \( \theta \).

\[
n_1 \sin \theta = n_2 \sin \phi
\]  

(2.17)

The \( Y \) coefficients can then be simplified as shown in Eqs. 2.18 from which the spectral, directional-hemispherical reflection coefficients, Eqs. 2.19, and the reflectivity of the boundary can be computed.

\[
Y_{1\pi} = \frac{n_1}{\cos \theta} \quad Y_{2\pi} = \frac{n_2}{\cos \phi} \\
Y_{1\sigma} = n_1 \cos \theta \quad Y_{2\sigma} = n_2 \cos \phi
\]  

(2.18)
Extending the derivation to a multi-layer structure such as multiple thin films deposited upon a silicon wafer changes the problem from an algebraic one to that of an array of algebraic equations. Consider the situation depicted in Fig. 2.5 where a plane wave is incident upon a multi-layer structure composed of two thin films upon a semi-infinite substrate. This situation is analogous to a vacuum surrounding a silicon wafer coated with silicon dioxide and polysilicon films.

Beginning with Snell’s law, Eq. 2.20, for the multi layer problem depicted above and repeatedly applying the boundary conditions at each interface, a matrix equation can be developed that relates the incident and reflected waves propagating in the vacuum to the transmitted wave in the silicon wafer, Eq. 2.21. The variable $M$ is a matrix representing the two thin films. The coefficient $\beta_{f1}$ in Eq. 2.22 is defined as $\beta_{f1} = n_{f1} k_0 \cos \psi$.

$$n_1 \sin \theta = n_{f1} \sin \psi = n_{f2} \sin \phi = n_2 \sin \gamma$$ (2.20)
Like the first example, the spectral, directional-hemispherical reflection coefficients can then be computed and are shown in Eqs. 2.23.

\[
\rho'_{\lambda, \text{12} \pi} = \frac{(a + bY_{2\pi})Y_{1\pi} - (c + dY_{2\pi})}{(a + bY_{2\pi})Y_{1\pi} + (c + dY_{2\pi})}
\]

\[
\rho'_{\lambda, \text{12} \sigma} = \frac{(a + bY_{2\sigma})Y_{1\sigma} - (c + dY_{2\sigma})}{(a + bY_{2\sigma})Y_{1\sigma} + (c + dY_{2\sigma})}
\]

2.5 Radiative Properties

As noted previously, accurate temperature control during film deposition requires the emissivity of the wafer be known. Employing the optical theory of thin films does not
directly calculate the wafer’s emissivity but instead another radiative property, reflectivity. Using the reflectivity calculated from optical theory, definitions of basic radiative properties, and an energy balance, the emissivity of the wafer can be determined.

Three basic radiative properties that are inherent to all surfaces are emissivity, absorptivity, and reflectivity. From Modest (1993), the spectral directional emissivity of a surface is defined as the ratio of the actual, spectral directional emissive power of an opaque surface divided by that of a black surface at the same temperature (Eq. 2.24). The spectral directional absorptivity of a surface, Eq. 2.25, is defined as the fraction of spectral directional irradiation absorbed divided by the total spectral directional irradiation. The last radiative property to be defined is reflectivity. Radiation theory has developed three definitions to describe reflectivity due to its dependence on both the incoming direction of radiation and the direction into which the reflected energy travels. The definition of reflectivity computed from the optical theory of thin films is the spectral, directional-hemispherical reflectivity, $\rho'_{\lambda}$. It is defined as the total reflected heat flux leaving a surface element into all directions due to spectral, directional irradiation.

$$
\varepsilon'_{\lambda}(T, \lambda, \tilde{s}_o) \equiv \frac{I_{\lambda}(T, \lambda, \tilde{s}_o)}{I_{b\lambda}(T, \lambda)}
$$

(2.24)

$$
\alpha'_{\lambda}(T, \lambda, \tilde{s}_i) \equiv \frac{G'_{\lambda, \text{abs}}}{G'_{\lambda}}
$$

(2.25)

Now that all of the basic radiative properties have been defined, an energy balance can be used to relate the emissivity of the wafer to its reflectivity. When an electromagnetic wave strikes a slab as depicted in Fig. 2.6, the wave can be reflected, absorbed, and transmitted. This situation is defined mathematically in Eq. 2.26 and Eq. 2.27. If the slab is assumed opaque, implying the transmission is zero, the energy balance can be simplified to Eq. 2.28. Employing Kirchhoff’s law, the spectral directional absorptivity is found to be equal to the spectral directional emissivity (Eq. 2.29). Substituting Kirchhoff’s law into the energy balance yields Eq. 2.30 relating the spectral directional reflectivity to the spectral directional emissivity.
Figure 2.6 Energy balance of infrared radiation incident upon a slab.

\[ G'_{\lambda} = G'_{\lambda, \text{abs}} + G'_{\lambda, \text{ref}} + G'_{\lambda, \text{tr}} \]  
\[ 1 = \alpha'_{\lambda} + \rho'_{\lambda} + \tau'_{\lambda} \]  
\[ 1 = \alpha'_{\lambda} + \rho'_{\lambda} \]  
\[ \alpha'_{\lambda} = \varepsilon'_{\lambda} \]  
\[ \varepsilon'_{\lambda} = 1 - \rho'_{\lambda} \]

### 2.6 Strategies for Controlling Rapid Thermal Processing

The need to improve the repeatability and uniformity of rapid thermal processing beyond that afforded by open loop, process recipe control has lead to numerous studies researching more advanced control techniques. The research conducted to date can broadly be classified into two categories: 1) closed loop, real-time control techniques which monitor key process variables during processing and attempt to manipulate tool parameters to produce the desired outcome, and 2) model-based approaches which develop processing strategies based upon theoretical analysis and computation modeling. In the paragraphs that follows, an overview of process recipe control is first detailed. This is followed by summaries of research efforts investigating real-time and model based control systems.
2.6.1 Process Recipe Control

Process recipe control is a technique based upon previous output. To setup a tool, a number of wafers are processed over a range of conditions. These are termed witness or monitor wafers. After processing, off-line measurements are made on each monitor wafer to characterize key attributes such as film thickness, film uniformity, or electrical properties. The processing conditions and measured wafer attributes are then compiled into a database defining the output of the tool. From the database, a set of operating conditions or process recipe is developed which define the setup of the tool. During production, monitor wafers are processed specifically for use in off-line analysis. Statistical process control is used to analyze the data from the monitor wafers and to identify out-of-tolerance results which indicate the need to modify the operation of the tool.

Efforts to improve process recipe or statistical process control have lead to enhanced statistical process control. This strategy works much the same as process recipe control but with the addition of in situ sensors. The sensors are used to gather additional data concerning the tool or wafers which can be used to update the process recipe.

Both process recipe and enhanced statistical process control are open loop, reactive control strategies requiring that at least one wafer be processed incorrectly before an unacceptable output can be identified and corrective actions initiated. A second limitation of these two control strategies is that they provide little or no information indicating what corrective action is necessary to fix the tool (Knight et al., 1997).

2.6.2 Real-Time Control

The limitations of process recipe control have led several investigators to study various closed loop control strategies. Closed loop control is fundamentally different from process recipe control in that data pertaining to the state of the process are collected in real-time. These data are then used to immediately modify the operation of the tool if necessary to ensure each wafer is processed within tolerance limits.
Two examples of such studies include the work of Rubloff et al. (1996) and Tedder et al. (1996). Both of these authors investigated real-time chemical sensing by mass spectrometry. The reaction rate of polysilicon deposited by means of rapid thermal chemical vapor deposition was resolved by monitoring the concentrations of key chemical species present in the exhaust gases. A dynamic simulation incorporating the real-time data with mathematical models of the process equipment, deposition process, and mass spectrometer. Results from the simulation were used to optimize the process recipe as well as begin a systematic study of fault detection.

Knight et al. (1997) have also developed a closed loop control system incorporating quadrupole mass spectrometry as a real-time sensor. Using the mass spectrometer chemical species concentration data, Knight applied his control strategy to the plasma enhanced chemical vapor deposition of silicon nitride. By controlling the partial pressures of specific chemical species, it was found that the electrical properties of the deposited film could be manipulated. Knight also found that his closed loop control system improved the stability of plasma enhanced deposition with regards to such common problems as a mass controller drifting out of tolerance.

A third example of real-time control is the work of Rashap et al. (1995) who applied the control strategy to reactive ion etching (plasma processing). Real-time data was collected by means of optical emission spectroscopy, which monitored the concentration of fluorine molecules, and combined with data from an inductive tap which measured the voltage applied to generate the plasma. The fluorine and voltage data were used in combination to optimize pressure and the energy level of the ions impinging upon the wafer. Results showed that the real-time control system improved the tool’s operation with regard to its etch rate. Improvements were seen in both the ability to achieve a desired etch rate and maintain that rate throughout the process.

2.6.3 Model Based Control

One problem common to open loop control of rapid thermal processing is that as deposition occurs the emissivity of the wafer changes resulting in erroneous pyrometer readings. By nature, open loop (process recipe) control has limited ability to correct for
emissivity changes because the rate of film deposition is not known or measured. Sorrell et al. (1990) attempted to improve the control of rapid thermal processing by a technique referred to as model based control. The objective of the research was to develop a computational model of an entire rapid thermal processing system including the wafer and pyrometer. Development of such a model would allow for improved temperature control by predicting the wafer’s emissivity using either an assumed or experimentally determined deposition rate. In addition to variations in emissivity affecting pyrometer measurements, corrections were also made to account for reflected light entering the pyrometer (Pettibone, 1986). Validation of the control strategy was done by modeling the depositing of polysilicon upon silicon dioxide using a target wafer temperature of 700 °C and a film deposition rate determine experimentally. Results indicated that improvements in the ability to maintain the target wafer temperature can be achieved relative to open loop control if the varying emissivity of the wafer is modeled.

Sorrell et al. (1994) further investigated model based control continuing the earlier work of correcting pyrometer readings for changes in wafer emissivity. Additional simulation results indicated that for deposition times less than 40 s the technique improved the accuracy of the pyrometer. However, for longer deposition times, emissivity correction did not result in any substantial improvement in the accuracy of pyrometer readings relative to open loop control. The reduced accuracy of the technique at later times was believed to be the result of a small difference between the actual and predicted deposition rates. Initially a small error in the predicted deposition rate does not produce a significant pyrometer error, but over time the error is compounded resulting in a significant difference between the actual and predicted thickness of the deposited film. This results in a large difference between the actual and predicted emissivity of the wafer. Simulation results showed that errors as small as 10 percent in the predicted deposition rate caused significant error in pyrometer readings at longer deposition time (~120 s).

The sensitivity of model based control to errors in the predicted deposition rate lead to the consideration of a different control strategy. The new strategy employed model based open loop control in the form of a preprogrammed, time dependent, lamp bank, power
Literature Review

22

curve designed to yield a constant temperature wafer. The power curve was predicted for
the entire deposition process based upon the expected deposition rate and resulting
changes in the wafer’s emissivity. Simulations showed that a preprogrammed power curve
was not highly sensitive to small errors in the predicted deposition rate and resulted in less
temperature variation than pyrometer correction control schemes.

2.7 Summary

Rapid thermal chemical vapor deposition has been demonstrated to be a fast and
thermally efficient technique for depositing high quality, thin films upon silicon wafers.
However, adequate control of the technique has not been achieved in terms of depositing
uniform films of a desired thickness on each wafer processed. This has limited adoption
of the technique in manufacturing applications.

A review of the literature regarding rapid thermal processing, applicable sensors, and
control strategies has shown that mass spectrometry can be used as a real-time sensor for
monitoring the process. Identification of the chemical species present in the exhaust gases
of the process can be used to monitor impurity levels in the vacuum system that effect the
quality of the deposited film as well as the rate of the deposition reaction.

Temperature control of the wafer has been the most difficult aspect of rapid thermal
chemical vapor deposition to control to date. Several sensors based on a variety of
different physical principles have been applied to the process. Experience has shown that
noninvasive infrared measurements of the wafer’s thermal emissions are the generally
preferred method for inferring the temperature of the wafer during processing. Infrared
measurements are non contact and therefore do not require equipment be placed inside the
vacuum chamber where it may adversely effect the temperature uniformity of the wafer
and must be able to withstand a hot, corrosive environment.

To correctly determine the temperature of the wafer, its emissivity must be known.
During processing, the wafer’s emissivity can vary with temperature, wavelength, and the
thickness of a deposited film. Studies have shown that over the range of temperatures
chemical vapor deposition occurs the emissivity of silicon remains constant with respect
to temperature. Careful selection of the wavelength or wavelengths monitored can also result in emissivity remaining constant with respect to wavelength. To account for the change in emissivity of the wafer caused by a depositing film, mathematical modeling must be employed. The deposition process can be modeled using the Arrhenius equation. Once the thickness of the deposited film has been computed, the emissivity of the wafer can then be predicted using formulas derived from Maxwell’s equations.

The potential benefits of using rapid thermal processing for semiconductor manufacturing have resulted in several studies investigating strategies for improving the control of the process beyond the current practice of a process recipe combined with statistical analysis. Several closed loop control systems using feedback from real-time sensors have demonstrated improved control in laboratory conditions. Alternative strategies for controlling rapid thermal chemical vapor deposition have also been investigated which derive tool operating conditions from theoretical analysis of the deposition process. Model based control employing a preprogrammed power curve for the lamp bank where consideration has been made for the changing emissivity of the wafer also can be used to improve the control of the process.
CHAPTER 3 EXPERIMENTAL FACILITY AND PROCEDURES

3.1 Introduction

An experimental facility has been built to develop a real-time control strategy for depositing polysilicon upon silicon wafers by means of rapid thermal chemical vapor deposition. The experimental facility is comprised of a furnace, sensors for monitoring essential process parameters, and a real-time data acquisition system capable of gathering data on all of the vital process parameters. In addition to the processing equipment, instrumentation for measuring the thickness and uniformity of deposited films was also used. Descriptions of the deposition chamber, sensors, real-time data acquisition system, film thickness measurement equipment, and processing procedures are detailed in this chapter.

3.2 Rapid Thermal Chemical Vapor Deposition Furnace

For this study, a rapid thermal chemical vapor deposition furnace was used for depositing polysilicon on wafers. The furnace was one module in a cluster of tools designed to investigate low thermal budget, single wafer, electronic materials processing. As part of a cluster tool, the furnace was designed to deposit both polysilicon and silicon oxide films as well as grow silicon oxide films and perform high vacuum anneal processes. To control these processes, the furnace has been equipped with temperature, pressure, and the gas flow rate control systems.

The design of the furnace consisted of a vacuum chamber, a lamp bank, and control systems. The lamp bank located at the top of the chamber as shown in Fig. 3.1 supplied energy to the system in the form of thermal radiation to heat the wafer to the desired processing temperature. The lamp bank is comprised of one dozen 2 kW tungsten halogen light bulbs arranged in a planar array. The lamps emit a maximum power of 24 kW which can yield a maximum wafer temperature of 950 °C. Measurement and control of the wafer’s temperature was achieved using two Omega model OS-G-B-WC-A5L pyrometers monitoring emissions of the wafer from 5.1 to 5.3 μm. The pyrometry data is then used in a control algorithm to modulate the power output of the lamp bank.
A MKS control valve model 253A-2-4CF-2 coupled with two MKS Baratron® manometers models 122AA-01000CD and 122AA-00010CD control the pressure and flow rate of gases through the furnace. The system is capable of developing pressures from 1 to 200 torr and flow rates ranging from 50 to 1000 sccm during processing. A more detailed description of the chemical vapor deposition furnace, its control systems, and its capabilities is provided by Bayoumi (1993), the system’s designer.

![Figure 3.1 Sketch of the rapid thermal chemical vapor deposition furnace.](image)

### 3.3 Sensors

Real-time data from a variety of sensors was recorded during processing. The sensors included a gas analyzer for measuring the concentrations of reaction products present in the exhaust gases. The temperature of the wafer was monitored using optical probes measuring the infrared radiation emitted by the wafer. The mass spectrometry and temperature data was combined with data from pressure sensors and the flow rate controller incorporated into the chemical vapor deposition tool to develop a comprehensive description on the state of the deposition process. A detailed description of each sensor is provided in the following paragraphs.
3.3.1 Gas Analyzer

The gas analyzer used for this study was a Leybold Inficon mass spectrometer model TSP TH200 (6633) with a H200M sensor head. The TH200 is a quadrupole instrument which measures the chemical species present in a gas using a three step process. First, the incoming gas is ionized by a hot cathode. The cathode emits electrons which bombard the gas molecules ionizing them. In the second step, the ionized molecules are separated by an applied potential according to their mass-to-charge ratios. Finally, the quantity of each chemical species present is determined by measuring the current discharged by each mass as the ions impact the instrument’s detector.

The Leybold mass spectrometer used in this study provided the ability to operate in two detection modes. In the first mode, the instrument used only a Faraday cup for its detector. A Faraday cup is typically a flat plate or cup shaped detector which ions impact after flowing through the instrument’s mass filter. If the signal is to weak to be measured by a Faraday cup, the instrument can operate in a second detection mode employing an electron multiplier and Faraday cup. The electron multiplier is located between the mass filter and the Faraday cup. It accelerates the ions exiting the mass filter by means of a large negative voltage, typically greater than -1 kV. This causes the ions to strike the electron multiplier and emit one or more secondary electrons. These electrons are then collected and measured by the Faraday cup. Operating with the electron multiplier on increases the sensitivity of the instrument, Leybold Inficon (1993). For a more detailed explanation of the operating theory of mass spectrometers, see O’Hanlon (1989).

Operation of the mass spectrometer requires the instrument be maintained at a pressure less than $10^{-4}$ torr. To meet this criteria, the mass spectrometer was integrated into the vacuum system shown in Fig. 3.2. The vacuum system is a two stage differentially pumped system which preforms two functions. First, the two stages work in combination to reduce the pressure of the exhaust gases to a pressure where the mass spectrometer can operate. Second, the system ensures that exhaust gases are quickly transported from the furnace to the mass spectrometer so that timely measurements of the deposition reaction can be made.
Figure 3.2 Mass spectrometry system attached to the chemical vapor deposition furnace.
The vacuum system operated by sampling a small portion of the exhaust gases from the deposition furnace through a 1 mm orifice located in the exhaust line. The pressure of the exhaust gases was reduced from 5 torr (the pressure inside the deposition chamber) to approximately 2x10^{-6} torr at the sensor head by the system’s six pumps and a metering valve. The pumps included two Leybold Turbovac 50 turbo pumps, two Alcatel 5011CP molecular drag pumps, and two Vacuubrand MZ 2C two stage diaphragm pumps. Of the two turbo pumps, only one pumped through the mass spectrometer. Assuming the turbo pumped its maximum capacity of 55 l/s at 2x10^{-6} torr while inside the deposition furnace gases flowed at 300 sccm, the percentage of the exhaust sampled by the mass spectrometer was much less than 0.1 percent.

3.3.2 Temperature Probes

A total of three optical probes were used to resolve the spatial temperature distribution of the wafer during processing. Two Omega pyrometers monitored infrared emissions from the center of the wafer while a custom built optical probe was used to monitor emissions near the edge of the wafer. All of the probes were mounted on the bottom of the furnace as shown in Fig. 3.3. From this position, the probes measured the infrared emissions from the bottom surface of the wafer.

A sketch of the custom built optical probe is shown in Fig. 3.4. The probe consisted of a lens, an optical filter, a photovoltaic detector equipped with a thermoelectric cooler, and a heat sink. To focus the radiation emitted by the wafer on the detector, a plano-convex, sapphire lens was used. Considering the distance from the wafer to the probe (~270 mm) and the diameter of the lens (7 mm), the diameter of the spot on the wafer monitored by the probe was approximately 10 mm.

Between the lens and the detector, an Optical Coating Laboratory narrow bandpass filter was used to restrict the wavelengths of radiation striking the detector to 3.720 ±0.07 μm. Radiation passing through the filter was then incident upon an EG&G Judson model J12TE2-66S-R02M indium arsenide photovoltaic photodiode. The detector is a two stage thermoelectrically-cooled unit with an active surface diameter of 1 mm and is sensitive
Experimental Facility and Procedures

Figure 3.3 Location of the pyrometers and custom built optical probe used to resolve the temperature of the wafer during processing.

Figure 3.4 Sketch of the custom built optical probe.
over the range of wavelengths from 1.0 to 3.8 \mu m. To minimize drift caused by variations in the ambient temperature and improve the sensitivity, the detector was cooled to -30 °C during operation by an EG&G Judson model TC2 thermoelectric controller coupled to a HS1-TO66-InAs-TC5 heat sink. The voltage output of the detector was amplified using an EG&G Judson PA-5 transimpedance gain preamplifier.

3.3.3 Pressure Gauges

Pressure measurements at specific locations within the mass spectrometer’s vacuum system were made during processing to ensure that the pumps were operating properly. The measurements were made using two different types of gauges and an electronic process controller.

A Granville Phillips series 275 Convectron gauge was used for measuring pressure from $10^{-3}$ to $10^4$ torr. The Convectron gauge uses both conductive and convective cooling to measure pressure over its entire range of operation. The resolution of the gauge is approximately $2 \times 10^{-3}$ torr. For this project, a Convectron gauge was located downstream of the inlet to the mass spectrometer’s vacuum system, see Fig. 3.2. In this location, the gauge monitored the pressure of gases just after entering the vacuum system.

A Granville Phillips nude ion gauge model 274028 was used to measure pressure below the operational range of the Convectron, from $4 \times 10^{-9}$ to $2 \times 10^{-2}$ torr. The ion gauge was a Bayard-Alpert type which measures pressure by creating a constant flow of electrons. The electrons collide with the gas molecules producing positive ions which are captured by a negatively charged collector. The rate of positive ion formation is proportional to the density of the gas for pressures below $10^{-2}$ torr. The Granville Phillips nude ion gauge has an accuracy of ±20%.

The nude ion gauge was located just upstream of the mass spectrometer’s sensor as shown in Fig. 3.2. In this location, the gauge monitored the pressure experienced by the sensor during processing. This ensured that variations in pressure which might effect the mass spectrometer’s results were detected.
Both the Convectron gauge and the ion gauge were connected to a Granville Phillips model 303 process controller. The controller provided the ability to monitor the pressure measured by both gauges plus degas the ion gauge, set the pressure readings of the gauges in terms of either argon or nitrogen, and generate analog signals which were recorded by the data acquisition system.

3.3.4 Rapid Thermal Processing System’s Sensors

In addition to the previously described signals, data pertaining to the pressure inside the rapid thermal processing furnace and the position of the throttle valve controlling the flow of gases through the chamber were also acquired for analysis. Both the pressure and valve position were collected from a MKS type 152 exhaust valve controller in the form of analog signals. On the deposition chamber, the exhaust valve controller was coupled to a MKS type 253 exhaust throttle valve and a MKS type 122 Baratron® 0 to 10 torr pressure transducer. The exhaust valve controller adjusted the pressure inside the deposition chamber by comparing the signal from the pressure transducer to a desired set point and then positioned the valve accordingly.

3.4 Real-Time Data Acquisition System

The development of a real-time rapid thermal processing control system required data characterizing the deposition process be acquired during processing. The data required to characterize the process included the temperature of the wafer, pressure inside the processing chamber, flow rate of the silane/argon gas mixture pumped through the chamber, and a mass spectrometry analysis of the exhaust gases. To capture all of this data, a custom designed data acquisition system was developed using National Instruments’ LabVIEW® software. A description of the data acquisition software and hardware used to acquire the real-time data is detailed below.

3.4.1 Data Acquisition Software

The acquisition of all the real-time data needed for this project presented two problems. First, communication with the various sensors would require the use of two different data acquisition boards--one serial card and one analog-to-digital (A/D) board.
Also, the sensors sampled and transmitted data at several different rates requiring each piece of data be time stamped so that temporal relations between events could be maintained.

To develop the data acquisition software needed, National Instruments’ LabVIEW® software was used. The data acquisition program created, DAQ.vi listed in Appendix B, provided the user the ability to independently set the rate of data acquisition of both the serial card and the analog board before beginning each experiment. Once initiated, data was automatically acquired from each board until the experiment was completed and the data saved to a file.

3.4.2 Data Acquisition Hardware

As noted above, communication with all of the sensors required the use of one serial and one analog data acquisition card. The serial card used was a RS-232 model AT-232/2 manufactured by National Instruments. The analog board was a ComputerBoards’ CIO-DAS1600/12 card. This is 12 bit board capable of acquiring a maximum of 16 signals simultaneously with a maximum frequency of 10 MHz. For this project, all of the signals were wired to the board in the differential mode. Differential wiring limits the maximum number of signals that can be acquired to eight but ensures that differences in the ground state of each signal’s source does not effect the data. Additionally, the board was configured in the unipolar mode measuring the voltage of each signal over the range from 0 to 10 V.

3.4.3 Data Signals

A summary of the data signals acquired during processing is listed in the following two tables. Table 3.1 tabulates the nine mass-to-charge ratios and the corresponding chemical species scanned by the mass spectrometer. These mass-to-charge ratios encompass the cracking patterns of the gases pumped into the rapid thermal chemical vapor deposition chamber as well as the products of the polysilicon deposition reaction.
Two analog pressure signals, one from the ion and one from the Convectron gauge, were acquired to monitor the mass spectrometer’s vacuum system—see Fig. 3.2 for the locations of the gauges. The signal from the ion gauge was used to monitor pressure at the mass spectrometer. Ideally, a constant pressure would be maintained at the sensor so that variations in pressure would not effect the instrument’s measurements. The Convectron gauge was incorporated into the system to monitor the pressure at the inlet of the vacuum system ensuring the system’s pumps on the bypass line were functioning properly. The temperature of the wafer was also monitored during processing by two pyrometers and one custom built optical probe. The last two analog signals acquired pertained to the processing conditions inside the deposition furnace. The position of the butterfly valve regulating gas flow through the furnace was recorded as well as the pressure inside the furnace.

<table>
<thead>
<tr>
<th>mass-to-charge ratios</th>
<th>signal description</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$H_2^+$, product of the deposition reaction</td>
</tr>
<tr>
<td>18</td>
<td>$H_2O^+$</td>
</tr>
<tr>
<td>20</td>
<td>$Ar^{++}$, cracking pattern of argon gas</td>
</tr>
<tr>
<td>28</td>
<td>$Si^+$ or $N_2^+$, nitrogen used to purge the system</td>
</tr>
<tr>
<td>29</td>
<td>$SiH^+$, cracking pattern of silane gas</td>
</tr>
<tr>
<td>30</td>
<td>$SiH_2^+$, cracking pattern of silane gas</td>
</tr>
<tr>
<td>31</td>
<td>$SiH_3^+$, cracking pattern of silane gas</td>
</tr>
<tr>
<td>32</td>
<td>$SiH_4^+$, cracking pattern of silane gas</td>
</tr>
<tr>
<td>40</td>
<td>$Ar^+$, cracking pattern of argon gas</td>
</tr>
</tbody>
</table>
In addition to the mass spectrometry data, a maximum of eight analog signals were simultaneously acquired—see Table 3.2. The analog signals included a constant 5 V signal from a Trygon model TL8-3-DV power supply. This signal was acquired to monitor the data acquisition hardware and ensure it was performing correctly.

<table>
<thead>
<tr>
<th>analog signals</th>
<th>signal descriptions</th>
</tr>
</thead>
<tbody>
<tr>
<td>power supply</td>
<td>constant voltage signal for monitoring the data acquisition hardware</td>
</tr>
<tr>
<td>ion gauge</td>
<td>pressure at the mass spectrometer</td>
</tr>
<tr>
<td>Convectron gauge</td>
<td>pressure immediately after the inlet to the mass spectrometer’s vacuum system</td>
</tr>
<tr>
<td>pyrometers</td>
<td>temperature at the center of the wafer</td>
</tr>
<tr>
<td>optical probe</td>
<td>temperature at the edge of the wafer</td>
</tr>
<tr>
<td>butterfly valve</td>
<td>position of the valve regulating flow through the rapid thermal chemical vapor deposition chamber</td>
</tr>
<tr>
<td>Baratron® manometer</td>
<td>pressure inside the rapid thermal chemical vapor deposition furnace</td>
</tr>
</tbody>
</table>

3.5 Silicon Wafers

The silicon wafers used for this project were purchased from Transition Technology International. Each of the wafers was test grade with a diameter of 100 mm. A complete list of the wafer’s specifications is given in Table 3.3.

<table>
<thead>
<tr>
<th>parameter</th>
<th>specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>diameter</td>
<td>100 mm</td>
</tr>
<tr>
<td>dopant</td>
<td>boron</td>
</tr>
<tr>
<td>flat</td>
<td>standard</td>
</tr>
<tr>
<td>grade</td>
<td>test</td>
</tr>
<tr>
<td>orientation</td>
<td>1-0-0</td>
</tr>
<tr>
<td>resistivity</td>
<td>0 - 100 Ω*cm</td>
</tr>
</tbody>
</table>
Experimental Facility and Procedures

3.6 Film Thickness Measurements

During this research, two instruments were used to measure the thickness of the deposited films. Thickness measurements of silicon dioxide (SiO$_2$) films were made using a Nanometrics NanoSpec/AFT while polysilicon films were measured using an ellipsometer. Below, a short description of each instrument is provided along with the operating setup of the instruments.

The Nanometrics resolves the thickness of a film by measuring the variation in intensity of electromagnetic waves incident upon the film. To determine a film’s thickness, the instrument scans the film from 480 to 790 nm measuring the change in intensity as a function of wavelength. The spectral fluctuation in intensity results from constructive and destructive interference of the electromagnetic waves as they travel through the film and reflect off the underlying substrate. From the spectral intensity distribution, the thickness of the deposited film can be computed.

The NanoSpec is capable of measuring silicon dioxide thicknesses from 400 to 30000 Å, deposited upon a silicon substrate, with an accuracy of two percent. For this project, 1000 Å silicon dioxide films were grown on each wafer to provide a plane of reference from which the thickness of the subsequent polysilicon film could be measured. The thickness of each silicon dioxide film was measured with the NanoSpec using a refractive index of 1.46. While the NanoSpec is also capable of measuring the thickness of polysilicon films, some of the films deposited were thinner than the NanoSpec could resolve. Therefore, an ellipsometer was used to measure the polysilicon films.

The ellipsometer used for this project was a J.A. Woollam Co. VASE (variable angle spectroscopic ellipsometer) 7000. The VASE resolves the thickness of the film by measuring the change in polarization of light reflected from the surface of a sample. Measurements are made by projecting a beam of light at various wavelengths onto the wafer specifications:

<table>
<thead>
<tr>
<th>thickness type</th>
<th>475 - 575 μm</th>
</tr>
</thead>
<tbody>
<tr>
<td>type</td>
<td>P</td>
</tr>
</tbody>
</table>

Table 3.3 Wafer Specifications.
work piece at a specific angle or angles. In the case of polysilicon, measurements were made over a range of wavelengths from 300 to 800 nm in increments of 100 nm. The light was incident on the wafer at 70° as shown in Fig. 3.5. The polarization of the reflected light measured as a function of wavelength and angle of incidence was used to compute the thickness of the deposited film. For the instrument to work properly, the wavelengths of light used to probe the film must be on the same order of magnitude as the thickness of the deposited film. This required that an estimate of the film’s thickness be known before using the instrument.

The accuracy of the VASE was not stated by the manufacturer who claims that no other technique of comparable accuracy exists with which to test the instrument. J.A. Woollam simply reported that data from their experiments closely matched results from other thin film measurement techniques such as Rutherford back scattering, transmission electron microscopy, and atomic force microscopy.

After a wafer had been processed, the thickness measurements were made at 21 points on the surface of the wafer surface as shown in Fig. 3.6 to characterize the thickness profile of the deposited film. The thickness measurements then used as input for the Matlab program *Polysurf.m*, see Appendix D, to compute the volume of film deposited. The volume deposited was later used in combination with the mass spectrometry data to develop models for predicting deposition.
3.7 Wafer Processing Procedures

To ensure the most accurate and repeatable experimental data possible, a procedure was developed for the handling and processing of the wafers. This procedure governed all aspects concerning the handling of wafers from initially receiving them to measuring the thickness of polysilicon films. A detailed description of the handling and processing procedure is provided below.

![Diagram of wafer locations](image)

**Figure 3.6** Location of film thickness measurements made to characterize the thickness and spatial variation of a deposited film.

The first task undertaken when handling a bare wafer was to scribe a number on it for identification purposes. Each wafer was then chemically cleaned in preparation for processing in the diffusion furnace. A layer of silicon dioxide was grown on each wafer using a Tylan/Tytag II diffusion furnace before depositing polysilicon. The oxide film was necessary so that the thickness of the subsequent polysilicon film could be measured. Without the oxide, the thickness of the polysilicon could not be measured because a
continuous silicon structure would have been created. Thus after the wafers were cleaned, they were processed in batches of 25 to 100 using the Tylan diffusion furnace to grow a 1000 Å layer of silicon dioxide on each wafer. Next, the Nanometrics was used to measure the thickness of each oxide film. The wafers were then chemically cleaned again and stored in a pressurized nitrogen box until transferred to the rapid thermal chemical vapor deposition tool for processing. Storage in the nitrogen box was a precautionary action designed to minimize contamination that might have occurred due to ambient sources.

Each day before any wafers were processed a start-up procedure was employed to ensure both the deposition furnace and mass spectrometer system were functioning properly. First, the ion gauge just upstream of the mass spectrometer sensor was degassed for 10 minutes and set to read pressure using argon as the reference gas. Next, the LabVIEW® program Startup.vi, see Appendix B, was run. This program automatically degasses the mass spectrometer for two minutes and then sequentially scans the charge-to-mass ratios from 1 to 100. The purpose of the charge-to-mass scans was to assess the background levels of chemical species present in the vacuum system and ensure the system was not contaminated.

Next, the mass spectrometer was calibrated. As will be shown later in the results, the sensitivity of the mass spectrometer can vary from day-to-day. The purpose of the calibration procedure was to set the voltage of the mass spectrometer’s electron multiplier so that the sensor’s sensitivity remained constant from one day to the next. To accomplish this task, the LabVIEW® program Sensor Calibrate.vi, see Appendix B, was used. This program works by sampling nitrogen at several electron multiplier voltage levels while pumping nitrogen gas through the deposition furnace at 5 torr. Various voltage levels were tested until a voltage level for that day was found that matched the target signal intensity.

Once all of the equipment had been readied, the wafers were processed in the deposition chamber one at a time over the range of operating conditions listed in Table 3.4. Between the processing of consecutive wafers, the furnace and mass spectrometer were
each purged with 200 sccm of nitrogen gas for two minutes. Once processing had been completed for the day, film thickness measurements were made as previously described.

Table 3.4  Process conditions employed while depositing polysilicon films.

<table>
<thead>
<tr>
<th>process variable</th>
<th>range of variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>wafer temperature</td>
<td>600 - 690 °C</td>
</tr>
<tr>
<td>time</td>
<td>5 - 65 s</td>
</tr>
<tr>
<td>chamber pressure</td>
<td>5 torr</td>
</tr>
</tbody>
</table>
CHAPTER 4 EXPERIMENTAL RESULTS

4.1 Introduction

In this chapter, a series of experimental results are presented for individual components of the real-time control system. These results are a precursor to the next chapter where the performance of the control system is discussed. In this chapter, the performance of both the mass spectrometer and the optical temperature probes is defined. Results are shown that define the level of control attainable by process recipe control in terms of depositing a polysilicon film of a desired thickness. An Arrhenius equation relating the deposition rate of polysilicon to temperature is also developed. Finally, the chapter concludes with a discussion explaining how the optical temperature measurements, film deposition model, and optical theory of thin films are combined to predict the emissivity of the wafer.

4.2 Mass Spectrometer

The prevailing presumptions about mass spectrometry are that neither the response time or the repeatability of the instrument is sufficient for the instrument to be used as a real-time sensor. One of the first tasks undertaken in this project was to build an experimental facility that would yield a mass spectrometer response time fast enough (~ 1 s) to warrant the instrument’s use in real-time applications. Once the desired response time had been achieved, additional experiments were conducted to establish the repeatability of the instrument under conditions that were both ideal and typical of those found during production. Results indicated that the sensitivity of the mass spectrometer varied from day-to-day. To overcome this problem, a calibration procedure was developed to improve the instrument’s repeatability. Finally, wafers were processed to assess the instrument’s ability to determine the total volume of film deposited from measurements of the chemical species present in the exhaust gases.

4.2.1 Response Time

The response time of the mass spectrometer can most easily be determined from the chronological order of two events that occur near the completion of wafer processing.
During processing once film deposition has been completed, the deposition furnace is programmed to automatically open its throttle valve, stop the flow of the silane/argon gas mixture, and begin flowing nitrogen to purge the system. By comparing the time difference between when the throttle valve opens and when the mass spectrometer detects the nitrogen, an accurate measure of the instrument’s response time can be made. The results of just such an experiment are shown in Fig. 4.1. As seen in the plot, just before 69.5 s the exhaust valve begins to open. The mass spectrometer does not sense the nitrogen purge until approximately one second later yielding a one second lag time for the instrument.

![Figure 4.1 Time lag between an event occurring in the chemical vapor deposition chamber and recognition of that event by the mass spectrometer ($P = 5$ torr, $V_g = 300$ sccm).](image)

4.2.2 Repeatability Experiments

Defining the repeatability of the mass spectrometer when used as a real-time sensor for monitoring rapid thermal chemical vapor deposition was a difficult task. Many variables of the processing technique are poorly understood and may affect the measurements of the
instrument in an unpredictable manner. For example, the temperature of the wafer varies temporally and also spatially during processing. This could cause the chemical composition of the exhaust gases to vary in an unpredictable manner if the temperature of the wafer was not adequately controlled. In order to determine the repeatability of the instrument, a series of experiments were designed that would eliminate or at least minimize as many of the process variables as possible. By flowing gas through the furnace without a wafer present and with the lamp bank turned off, the repeatability of the mass spectrometer could be analyzed without concern for the temporal and spatial variations in the exhaust gases caused by processing. Using this concept, repeatability experiments were conducted by pumping both pure nitrogen and a 10 percent silane 90 percent argon mixture (by volume) through the furnace at the same pressure (5 torr) and gas flow rate (300 sccm) as used during film deposition.

4.2.2.1 Nitrogen Experiments

The nitrogen repeatability experiments were conducted by monitoring the charge-to-mass ratio 28 while pumping only nitrogen gas through the chamber. Measurements were taken with the instrument’s electron multiplier turned both on and off. When the electron multiplier was on, measurements were taken at several voltage levels. The experiments were repeated seven times over a one month period to establish the repeatability of the instrument under ideal conditions.

The results from the experiments conducted with the electron multiplier on are shown in Fig. 4.2. From the figure, the measured signal is directly proportional to the electron multiplier’s voltage setting. Also, the signal measured at any voltage level can vary from day-to-day. To illustrate this point, consider the signal measured at a level of 1100 V on days one, two, and three. The data from day one was taken prior to processing the wafers on that day for the purpose of establishing a baseline to which future results could be compared. On day two, the nitrogen data was collected again before processing any wafers. Clearly, the intensity of the \( \text{N}_2^+ \) signals on day two was less than that of day one indicating a drop in the sensitivity of the instrument. Similar results were also found when
Experimental Results

Comparing the data from day two to day three. The findings from these first three days appear to indicate that the instrument’s sensitivity decreases with use. However, the data from days four, five, and six do not support this conclusion because the intensity of the nitrogen signal increased relative to that measured on day three. The key to understanding the instrument’s performance in light of the latest findings is to realize wafers were not processed on days three or four. Thus, the mass spectrometer was not exposed to silane from the end of day two until after the $N_2^+$ data was taken on day five. The results plotted in Fig. 4.2 suggest the instrument is highly repeatable when sampling a non-reactive gas such as nitrogen. However, flowing a corrosive, reactive gas like silane through the mass spectrometer degrades its sensitivity in direct proportion to the amount of exposure.

![Figure 4.2](image-url)

Figure 4.2 Variability in the signal intensity of nitrogen as measured by the mass spectrometer operating with the electron multiplier turned on ($P = 5$ torr, $V_g = 300$ sccm).

Nitrogen repeatability experiments were also run with the electron multiplier turned off (Faraday cup mode). Discussions with the instrument’s manufacturer, Leybold-
Inficon, indicated that the repeatability of the instrument might be improved if operated in such a manner. Investigating the performance of the instrument when operating in the Faraday cup mode was accomplished by performing a second series of nitrogen experiments. Operating with the electron multiplier turned off did not yield the desired results as shown by the data in Fig. 4.3. The instrument’s signal intensity was still degraded by exposure to silane. Furthermore, turning off the electron multiplier, which functions as a gain for the sensor, decreased the sensitivity of the instrument by approximately two orders of magnitude. For these two reasons, all other mass spectrometry data was collected with the electron multiplier turned on.

![Figure 4.3](image)

*Figure 4.3 Variability in the signal intensity of nitrogen as measured by the mass spectrometer operating with the electron multiplier turned off ($P = 5$ torr, $V_g = 300$ sccm).*

To ensure the mass spectrometer could be cleaned if contaminated while in use without being sent back to the factory, the instrument was designed with a degassing feature. Degassing raises the temperature of the instrument which in turn helps drive off
any contaminates that may have deposited. Once silane exposure was identified as degrading the instrument’s performance, degassing was explored as a means of restoring the instrument’s sensitivity. To test degassing, a series of experiments were conducted after the mass spectrometer was known to be contaminated by silane. The instrument was degassed for a total of 20 minutes. The effect of degassing was not investigated beyond 20 minutes because it was assumed that in a manufacturing environment production schedules would only allow for a degassing period of a few minutes. After 5, 10, and 20 minutes of degassing, nitrogen was pumped through the system while the signal intensity of the charge-to-mass ratio 28 was monitored at several voltage levels. The results the experiment are shown in Fig. 4.4. The data shows that degassing did not effect the sensitivity of the instrument at all. The only way found to eliminate the detrimental effects of silane exposure was to keep the instrument at the baseline pressure of the vacuum system and not flow any gases through it for a period of several days.

4.2.2.2 Silane Experiments

The nitrogen repeatability experiments investigated the performance of the mass spectrometer under ideal conditions. Nitrogen gas is neither corrosive or reactive and therefore should have little detrimental effect on the instrument. To test the instrument under conditions that would exist during wafer processing, a second set of repeatability experiments was preformed using the silane/argon gas mixture employed for depositing polysilicon. These experiments investigated the performance of the mass spectrometer when exposed to a corrosive, reactive gas.

The silane repeatability experiments were run on two separate days with the mass spectrometer operating with its electron multiplier turned on. The data from these experiments displayed in Fig. 4.5 indicate that: 1) the intensity of the measured signal is directly proportional to the voltage setting of the electron multiplier, and 2) exposure to silane decreases the sensitivity of the instrument. Thus, the mass spectrometer was found to performed in a similar fashion when measuring silane as it did when sampling nitrogen.
4.2.3 Mass Spectrometer Calibration Technique

The daily fluctuation in the sensitivity of the mass spectrometer is the instrument’s limiting characteristics in regards to employing it in a production application. Improved results might be obtained if a calibration procedure existed to compensate for any decrease in sensitivity the instrument may experience resulting from use.

The idea behind a calibration procedure was to correct for the varying sensitivity of the instrument by adjusting the voltage of its electron multiplier so that the same signal intensity for nitrogen could be maintained from day to day. By employing LabVIEW®, software was developed to calibrate the instrument. During calibration, nitrogen was pumped through the deposition chamber at the same pressure and gas flow rate as used during polysilicon deposition. All calibration experiments were conducted without a wafer present in the furnace. The LabVIEW® program, Sensor Calibrate.vi listed in Appendix B, scanned a series of five electron multiplier voltage settings and plotted the

Figure 4.4 Effect of degassing the mass spectrometer on the measured signal intensity of nitrogen gas ($P = 5$ torr, $\bar{V}_g = 300$ sccm).
recorded signal intensity of the charge-to-mass ratio 28 against the voltage level of the electron multiplier. From this data, the electron multiplier was adjusted so that the instrument maintained a constant measured signal intensity for $\text{N}_2^+$. 

![Figure 4.5 Daily variability in the signal intensity of silane gas as measured by the mass spectrometer operating with the electron multiplier turned on ($P = 5$ torr, $\dot{V}_g = 300$ sccm).](image)

To illustrate the application of the calibration program, the electron multiplier voltage settings used for the data shown in Fig. 4.2 are listed in Table 4.1. The data shows that the voltage settings required to maintain a constant nitrogen signal can easily span a 100 V range and vary unpredictably from one day to the next.
4.2.4 Polysilicon Experiments

Once the initial experiments had been completed characterizing the performance of the mass spectrometer under ideal conditions, the investigation was expanded to test the instrument’s performance during polysilicon deposition. A series of 52 wafers were processed over a three month period to determine the accuracy and repeatability with which the data collected by the mass spectrometer could be used to predict the total volume of polysilicon deposited. Each wafer was processed individually according to a process recipe which specified the deposition temperature, 670 °C, the pressure inside the deposition furnace, 5 torr, and the flow rate of gases through the furnace, 300 sccm. By holding constant the temperature, pressure, and gas flow rate, the variables for this series of experiments were the dwell time, the length of time the wafer was processed once the deposition temperature had been reached, and the variability of the instrument. To minimize variability, the calibration procedure previously described was employed each day prior to processing any wafers.

The results of the polysilicon experiments, shown in Fig. 4.6, demonstrate the correlation found between the time integrate $\text{H}_2^+$ signal measured by the mass spectrometer and the total volume of polysilicon deposited upon the wafer. Using least squares, a straight-line model correlating the two parameters was developed. The

<table>
<thead>
<tr>
<th>day</th>
<th>electron multiplier setting [V]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1087</td>
</tr>
<tr>
<td>2</td>
<td>1120</td>
</tr>
<tr>
<td>3</td>
<td>1143</td>
</tr>
<tr>
<td>4</td>
<td>1097</td>
</tr>
<tr>
<td>5</td>
<td>1099</td>
</tr>
<tr>
<td>6</td>
<td>1113</td>
</tr>
<tr>
<td>7</td>
<td>1174</td>
</tr>
</tbody>
</table>
Experimental Results

A coefficient of linear correlation, $r^2$, for the model was found to be 0.9594 indicating a strong, positive relationship between the measured $\text{H}_2^+$ signal and the volume of polysilicon deposited.

![Graph showing correlation between time integrated $\text{H}_2^+$ signal and volume of polysilicon deposited.](image)

Figure 4.6 Correlation between the time integrated $\text{H}_2^+$ signal measured by the mass spectrometer and the total volume of polysilicon deposited upon the wafer using process recipe control ($T = 670 \, ^\circ\text{C}, P = 5 \, \text{torr}, \dot{V}_g = 300 \, \text{sccm}$).

One premise of this project was the control of rapid thermal chemical vapor deposition afforded by process recipes could be improved upon by developing a real-time control system. The repeatability of process recipe control can be determined by considering the data plotted in Fig. 4.7. The figure contains the same data as shown in Fig. 4.6 however this time the data has been plotted to highlight the dwell time of each experiment. For the wafers processed with a dwell time of 35 s, the volume of polysilicon deposited varied from 0.59 to 0.89 mm$^3$. This variability is illustrated graphically in Fig. 4.8 where the...
Experimental Results

The volume of polysilicon deposited on each wafer processed with a dwell time of 35 s has been plotted as a histogram. From the figure, the range over which the volume of polysilicon deposited varied from 0.59 mm$^3$ to 0.81 mm$^3$, if the single observation at 0.89 mm$^3$ is assumed to be an outlier. The 0.22 mm$^3$ change in the volume of material deposited equates to a variation of 280 Å in the average thickness of the deposited films.

4.3 Optical Temperature Probes

Resolving the wafer’s spatial temperature profile during processing was accomplished by employing two optical sensors. The first, a pyrometer shown in Fig. 3.3 on page 29, was part of the chemical vapor deposition chamber’s control system. It monitored infrared emissions from the center of the wafer. The second a custom built optical probe, also shown in Fig. 3.3, monitored emissions along the wafer’s radial edge. Limitations in the original design of the furnace restricted optical access to only these two probes. Additional probes could not be added because of the extensive modifications required to upgrade the furnace.

Figure 4.7  Variation in the thickness of deposited polysilicon films when employing process recipe control ($T = 670$ °C, $P = 5$ torr, $\dot{V}_g = 300$ sccm).
An example of the data collected by the pyrometer and optical probe during the deposition of polysilicon is shown in Fig. 4.9. For the particular experiment shown, the target processing temperature was 650 °C. Close inspection of the pyrometer signal reveals that shortly after the lamp bank was turned on the wafer briefly exceeded the target temperature. The observed overshoot is believed to be the result of the wafer being partially transparent at temperatures less than approximately 600 °C. Once the overshoot had been corrected, the pyrometer indicates the temperature of the wafer was held constant at the target temperature for the duration of the experiment. Temperature data recorded by the optical probe is also shown in the figure. It indicates the edge of the wafer was cooler than the center.

Calibration of both the pyrometer and optical probe was accomplished using a 150 mm (6 in.) diameter wafer embedded with three thermocouples. The wafer was a bare silicon substrate without an oxide coating. The thermocouples were located with one at...
the center of the wafer, one 38 mm (1 1/2 in.) from the center, and the last one 6 mm from
the edge of the wafer.

Figure 4.9 Temperature measurements of the pyrometer and optical probe
recorded during polysilicon deposition.

To calibrate the probes, the thermocouple wafer was placed inside the deposition
furnace, and the pressure of the furnace reduced to 5 torr while flowing 300 sccm of
nitrogen. Once 5 torr was reached, the lamp bank was activated to initiate the calibration
procedure. The power output of the lamp bank was varied to yield pyrometer
temperatures ranging from 400 to 750 °C at increments of 50 degrees. Once the wafer had
reached steady state at each temperature increment, the voltage outputs of the three
thermocouples were recorded along with the optical probe’s signal. This procedure was
repeated four times. When all of the data had been collected, the voltage outputs of the
thermocouples, the data from the probe, and the wafer’s calibration table relating voltage
to temperature were used to derive a temperature correlation for the optical probe.
Examples of several temperature profiles recorded from the thermocouple wafer during calibration are shown in Fig. 4.10. The data clearly indicate the center of the wafer was hotter than the edge. Shown in Fig. 4.11 is some additional calibration data that relates to the repeatability of the measurements. The figure shows the voltage outputs for both the center and edge thermocouples from the four calibration experiments conducted. The data reveal that the voltage output of each thermocouple varied as much as 0.3 mV which corresponds to approximately 20 °C based upon the calibration table provided with the wafer. Possible sources of error that could produce the observed drift include both the optical sensors and the thermocouple wafer. In regard to the sensors, drift in the detectors is the most likely source of error. For the thermocouple wafer, likely sources of error are the bonds adhering the thermocouples to the wafer and the thermocouple wires.

### 4.4 Effect of Temperature on the Deposition Rate of Polysilicon

For the chemical vapor deposition of polysilicon, the material to be deposited first enters the system as a gas. Energy in the form of thermal radiation, from the lamp bank, is used to heat the wafer. Silane gas molecules that absorb energy from either the wafer or lamp bank and exceed the activation energy of the deposition reaction deposit. Once deposition begins and assuming the reaction is not mass limited, the kinetic theory of gases predicts the rate of deposition at any particular spot on the wafer will be directly proportional to the wafer’s local temperature.

To investigate the effect of temperature on the deposition rate of polysilicon, a series of wafers was processed varying only the temperature. The span of temperatures investigated varied from 600 to 700 °C bounding the range employed to deposit polysilicon. The results of the experiment are shown in Fig. 4.12 where the volume of polysilicon deposited is plotted as a function of temperature. Inspection of the data verifies that depositing polysilicon by means of rapid thermal chemical vapor deposition obeys the kinetic theory of gases.

The temperature dependent deposition data was then used to develop an Arrhenius equation, see Eq. 2.5 on page 10, which was incorporated into the real-time control system for the purpose of modeling deposition. The coefficients of the Arrhenius equation, see
Figure 4.10  Examples of the thermocouple wafer’s temperature profile during calibration of the pyrometer and optical probe.

Figure 4.11  Repeatability of the thermocouple wafer’s data used to calibrate the pyrometer and optical probes.
Eq. 4.1, were determined from Fig. 4.13, where the deposition data has been replotted using different axes to facilitate the analysis. The activation energy required to initiate the deposition of polysilicon was found to be 122 kJ/mol.

\[ u = 142059e^{(-14717/T)} \]  

(4.1)

When computing the coefficients of the Arrhenius equation (the deposition constant, \( C \), and the activation energy, \( E_a \)), it was assumed that the pyrometer data represented the temperature of the entire wafer, and the wafer’s temperature was uniform throughout the entire deposition process. As will be shown below, measured film thickness profiles suggest these two assumptions were not entirely accurate.

The result of making these two assumptions was that both of the Arrhenius equation coefficients could contain errors. In the Arrhenius equation, the activation energy appears as a constant in the exponential term. A small error in its value would result in predictions
for deposited films that were grossly inaccurate. As will be shown later, this was not the case indicating that the computed activation energy was fairly accurate. If an error was introduced into the equation, it is most likely to effect the deposition constant. It appears as a first-order multiplier of the exponential term.

Because the number of optical probes was limited to two, the wafer’s spatial temperature profile could not be measured with as much spatial resolution as desired. To overcome this problem, two assumptions were made. First, the wafer’s temperature profile was assumed to be axially uniform. Second, a radial temperature profile was assumed based upon data from the pyrometer, optical probe, and thermocouple wafer. While these assumptions facilitating the development of the control system, the data in Fig. 4.14 and Fig. 4.15 shows their shortcomings.

In Fig. 4.14, thickness profiles of deposited films are plotted from a series of wafers processed varying only the dwell time. From the figure, the profiles vary radially, axially,
Figure 4.14 Profiles of deposited polysilicon films for wafers processed with dwell times varying from 5 to 65 s ($T = 670 \, ^{\circ}\text{C}$, $P = 5$ torr, $\dot{V}_g = 300$ sccm).
and with the time. Assuming that the deposition process is governed by the kinetic theory of gases, the profiles suggest the temperature of the wafer was also a function of these three variables. Analysis of the $\text{H}_2^+$ signal from the same set of wafers also supports this conclusion. Show in Fig. 4.15 is the $\text{H}_2^+$ data for the same series of wafers. From the shape of the curves, the slope of the signals can clearly be seen to be continually changing. This suggest the rate of the deposition reaction was continually varying providing further evidence the temperature of the wafer was not constant with respect to time.

![Figure 4.15](image.png)

Note: dwell times listed next to curves

Figure 4.15  Mass spectrometer $\text{H}_2^+$ data for wafers processed with dwell times varying from 5 to 65 s ($T = 670$ °C, $P = 5$ torr, $\dot{V}_g = 300$ sccm).

All of this data leads to the conclusion that the simple radial temperature model assumed clearly does not have enough degrees of freedom to accurately generate a temperature map for the entire surface of the wafer. Additionally, the data also highlights the importance of designing rapid thermal chemical vapor deposition system’s that are at a
minimum able to heat the wafer with axial uniformity. Without axial temperature uniformity, additional optical probes would be required to resolve the wafer’s spatial temperature distribution.

4.5 Temperature Measurement, Film Deposition, and the Optical Theory of Thin Films

During rapid thermal chemical vapor deposition, several interrelated events are occurring simultaneously that in combination make controlling the deposition of thin films a difficult task. For example, simultaneously the wafer is being heated, deposition is occurring, and the optical properties of the wafer are varying both temporally and spatially. The purpose of this section is two fold. First, it explains how the data collected by the real-time control system is combined with the optical theory of thin films to predict the changing emissivity of the wafer. Second, it discusses some radiation heat transfer theory that must be addressed to develop the control system.

The problem of controlling rapid thermal processing arises from resolving the temperature of the wafer correctly at each time step during processing. Accurate temperature data is required to correctly predict the spatial thickness distribution of the deposited film using the Arrhenius equation. With accurate deposited film data, the emissivity of the wafer can then be updated to account for any changes. The new emissivity values can then be used at the next time step to compute the wafer’s temperature. Any error in this process may be compounded throughout the duration of deposition resulting in a deposited film of unintended thickness.

To illustrate the range of emissivity values a wafer can assume during polysilicon deposition, consider the spectral, hemispherical emissivity data plotted in Fig. 4.16, for a silicon wafer coated with 1000 Å of silicon dioxide. The data was generated using the Maple program Emissivity, see Appendix C, and is derived from the optical theory of thin films as developed by Stone (1963). In the plot, the wafer’s emissivity is shown to vary from approximately 0.3 to 0.95 depending upon the thickness of the deposited polysilicon film and the wavelength of interest. As an example, consider the wavelength 3.720 μm. The custom built optical probe monitored a narrow band of radiation centered at this
Experimental Results

wavelength. During deposition, the emissivity of the wafer could vary as much as ±15 percent from its initial value of 0.69. Additional curves are also plotted for other wavelengths of interest. The wavelengths 2.898 and 3.312 μm represent the wavelengths at which blackbodies of 1000 and 875 K, respectively, emit the most power. This bounds the range of temperatures over which polysilicon was deposited during this project. While a wafer cannot be considered a blackbody, the data highlights the fact that at shorter wavelengths the emissivity of the wafer varies over a wider range. The 5.200 μm curve represents the wavelength monitored by the pyrometer.

The last curve plotted in Fig. 4.16 is for 0.966 μm. This corresponds to the wavelength at which a 3000 K blackbody emits the most power. The tungsten halogen lamps employed by the furnace operated at 3000 K and can reasonably be assumed black. The wavelength 0.966 μm is important in regards to the absorptivity of the wafer. Absorptivity by definition is not a surface property as is emissivity but instead a function of the incident radiation, see Eq. 2.25 on page 17. By employing Kirchhoff’s law and assuming the surface of the wafer to be diffuse-spectral (independent of direction), the spectral, hemispherical emissivity for 0.966 μm plotted in Fig. 4.16 also represents the spectral, hemispherical absorptivity of the wafer at that wavelength. The curve indicates that the absorptivity of the wafer is changing at a rate faster than the emissivity of the wafer.

The importance of wavelength and the role it plays in radiation heat transfer and the design of optical probes is further illustrated in Fig. 4.17. The data shows the band of wavelengths over which blackbodies of 875, 1000, and 3000 K emit 90 percent of their power. The temperatures 875 and 1000 K bound the wafer’s temperature range during film deposition. Based upon the curves, the wafer would emit most of its energy from approximately 1.3 to 9 μm. The lamp bank because it is hotter will emit 90 percent of its energy at shorter wavelengths from approximately 0.4 to 3 μm.
Experimental Results

Figure 4.16  Select spectral, hemispherical emissivity curves for polysilicon deposited on a silicon wafer coated with 1000 Å of silicon dioxide.

Figure 4.17  Spectral, blackbody emissive power curves for blackbodies of 875, 1000, and 3000 K.
CHAPTER 5 REAL-TIME CONTROL APPLICATIONS

5.1 Introduction

The purpose of this chapter is to demonstrate the real-time control system developed for this project. To ensure a comprehensive understanding of how the system operated, this chapter begins with a description of the deposition process and the key variables monitored. This is followed by a description of experiments performed to test the system. Once the fundamentals of how the control system operated and was tested have been described, data is presented which characterizes the ability of the control system to deposit a film of a desired thickness. These results are then compared to the level of control obtained when depositing films using process recipe control. Finally, results from a computer algorithm which predict the thickness profile of deposited films from the real-time data are presented.

5.2 Deposition Process and the Real-Time Control System

The processing of a wafer begins after all of the wafers have been loaded into the furnace’s wafer handling chamber. The first step entails pumping the deposition chamber down to its base vacuum pressure. With the system at its base pressure, the 10% silane 90% argon mixture is pumped into the furnace while the throttle valve regulating flow out of the chamber is kept closed. The valve remains closed until the target pressure is reached as shown in Fig. 5.1. Adjustments to the position of the valve are then automatically made by the unit’s control module to maintain the desired pressure.

Immediately after the target pressure has been reached, the lamp bank is activated, see Fig. 5.1 and Fig. 5.2. Approximately seven to ten seconds are required to heat the wafer to its target processing temperature. Once the target temperature has been achieved, the power output of the lamp bank is modulated to maintain the temperature of the wafer for the duration of the run. At the end of processing, the lamp bank is turned off, see Fig. 5.2, and simultaneously the throttle valve is opened 100 percent, see Fig. 5.1. Nitrogen is then pumped through the vacuum chamber to purge it of all reactive gases.
Figure 5.1 Throttle valve position and pressure inside the deposition chamber during processing \((P = 5 \text{ torr}, \dot{V}_g = 300 \text{ sccm})\).

Figure 5.2 Wafer temperature during processing as measured by the pyrometer \((T = 650 \degree \text{C}, \dot{V}_g = 300 \text{ sccm})\).
Shown in Fig. 5.3 and Fig. 5.4 are the crucial mass spectrometry signals that correspond to the pressure and temperature data plotted in the previous two figures. At the onset of processing, the hydrogen ion signal increased due to the rising pressure within the deposition furnace. Once the target deposition pressure had been reached, the $\text{H}_2^+$ signal leveled off to what was defined as its background level. Both the beginning and end of deposition are marked by rapid changes in the $\text{H}_2^+$ signal as shown in the figure. The time integrated hydrogen signal, which was correlated to the volume of polysilicon deposited, was computed from the hatched area under the hydrogen curve. In Fig. 5.4, the signal for the charge-to-mass ratio 28 ($\text{Si}^+$ and $\text{N}_2^+$) is plotted. The signal for mass 28 initially rises as the chamber is pressurized with the silane argon mixture. Once deposition begins, silicon is deposited causing the $\text{Si}^+$ signal to decrease. The large increase in mass 28 at approximately 87 s marks the end of deposition and the beginning of the nitrogen purge.

![Figure 5.3 $\text{H}_2^+$ signal measured by the mass spectrometer during processing.](image-url)
5.3 Real-Time Control Experiment

The primary goal of this project was to develop a real-time control system capable of depositing thin films with greater control and accuracy than possible using process recipe control. In this section, a three step experiment is described which explains how the real-time control system was tested.

In the first step, a series of four wafers were processed to develop a deposition equation correlating the time integrated $H_2^+$ signal measured by the mass spectrometer to the volume of material deposited. The wafers were processed using process recipe control and the same temperature, pressure, and gas flow rate used for all wafers processed that day. Only the dwell time of each wafer was varied—10, 25, 35, and 50 s. Once films had been deposited on the four wafers, processing was temporarily halted while film thickness measurements were made to determine the volume of material deposited on each wafer.
The Matlab programs *Insight.m* and *Massspec.m*, see Appendix D, were then run to compute the time integrated $H_2^+$ signal from the mass spectrometry data. The film thickness measurements and $H_2^+$ data were then combined to produce the deposition correlation used in the next step.

The purpose of this first step was to generate a deposition correlation that accounted for variations in the performance of both the mass spectrometer and the deposition chamber. Experience had shown that even though a calibration procedure had been developed for the mass spectrometer to compensate for variable sensitivity caused by silane contamination, the correlations relating the $H_2^+$ signal of the mass spectrometer to the volume of film deposited could vary from day-to-day as evidenced by the data in Fig. 5.5. Therefore, it was necessary to develop a deposition correlation for each day the real-time control system was employed in order to maximize the potential of the control technique.

In the second step, wafer processing was resumed employing real-time control. The goal was now to evaluate the ability of the real-time control system to deposited a film of a desired, average thickness. Control of the deposition process was accomplished with the use of the LabVIEW® program *DAQ.vi*, see Appendix B. Prior to processing each wafer, the desired, average film thickness was entered into the program. During processing, the $H_2^+$ signal was analyzed to determine when film deposition should be terminated based upon the correlation developed in the first step.

The final step of the experiment entailed quantitatively characterizing the films deposited using the real-time control system. Film thickness measurements were made from which the total volume and average thickness of each film was computed. This data was then compared to the target film thickness values input into the real-time control software.
5.4 Real-Time Control Results

The ability of the real-time control system to deposit a film of a desired, average thickness was tested by processing three series of wafers on separate days. Shown in Fig. 5.5 are the correlations developed in step one of the experiment relating the volume of polysilicon deposited to the time integrate H$_2^+$ signal. These correlations were developed at the beginning of each day from the four wafers processed using process recipe control. Inspection of the data highlights the problem of employing process recipe control. From day-to-day, the quantity of film deposited for a selected recipe can vary. For example, the change in the volume of material deposited between days one and two for a dwell time of 35 s equates to a variation of 121 Å in the average thickness of the two films.

![Graph showing deposition correlations](image)

Figure 5.5 Deposition correlations relating the volume of polysilicon deposited to the H$_2^+$ signal used to control processing in real-time ($T = 670$ °C, $P = 5$ torr, $V_g = 300$ sccm).

Evaluation of the real-time control system’s ability to deposit a film of desired thickness was tested by depositing films varying from 800 to 1200 Å. In Fig. 5.6, the
average thickness of films deposited using the real-time control system is plotted against
the target, average film thickness. From the data labeled day one, the first time the real-
time control system was used all of the deposited films were approximately 125 Å thicker
than intended. It is believed this resulted from the deposition reaction continuing on for a
few seconds after the intended termination point. At the end of deposition, the real-time
control system is programmed to issue a command to the deposition furnace to turn off the
lamp bank, stop the flow of the silane/argon gas mixture, and begin the nitrogen purge.
Conceptually this was intended as the end point of deposition. However, physical
evidence suggests the deposition reaction continued on for a few seconds until either the
wafer cooled sufficiently or all of the silane gas had been depleted. Referencing Fig. 5.3
on page 64, note the additional H₂⁺ detected after the lamp bank had been turned off.
Initially, this was thought to be hydrogen that was generated prior to the lamp bank being
turned off but not detected until later. It appears now this signifies the continuation of the
deposition reaction past the intended termination point. Similar results were also observed
in the second test of the control system (see the data labeled day 2, series a).

To overcome the problem of depositing films of greater thickness than intended, the
desired film thickness input into the real-time control system was decrease by 125 Å. The
results of the wafers processed under these conditions are shown in Fig. 5.6 labeled as day
2, series b. The films deposited on the series b and day 3 wafers deviated from the
intended, average thickness by as little as 6 Å to as much as 74 Å. On average, the films
varied 39 Å from the intended, average thickness. This compares quiet favorably to
process recipe control which yielded films of average thickness varying over a range of
280 Å when repeatedly using the same recipe.

Repeatability was the second metric used to compare the performance of the two
control strategies. The repeatability of process recipe control was tested by processing a
series of 24 wafers--eight wafers per day on three separate days. Each wafer was
processed using the same recipe--670 °C, 5 torr, 300 sccm gas flow rate, and a dwell time
of 35 s. The film deposited upon the first wafer processed each day was used as the
baseline to which the following seven films were compared. The results shown in Fig. 5.7 indicate that when employing process recipe control the average thickness of deposited films varied from 5 Å to 140 Å with an average deviation of 48 Å. The repeatability of the real-time control system was tested in a similar manner. The results of the deposited films varied in average thickness from 4 to 38 Å with an average variation of 19 Å. A 60 percent improvement over process recipe control.

![Figure 5.6](image.png)

Figure 5.6 Real-time control system’s ability to deposit a film of a desired, average thickness ($T = 670 \, ^\circ\text{C}$, $P = 5$ torr, $V_g = 300$ sccm).

5.5 Numerical Predictions

In addition to being able to deposit a film of a desired, average thickness, another key objective of this project was developing the ability to predict the spatial thickness profile of the deposited film. To successfully accomplish this task, the data from both the mass spectrometer and optical temperature probes was combined with the Arrhenius deposition equation and developed into a computer model. The Fortran program developed for this task, *RTCVD Control*, is listed in Appendix A.
In the development of the Fortran code, three assumptions were made that are key to understanding the results of the program. First, the wafer’s temperature was assumed axially symmetric. While axially varying film thickness measurements indicate the wafer’s temperature most likely was not axially symmetric during processing, the limited optical access afforded by the deposition furnace made this assumption necessary. The limited optical access also required an assumption be made concerning the wafer’s radial temperature profile. The data from the two optical probes was used as the end points for an assumed elliptical temperature profile. Other profiles, examples include uniform, straight line, and parabolic, were investigated, but the elliptical profile was found to yield the best results. Finally, the Fortran code was not run during processing. It was developed to run during the period of time between when two wafers were processed. By executing between processing runs, the program was able to generate valuable data concerning the

Figure 5.7 Ability of the process recipe and real-time control strategies to repeatedly deposit films of the same average thickness.
performance of the deposition furnace during the time wafer handling tasks were completed.

Shown below in Fig. 5.8 are film thickness profiles both measured and predicted for one wafer processed using the real-time control system. The first two profiles are contours generated from thickness measurements made diametrically separated by 90 degrees. The remaining three profiles are all predictions generated using the Fortran program. From the figure, if a uniform temperature model (temperature is the same everywhere on the wafer) is assumed the deposited film thickness is under predicted at radial locations less than approximately 35 mm and over predicted at radial locations greater than 35 mm. This result is in line with the wafer’s temperature profile during processing and the radial distribution of surface area for a 100 mm diameter wafer.

Of all of the temperature profiles investigated, the elliptical profile with an assumed 15 °C temperature gradient yielded predictions that most closely matched the thickness profiles of deposited films. The temperature gradient assumed the center of the wafer was always 15 °C hotter than the edge. A comparison of the predicted and measured film thickness results for the center of the wafer revealed a difference of only 12 Å. In terms of predicting the wafer’s emissivity and in turn its temperature, 12 Å would not yield any appreciable error. However, results with the same degree of accuracy were not obtained at the radial edge of the wafer. The predicted thickness varied as little as 46 to as much as 160 Å from the measured values. A difference of 160 Å between the prediction and actual film thickness only results in an 1.12 percent error in the calculation of the wafer’s emissivity.

As noted earlier, the real-time control system was initially developed with the intention of using the temperature measurements of the optical probes as the two end points of the temperature profile. In practice, the application of this concept did not meet expectations. Experience with the optical probes and the thermocouple wafer used to calibrate the probes indicated the resolution of the temperature measurements was at best 5 °C. Even worse the accuracy of the custom built optical probe was only 20 °C. The
importance of developing optical temperature measurement equipment that can quickly and easily be calibrated using a known standard cannot be over stated (see DeWitt, 1997).

Shown in Fig. 5.9 are some predicted film thickness and emissivity data computed using the Fortran program *RTCVD Control*. The data encompasses a chronological period that includes the deposition process as well as a few seconds before and after. At the start of processing, the emissivity of the wafer was 0.69. Once the film began depositing, the emissivity of the wafer began to vary with both space and time. The spatial variations reflect nonuniform deposition rates resulting from uneven heating while the time variations represent the increasing thickness of the depositing film. At the onset of deposition, a step increase in the film thickness and emissivity of the wafer is predicted. This event does not physically occur but instead highlights a problem with the control strategy. Prior to turning on the lamp banks the pressure within the vacuum system was increased to the target processing pressure. Once this was done, the lamp bank was turned
on to heat the wafer. The problem with this chain of events is that the deposition rate jumps from zero to roughly 25 Å/s almost instantaneously. This combined with the one second response time of the mass spectrometer yields modeling results that indicate a step increase in the emissivity of the wafer. In addition to decreasing the response time of the mass spectrometer, this problem may be solved by initiating the deposition process at a lower pressure.

Figure 5.9 Spatial and temporal variation of the wafer’s emissivity during the deposition of polysilicon.
CHAPTER 6 CONCLUSIONS AND RECOMMENDATIONS

A study has been conducted to develop a real-time control system for rapid thermal chemical vapor deposition. A control system was developed for depositing polysilicon that employed multiple sensors and a computer model to predict the state of the deposition process. Specific findings relating to individual components and the overall performance of the system are categorized into three sections—mass spectrometer, optical temperature probes, and real-time control strategy. In addition, the experience of developing the control system taught many valuable lessons that cannot be classified as conclusions but are better defined as recommendations for developing future systems. These recommendations are also detailed below.

6.1 Mass Spectrometer

1. The length of time between when an event occurs in the deposition chamber and when the mass spectrometer detects that event has been defined as the response time of the instrument. The mass spectrometer’s response time was found to be approximately one second. This lag time was determined to be short enough to warrant the instrument’s use as a real-time sensor for monitoring the deposition reaction.

2. When exposed to and sampling only nitrogen gas, the mass spectrometer was found to repeatedly measure the same signal from one day to the next. No decrease in the sensitivity of the instrument was observed due to nitrogen exposure.

3. Exposure to the corrosive, reactive gas silane produced a decrease in the sensitivity of the instrument. The decrease in sensitivity was found to be directly proportional to the length of exposure. A maximum decrease in the sensitivity of the instrument was never observed. Exposure to silane always produced an additional decrease in the sensitivity of the instrument.
Conclusions and Recommendations

4. A calibration procedure was developed for the mass spectrometer which provided a means to maintain the sensitivity of the instrument after exposure to silane. The calibration procedure entailed sampling nitrogen gas while noting the signal intensity measured at several electron multiplier voltage settings. From the data, the voltage of the electron multiplier was then adjusted to maintain the same signal intensity for nitrogen from one day to the next.

5. When operating in the Faraday cup mode (with the electron multiplier turned off), the sensitivity of the instrument was found to decrease by approximately two orders of magnitude relative to when the electron multiplier was on. The effect of silane exposure when operating in the Faraday cup mode was found to be consistent with previous results in that exposure still decreased the sensitivity of the instrument.

6. Degassing the mass spectrometer, which was supposed to clean the instrument, was found to have no effect on the sensitivity of the instrument once exposed to silane. The only technique found to reverse the effects of silane exposure was to leave the instrument unused for a period of days while it was maintained at the base pressure of its vacuum system (≤1x10⁻⁸ torr).

7. Experience gained during polysilicon deposition indicated that the sensitivity of the mass spectrometer could be significantly decreased after as little as 30 minutes of silane exposure. Without a means to quickly reverse the effects of silane, the mass spectrometer cannot be considered a viable sensor for production applications.

6.2 Optical Temperature Probes

8. Data recorded by the optical probes indicated the wafer’s radial temperature distribution was not uniform during processing. The resolution of the probes was found to be 5 °C while their accuracy was approximately 20 °C. Improved resolution and accuracy may have been achieved if a quick and accurate calibration
technique could be integrated into the design of the furnace. This would eliminate
the time consuming task of placing a thermocouple wafer inside the furnace to
calibrate the optical probes.

9. The design of the deposition furnace plays a crucial role in determining the
number of optical probes needed to resolve the spatial temperature distribution of
the wafer. The ability of the furnace to heat the wafer axially uniformly greatly
reduces the number of optical probes required.

6.3 Real-Time Control Strategy

10. Accuracy and repeatability were the two metrics used to compare the real-time and
process recipe control systems. When attempting to deposit films of an average
thickness ranging from 800 to 1200 Å, the films deposited using the real-time
control system varied as little as 6 to as much as 74 Å. On average, each deposited
film was 39 Å off from the intended thickness. This compares quiet favorably to
process recipe control which produced films varying over a range of 280 Å when
the same process recipe was used repeatedly. In terms of repeatability, real-time
control system produced films that varied in average thickness from 4 to 38 Å with
an average variation of 19 Å. The repeatability of process recipe control was
found to range from 5 to 140 Å with an average variation of 48 Å.

11. The Arrhenius equation was shown to be a good model for predicting deposition
based upon the accuracy with which predicted and deposited film profiles matched.
The assumptions of a uniform and constant temperature profile for the wafer made
prior to computing the equation’s coefficients did not affect the accuracy of the
coefficients to a degree that rendered the predicted film profiles inaccurate.

12. One problem not initially anticipated that adversely affected the ability of the real-
time control system to deposit a film of a desired thickness was the manner in
which the deposition reaction was stopped. Once it was determined that the
desired thickness had been deposited, the deposition reaction was stopped by
turning off the lamp bank. This resulted in deposition continuing on for a few seconds until either the wafer cooled sufficiently or all of the silane gas had been depleted. Ideally, the deposition reaction could be stopped instantaneously. However in practice, this is not viable. A more practical approach would be to decrease the rate of the deposition reaction shortly before the target film thickness is reached and then shut off the lamp bank. This could be done by either decreasing the gas pressure inside the deposition chamber or decreasing the temperature of the wafer.

6.4 Additional Recommendations

13. While the mass spectrometer was found not to be the ideal sensor for measuring the exhaust products of polysilicon deposition, the concept of determining the deposition reaction rate from the exhaust gases proved viable. To overcome the problems associated with the mass spectrometer, two possibilities seem likely. First, the mass spectrometer could be redesigned to address its contamination problem. Second, an optical sensing technique could be developed to replace the mass spectrometer. From the experience gained during this project, optical techniques seem to possess several inherent advantages over the mass spectrometer. First, optical measurements are non-contact and therefore would not be affected by corrosive, reactive gases. Second, optical techniques could operate at the pressure of the furnace and thus not require a separate vacuum system to reduce the pressure of the exhaust gases. Finally, without the need for a separate vacuum system, optical systems would require fewer mechanical components which should yield lower capital costs and less maintenance.

14. Experience gained during this project with the mass spectrometer and thermocouple wafer has taught that ideally all sensors used to monitor chemical vapor deposition should be placed outside the deposition chamber. By following this recommendation, sensors will not be exposed to the high temperatures and reactive gases that can quickly foul an instrument.
LIST OF REFERENCES


2. Brady, James E., and Humiston, Gerard E.

3. Buckley, M.E.


5. DeWitt, D.P., Sorrell, F.Y., and Elliott, J.K.


7. Hecht, Eugene

8. Knight, Thomas J., Greve, David W., Cheng, Xu, and Krogh, Bruce H.

9. Leybold Inficon Inc.
10. Modest, Michael F.  

11. Müller, N.  
   1993 “Use of Quadrupole Mass Spectrometers in Ultrahigh Vacuum Systems.”  

12. O’Hanlon, John F.  
   Sons: New York.

13. Öztürk, Mehmet C., Sorrell, F. Yates, Wortman, Jimmie J., Johnson, F. Scott, and  
    Grider, Douglas T.  
    1991 “Manufacturability Issues in Rapid Thermal Chemical Vapor Deposition.”  

    1986 “The Effect of Thin Dielectric Films on the Accuracy of Pyrometric  

15. Peuse, Bruce and Rosekrans, Allan  
    1993 “In-situ Temperature Control for RTP via Thermal Expansion Measurement.”  

    1995 “Control of Semiconductor Manufacturing Equipment: Real-Time Feedback  
    Control of a Reactive Ion Etcher.” IEEE Transactions on Semiconductor  

17. Rubloff, Gary W., Tedder, Laura L., and Lu, G. Brian  
    1996 “Real-Time Sensing and Dynamic Simulation for CVD Optimization and  
    Control.” Proceedings of the XIII International Conference on Chemical  
    Vapor Deposition (May 5-10, 1996): Los Angeles, CA.

18. Satō, Tsutomu  

19. Semiconductor Industry Association  
20. Semiconductor Industry Association


22. Sorrell, F. Yates and Gyurcsik, Ronald S.
   1993  “Model-Based Emissivity Correction in Pyrometer Temperature Control of
          Rapid Thermal Processing Systems.” IEEE Transactions on Semiconductor

   1994  “Applied RTP Optical Modeling: An Argument for Model-Based Control.”
          IEEE Transactions on Semiconductor Manufacturing (November 1994):
          7(4): 454-459.

24. Stone, John M.,

25. Tedder, L.L., Rubloff, G.W., Cohaghan, B.F., and Parsons, G.N.
   1996  “Dynamic Rate and Thickness Metrology during Poly-Si Rapid Thermal
          Chemical Vapor Deposition from SiH₄ using Real Time in Situ Mass
          Spectrometry.” Journal of Vacuum Science Technology A (March/April
APPENDICES
module global_data
    implicit none
    save
    integer:: ircells,ithetacells,izcells
    real*8,allocatable,dimension(:,:,:):: are,arn,ars,arw,key_data,u,vol
    real*8,allocatable,dimension(:,:):: A,emissivity,film
    real*8,allocatable,dimension(:):: rcv,thetacv,zcv
end module global_data
!
! Program Name: RTCVD_control
!
! Program Overview:
! Fortran program for predicting the film thickness deposited upon
! a Si wafer during Rapid Thermal Chemical Vapor Deposition
! (RTCVD). The program reads a text file containing real-time
! data collected during processing using Labview. The data is
! then used to predict the thickness of the deposited film.
!
! Author: Robert M. Smith
! Project: PhD research
!
! Last Revision: 3/5/98

program RTCVD_control
!
! descriptions of variables

! i1 - index of analog time loop
! irowA - last row of analog data
! isec - time [s]
! rl - length of radial domain [m]
!

! variable declarations


implicit none
integer:: i1,irowA,isec
real*8:: rl
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
call subroutines
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
call wafer_grid(rl) ! wafer grid
call labview_data(irowA) ! reads real-time data
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! analog data time loop
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
isec=1
!
doi1=1,irowA
    call deposition_process(i1,rl) ! deposition status
    call output(i1,irowA,isec) ! save data for file
end do
!
!
end program RTCVD_control
Fortran Subroutine: Wafer Grid

subroutine wafer_grid(rl)
use global_data, only: are,arn,ars,arw, &
    & emissivity,film,key_data,ircells, &
    & ithetacells,izcells,rcv,thetacv, &
    & u,vol,zcv
!
!
!**********************************************************************
! Subroutine Name: wafer_grid
!
! Subroutine Overview:
! Fortran subroutine for gridding the wafer. The subroutine also
! initializes the temperature of each cell, sets the thickness of
! the deposited film to zero of each surface cell, and defines the
! emissivity of each surface cell.
!
!
! Author: Robert M. Smith
! Project: PhD research
!
! Last Revision: 5/26/98

!**********************************************************************
!
!**********************************************************************
! descriptions of variables passed to the master program
!**********************************************************************
!
! rl    - length of radial domain [m]
!
!**********************************************************************
!
! descriptions of variables used in this subroutine
!**********************************************************************
!
! are    - area of east face of cell [m^2]
! arn    - area of north face of cell [m^2]
! ars    - area of south face of cell [m^2]
! arw    - area of west face of cell [m^2]
! emissivity    - emissivity of wafer per cell
! film    - thickness of deposited film on each cell [nm]
! key_data    - process data saved to disk
! ircells    - number of cells in the radial direction (j1 index)
ithetacells - number of cells in the theta direction (j2 index)
izcells - number of cells in the z direction (j3 index)
j1 - index for r direction
j2 - index for theta direction
j3 - index for z direction
pi - 3.14159...
rcv - location of radial control volume faces [m]
t# - temporary variable (examples: t1, t2, etc.)
thal cv - location of theta control volume faces [m]
thal - radians of theta domain [rad]
u - temperature of each cell [K]
vol - volume of cell [m^3]
zc v - location of z control volume faces [m]
zl - length of z domain [m]

**********************************************************************
variable declarations
**********************************************************************
imPLICIT NONE
INTEGER:: j1,j2,j3
REAL*8:: pi,rl,t1,t2,t3,t4,t5,t6,thetal,zl
ircells=5
ithetacells=2
izcells=2
pi=4.0d0*ATAN(1.0d0)
rl=0.05d0 ! 50 mm
thetal=2.0d0*pi
zl=0.0006d0 ! 0.6 mm

**********************************************************************
allocate size of arrays based upon number of cells in grid
**********************************************************************
allocate(are(1:ircells,1:ithetacells,1:izcells))
allocate(arn(1:ircells,1:ithetacells,1:izcells))
allocate(ars(1:ircells,1:ithetacells,1:izcells))
allocate(arw(1:ircells,1:ithetacells,1:izcells))
allocate(emissivity(1:ircells,1:ithetacells))
allocate(film(1:ircells,1:ithetacells))
allocate(key_data(1:ircells,1:5,1:200))
allocate(rcv(0:ircells))
allocate(thetacv(0:ithetacells))
allocate(vol(1:ircells,1:ithetacells,1:izcells))
allocate(u(1:ircells,1:ithetacells,1:izcells))
allocate(zcv(0:izcells))
key_data(1:ircells,1:5,1:200)=0.0d0

!**********************************************************************
! defining location of radial, theta, and z control volume faces
! Notes:
! 1) The radial distances between control volume faces are define so
! that each cell has the same polar area (r-theta area).
!**********************************************************************

rcv(0)=0.0d0

! calculate the face areas and volume of each cell
!**********************************************************************

! do j2=1,ithetacells
! do j3=1,izcells
! do j1=1,ircells

end do
vol(j1,j2,j3)=are(j1,j2,j3)*t5
end do
end do
end do
!
!**********************************************************************
! initialize the deposited film thickness of all surface cells to zero,
! and initialize the temperature of all wafer cells to 298K
!**********************************************************************
!
film(1:ircells,1:ithetacells)=0.0d0
u(1:ircells,1:ithetacells,1:izcells)=0.0d0
!
!**********************************************************************
! initialize the spectral, hemispherical emissivity of all surface
! cells. the emissivity defined below is calculated from the thin
! films theory for 1000 Angstroms of SiO2 deposited upon the wafer.
! emissivity calculations assumed radiation is directionally dependent
! upon the polar angle.
!**********************************************************************
!
emissivity(1:ircells,1:ithetacells)=0.689383d0 ! wafer + SiO2
!
return
end subroutine wafer_grid
Fortran Subroutine: Labview Data

subroutine labview_data(irowA)
use global_data, only: A

! Subroutine Name: labview_data

! Subroutine Overview:
! Fortran subroutine for reading the real-time data collected by
! Labview into memory. Analog signals must be converted from
! voltages to physical data. The data file has the following
! format:
! row 1: header describing the data in each column
! row 2+: data

! Author: Robert M. Smith
! Project: PhD research
! Last Revision: 7/17/98

! descriptions of variables passed to the master program

! irowA - last row of analog data

! descriptions of variables used in this subroutine

! A - Labview data
! dataerr - verification of file i/o error message
! header - column description of data in the real time data file
! i1 - index
! i2 - index
! ioerror - iostat variable for trapping errors reading data file
! t1 - A/D board conversion factor, voltage
! t2 - A/D board conversion factor, digital equivalent of t1

Appendix A

! expected format of real-time data file
! Notes:
! 1) the format listed below is the default output of the Labview data acquisition program Fiber9.vi
! 2) units listed are for after conversion to physical data
! 3) all mass spec data is in terms of intensity [A]

!**********************************************************************
!
! column #1  time stamp for analog signals
! column #2  5.00 V dc signal from power supply [V]
! column #3  ion guage (mass spec) [Torr]
! column #4  convectron guage (mass spec) [mTorr]
! column #5  fiber optic probe #1 [K]
! column #6  fiber optic probe #2
! column #7  pyrometer (RTP)
! column #8  butterfly valve position (RTP) [% open]
! column #9  pressure guage (RTP) [Torr]
! column #10 time stamp for mass spec signals
! column #11 H2+   signal (AMU=2)
! column #12 H2O+  signal (AMU=18)
! column #13 Ar++  signal (AMU=20)
! column #14 Si+   signal (AMU=28)
! column #15 SiH+  signal (AMU=29)
! column #16 SiH2+ signal (AMU=30)
! column #17 SiH3+ signal (AMU=31)
! column #18 SiH4+ signal (AMU=32)
! column #19 Ar+   signal (AMU=40)
!
!**********************************************************************
!
! variable declarations
!**********************************************************************
!
implicit none
integer:: i1,i2,ioerror,irowA
real*8:: t1,t2
real*8:: temp(3500,19)
character(len=10):: dataerr
character(len=274):: header
!
!**********************************************************************
!
read data file
!**********************************************************************
!
open(unit=9,file="c:\bsmith\exp17\testque1.txt" &
 & ,status="old",iostat=ioerror)
if (ioerror /= 0) then
  print *,"Error opening the data file"
  read *,dataerr
  stop
end if
read(unit=9,fmt=201) header
do i1=1,3500
  read(unit=9,fmt=*,end=20) (temp(i1,i2),i2=1,19)
end do
20 close(9)
irowA=i1-1
201 format(A)

allocate(A(1:irowA,1:19))
A(1:irowA,1:19)=temp(1:irowA,1:19)

allocate variable 'A', copy data from 'temp' to 'A'

convert analog signals to physical data
Notes:
  1) digital data is first converted to an analog voltage
  2) the analog voltage is then converted to physical data
  3) the conversion formula for the Convectron and ion gauges is
     based upon the output signal format of the Granville-Phillips
     303 process controller
  4) optic probe data not converted to temperature until later
     when the emissivity of the wafer's surface is known
  5) no signal from fiber #2
  6) pyrometer signal from RTP1, data converted to temperature now
     because the signal represents the temperature used by RTP1 to
     control the deposition process
  7) mass spec data are serial signals which don't require converting

t1=9.985d0
t2=4090d0
A(1:irowA,2:9)=A(1:irowA,2:9)*t1/t2 ! digital to voltage
A(1:irowA,3:4)=(20.0d0*(A(1:irowA,3:4)- &
 & floor(A(1:irowA,3:4)))-10.0d0* &
& floor(2.0d0*(A(1:irowA,3:4)- &
& floor(A(1:irowA,3:4)))))*10.0d0** &
& (-11+floor(2.0d0*A(1:irowA,3:4)))
A(1:irowA,4)=A(1:irowA,4)*1000.0d0
A(1:irowA,6)=0.0d0 ! no signal
A(1:irowA,7)=A(1:irowA,7)*1.0d3/5.0d0+2.7315d2 ! pyrometer [K]
A(1:irowA,8)=A(1:irowA,8)*10.0d0
!
!
return
end subroutine labview_data
Fortran Subroutine: Deposition Process

subroutine deposition_process(i1,rl)
use global_data, only: A, emissivity, ircells, &
  & ithetacells, izcells, rcv, u
!
!
!**********************************************************************
! Subroutine Name: deposition_process
!
! Subroutine Overview:
! Fortran subroutine that uses the real-time data collected by
! Labview to determine when important events during the processing
! of a wafer occur.
!
! Author: Robert M. Smith
! Project: PhD research
!
! Last Revision: 7/17/98
!**********************************************************************
!
!**********************************************************************
! descriptions of variables passed to the master program
!**********************************************************************
!
! i1 - index of analog time loop
! rl - length of radial domain [m]
!
!**********************************************************************
! descriptions of variables used in this subroutine
!**********************************************************************
!
! A - Labview data
! eff_emiss - effective emissivity corrected for chamber reflectivity
! emissivity - emissivity of wafer per cell
! h2bckgrd - H2+ signal intensity when deposition starts
! h2step - H2+ generated per each time step during deposition [A]
! h2total - total H2+ generated during deposition [A]
! i2 - index of mass spec time loop
! idepend - deposition over switch (0=off, 1=on)
! idepstart - Hydrogen background switch (0=off, 1=on)
! intercept - intercept of straight line temperature function [K]
! ipdep  - target pressure switch (0=off, 1=on)
! iprofile  - select temperature profile
! itdep  - target temperature switch (0=off, 1=on)
! j1  - index for r direction
! j2  - index for theta direction
! p  - directrix y=-p of the parabolic temperature curve [m]
! pi  - 3.1416...
! ptarget  - target deposition pressure in RTCVD chamber [Torr]
! ptol  - allowable variation from pressure tolerance [Torr]
! Rch  - chamber reflectivity [0,1]
! rcv  - location of radial control volume faces [m]
! rnode  - radial location of cell's center [m]
! slope  - slope of straight line temperature function [K/m]
! ttarget  - minimum wafer deposition temperature [K]
! u  - temperature of each cell [K]
!
**********************************************************************
! variable declarations
**********************************************************************
!
implicit none
integer:: i1,i2,idepend,idepstart, &
   & ipdep,iprofile,itdep,j1,j2
real*8:: eff_emiss,h2bckgrd,h2step, &
   & h2total,intercept,p,phi,pi,ptarget, &
   & ptol,Rch,rl,rnode,slope,ttarget
if (i1 == 1) then ! declare only @ start
   i2=1 ! mass spec time index
   idepend=0 ! idepend off
   idepstart=0 ! idepstart off
   ipdep=0 ! ipdep off
   iprofile=3 ! temperature profile
   itdep=0 ! itedp off
   h2step=0.0d0 ! H2+ per time step
   h2total=0.0d0 ! total H2+
   pi=4.0d0*atan(1.0d0) ! 3.1416...
   ptarget=5.0d0 ! target pressure
   ptol=0.1d0 ! pressure tolerance
   Rch=1.0d0 ! chamber reflectivity
   ttarget=873.0d0 ! 600 C
if (iprofile == 1) then
   write(6,*) 'elliptic temperature profile'
endif
if (iprofile == 2) then
write(6,*),'parabolic temperature profile'
endif
if (iprofile == 3) then
  write(6,*),'straight line temperature profile'
endif
end!

!**********************************************************************
! analog data time loop
! Notes:
! 1) Both the analog data and the mass spec data each have their own
!    timestamp.
! 2) For deposition to begin, two events must occur. First, the target
!    pressure must be reached and maintained. Second, the target wafer
!    temperature must be reached.
! 3) Once deposition begins, the intensity of the Hydrogen signal is
!    recorded so that the background H2+ signal can be subtracted
!    from the total amount of H2+ measured during deposition.
! 4) After deposition begins, the total H2+ generated, which
!    correlates with the total material deposited upon the wafer, must
!    be calculated.
! 5) Finally, the time when deposition ends must be resolved.
!    Deposition ends when the butterfly valve, which controls the
!    flow of gases through the RTCVD, is more than 80% open. The
!    selection of when deposition ends should take into consideration
!    the ~2 second lag between events occurring inside the RTCVD and
!    the massspec.
!**********************************************************************

!**********************************************************************
! temperature calculations
!**********************************************************************

!**********************************************************************
! optical probe
! Notes:
! 1) Insufficient signal for probe if the signal < 0.48 V.
! 2) Emissivity of the wafer accounted for in the calculation.
! 3) A geometric correction factor is also part of the temperature
!    calculation to account for stray light reflecting into the
!    probe. The correction factor is based upon the paper by
!    D.W. Pettibone, J.R. Suarez, and A. Gat "The Effect of Thin
! Dielectric Films on the Accuracy of Pyrometric Temperature
! Measurement

if (A(i1,5) >= 0.48d0) then
  j1=ircells
  do j2=1,ithetacells
    eff_emiss=emissivity(j1,j2)/(1.0d0 - &
    & (1.0d0-emissivity(j1,j2))*Rch)
    u(j1,j2,izcells)=881.31d0+638.22d0* &
    & log10(A(i1,5)/eff_emiss)
  enddo
else
  u(1:ircells,1:ithetacells,izcells)=298.0d0
endif

! RTP1 pyrometer

do j2=1,ithetacells
  u(1,j2,izcells)=A(i1,7)* & ! correcting temp.
  & (emissivity(1,j2)/0.68934d0) ! for new emissivity
enddo
u(ircells,1:ithetacells,izcells)= & ! define edge temp.
& u(1,1:ithetacells,izcells)-5.0d0!

if (iprofile == 1) then
  do j1=2,ircells-1
    rnode=(rcv(j1)+rcv(j1-1))/2.0d0
    do j2=1,ithetacells
      u(j1,j2,izcells)=sqrt(1.0d0- &
      & (rnode/0.05d0)**2)* &
      & (u(1,j2,izcells)- &
      & u(ircells,j2,izcells)) &
      & u(ircells,j2,izcells)
  enddo
  enddo
endif
if (iprofile == 2) then
  do j1=2,ircells-1
    rnode=(rcv(j1)+rcv(j1-1))/2.0d0
    do j2=1,ithetacells
      p=(u(1,j2,izcells)- &
         & u(ircells,j2,izcells))**2/ &
         & (4.0d0*rl)
      u(j1,j2,izcells)=sqrt(-4.0d0*p* &
         & (rnode-rl))+u(ircells,j2,izcells)
    enddo
  enddo
endif
if (iprofile == 3) then
  do j1=2,ircells-1
    rnode=(rcv(j1)+rcv(j1-1))/2.0d0
    intercept=u(1,1,izcells)
    slope=(u(ircells,1,izcells)- &
           & u(1,1,izcells))/rl
    do j2=1,ithetacells
      u(j1,j2,izcells)=slope*rnode+ &
      & intercept
    enddo
  enddo
endif
!
!**********************************************************************
! loop to find the massspec time that is equivalent to time stamp of
! the analog data.
!**********************************************************************
!
do while (A(i2,10) < A(i1,1)) ! equivalent ms time
  i2=i2+1
enddo
!
!**********************************************************************
! the target pressure for deposition must be achieved before
! deposition can begin
!**********************************************************************
!
if (ipdep == 0 .and. A(i1,9) >= ptarget-ptol &
     & .and. idepstart == 0) then
  ipdep=1
endif
!
the target temperature for deposition must be achieved before
 deposition can begin

! if (itdep == 0 .and. u(1,1,izcells) >= ttarget &
 & .and. idepstart == 0) then
 itdep=1
endif

! deposition begins once both the target pressure and target wafer
! temperature have been achieved

! if (ipdep == 1 .and. itdep == 1 .and. &
 & idepstart == 0) then
 idepstart=1
 h2bckgrd=abs(sum(A(i2-2:i2+2,11))/5.0d0) ! H2+ background
endif

! once deposition begins the amount of H2+ generated is computed.
! Notes:
! 1) The H2+ generated that needs to be measured occurs after
!    deposition begins but before deposition end.
! 2) The subroutine arrhenius is called here to calculate the spatial
!    distribution of the depositing film and update the thickness of
!    the depositing film.
! 3) If h2step <= 0, no film deposition and no emissivity change of
!    the wafer occurs.

! if (idepstart == 1 .and. idepend == 0) then
 h2step=(A(i2,11)-h2bckgrd)*(A(i1,1)-A(i1-1,1))
 if (h2step > 0) then
  h2total=h2total+h2step
  call film_deposition(h2total)
  call optics
 endif
endif

! deposition ends after deposition has started, before deposition
! had ended, and the butterfly valve's position exceeds 80% open
!***************************************************************************
!
if (idepstart == 1 .and. idepend == 0 .and. 
   & A(i1,8) > 80.0d0) then
   idepend=1
write(6,'(A10,1X,3A10)') 'deposition over',A(i1,1),A(i2,10)
endif
!
!
return
end subroutine deposition_process
Fortran Subroutine: Film Deposition

subroutine film_deposition(h2total)
use global_data, only: arw,film,ircells, &
    & ithetacells,izcells,u
!
!
!**********************************************************************
! Subroutine Name: film_deposition
!
! Subroutine Overview:
! Fortran subroutine models the deposition of film upon the wafer.
! Two models are employed to calculate the spatial film deposition
! rate. The first model is empirical based upon data collected
! with the mass spectrometer. The model uses the cumulative H2+
! signal to calculate the total volume of film deposited. An
! Arrhenius model is then used to determine the spatial
! distribution of the depositing film. The second model assumes
! uniform film deposition.
!
!
! Author: Robert M. Smith
! Project: PhD research
!
! Last Revision: 7/13/98
!**********************************************************************
!
!**********************************************************************
! descriptions of variables passed to subroutine deposition_process
!**********************************************************************
!
! h2total - total H2+ generated during deposition [A]
!
!**********************************************************************
! descriptions of variables used in this subroutine
!**********************************************************************
!
! Aconst - proportionality constant of Arrhenius Eq. [mm^3/s]
! arw - area of west face of cell [m^2]
! delta_vol - volume of film deposited since last time step [mm^3]
! dia - wafer diameter [mm]
! Ea - activation energy of Arrhenius Eq. [J/mole]
! film - thickness of deposited film on each cell [nm]
Appendix A

- average deposited film thickness [nm]
- film deposition model
- switch to limit execution of if-then statements
- number of cells in the radial direction (j1 index)
- number of cells in the theta direction (j2 index)
- number of cells in the z direction (j3 index)
- index for r direction
- index for theta direction
- volume fraction of film deposited on each cell
- deposition rate of Arrhenius Eq. [mm^3/s]
- constant of empirical deposition model [mm^#/A]
- 3.14159...
- universal gas constant [J/(mole*K)]
- temperature of each cell [K]
- volume of film deposited up to current time step [mm^3]
- volume of film deposited up to last time step [mm^3]

**********************************************************************
! variable declarations
!**********************************************************************

implicit none
integer:: iexec,imodel,j1,j2
real*8:: Aconst,dia,Ea,h,h2total,m0,m1,m2, &
         pi,R,delta_vol,vol,vol_old
real*8:: k_dep(1:ircells,1:ithetacells), &
         k_rate(1:ircells,1:ithetacells)
imodel=1
k_dep(1:ircells,1:ithetacells)=0.0d0
k_rate(1:ircells,1:ithetacells)=0.0d0
pi=4.0d0*atan(1.0d0)

**********************************************************************
! noting deposition model used on screen
**********************************************************************

if (imodel == 1 .and. iexec == 0) then
   write(6,*) 'Arrhenius deposition model'
   iexec=1 ! 1 execution only
endif
if (imodel == 2 .and. iexec == 0) then
   write(6,*) 'uniform film deposition model'
   iexec=1 ! 1 execution only
endif
Appendix A

! constants of empirical film deposition model (y=m0+m1*x+m2*x^2)
! y - volume of posilicon deposited
! x - H2+ signal from mass spectrometer
! model developed for wafers 111-118

m0=2.7514d-1
m1=1.9765d6
m2=-7.5379d11

! constants of Arrhenius equation

Aconst=142059.0d0
Ea=122357.0d0
R=8.3140d0 ! gas constant

! total volume of film deposited & volume deposited between time steps

vol_old=vol
vol=m0+m1*h2total+m2*h2total**2
delta_vol=vol-vol_old

! Arrhenius model for predicting spatial distribution of deposited film.

if (imodel == 1) then
    k_rate=Aconst*exp(-Ea/ &
    & (R*u(1:ircells,1:ithetacells,izcells)))
k_dep=k_rate/sum(k_rate)
do j1=1,ircells
    do j2=1,ithetacells
        film(j1,j2)=film(j1,j2)+k_dep(j1,j2)* &
        & delta_vol/arw(j1,j2,izcells)
    enddo
endo
dendif
! uniform film deposition model.
!
if (imodel == 2) then
    dia=100.0d0
    h=4.0d0*vol/(pi*dia**2)*1.0d6
    film(1:ircells,1:ithetacells)=h
endif
!
return
end subroutine film_deposition
Fortran Subroutine: Optics

subroutine optics
use global_data, only: emissivity, film, &
   & ircells, ithetacells
!
!**********************************************************************
! Subroutine Name: optics
!
! Subroutine Overview:
! Thin films optical model.
! Thin films model developed from "Radiation and Optics" by John M.
! Stone.
!
! Author: Robert M. Smith
! Project: PhD research
!
! Last Revision: 1/23/98
!**********************************************************************
!
!**********************************************************************
! descriptions of variables passed to subroutine deposition_process
!**********************************************************************
!
! none
!
!**********************************************************************
! descriptions of variables used in this subroutine
!**********************************************************************
!
! anglerad  - angle [rad]
! beta2     - constant for polysilicon film
! beta3     - constant for SiO2 film
! dangle    - angle, 1 deg. expressed in [rad]
! d2        - thickness of polysilicon film [micrometers]
! d3        - thickness of SiO2 film [micrometers]
! emissivity - emissivity of wafer per cell
! eps       - spectral, directional emissivity
! epslambda - spectral, hemispherical emissivity
! film      - thickness of deposited film on each cell [nm]
! f0-f3     - coefficients of Simpson's rule
! iangle    - angle [degrees]
! ircells - number of cells in the radial direction (j1 index)
! ithetacells - number of cells in the theta direction (j2 index)
! j1 - index for r direction
! j2 - index for theta direction
! k0 - vacuum wave number
! lambda - wavelength [micrometers]
! Mpi - films pi coefficient matrix
! Msigma - films sigma coefficient matrix
! n1 - refractive index of vacuum (Argon)
! n2 - refractive index of poly-Si
! n3 - refractive index of SiO2
! n4 - refractive index of Si wafer
! Pi - Pi
! R - reflectivity
! rpi - reflection coefficient
! rsigma - reflection coefficient
! t# - temporary variable
! theta1 - incident angle at vacuum/poly-Si interface [rad]
! theta2 - reflection angle in poly-Si [rad]
! theta3 - reflection angle in SiO2 [rad]
! theta4 - reflection angle in Si wafer [rad]
! Y1pi - film coefficient
! Y1sigma - film coefficient
! Y2pi - film coefficient
! Y2sigma - film coefficient
! Y3pi - film coefficient
! Y3sigma - film coefficient
! Y4pi - film coefficient
! Y4sigma - film coefficient

!**********************************************************************
! variable declarations
!**********************************************************************

! implicit none
integer:: iangle,j1,j2
real*8:: angerad,beta2,beta3,dangle,d2,d3, &
& epslambda,f0,f1,f2,f3,k0,lambda,n1, &
& n2,n3,n4,Pi,R,theta1,theta2,theta3, &
& theta4,Y1pi,Y1sigma,Y2pi,Y2sigma, &
& Y3pi,Y3sigma,Y4pi,Y4sigma
real*8:: t1,t2,t3,t4,t5,t6,t7,t9,t10,t16,t19
real*8:: eps(0:90)
complex*16:: rpi,rsigma,t13,t14,t20,t21
complex*16:: Mpi(1:2,1:2),Msigma(1:2,1:2)

Pi=4.0d0*datan(1.0d0)
!

! defining wavelength & vacuum wave number
!**********************************************************************
!
lambda=3.4188d0
k0=2.0d0*Pi/lambda
!

!**********************************************************************
!
! defining refractive index data
!
! layer 1: Ar/SiH4 gas
! layer 2: poly-Si film
! layer 3: SiO2 film
! layer 4: Si wafer
!
! dispersion data from "Handbook of Infrared Optical Materials" edited
! by Paul Klocek. Dispersion data for SiO2 for wavelengths [0.185-7]
!**********************************************************************
!
n1=1.000259d0 ! n of Ar gas
if (lambda <= 5.0d0) then ! n of poly-Si
    n2=0.35241D1-0.55415D-1*lambda+ &
        & 0.11016D-1*lambda**2-0.77091D-3*lambda**3
else if (lambda >= 5.0d0 .and. &
    & lambda <= 12.0d0) then
    n2=0.34465D1-0.66634D-2*lambda+ &
        & 0.60911D-3*lambda**2-0.19207D-4*lambda**3
else if (lambda >= 12.0d0 .and. &
    & lambda <= 25.0d0) then
    n2=0.34226D1-0.16155D-3*lambda+ &
        & 0.25901D-5*lambda**2
else
    n2=3.4201d0
endif
if (lambda <= 0.508d0) then ! n of SiO2
    n3=0.21509D1-0.41098D1*lambda+ &
        & 0.96671D1*lambda**2-0.76716D1*lambda**3
else if (lambda >= 0.508d0 .and. &
    & lambda <= 7.0d0) then
    n3=0.157D1-0.39D-1*lambda+0.115D-1* &
        & 0.2D-2*lambda**2-0.2D-2*lambda**3
else
n3=1.167d0
endif
n4=n2 ! n of Si wafer
!
**********************************************************************
! SiO2 film thickness [Angstroms --> micrometers]
! Notes:
! 1) film is 1000 Angstroms thick
! 2) dividing by 1.0e4 converts Angstroms to micrometers
**********************************************************************
!
d3=1000.0d0/1.0d4 ! SiO2 film
!
**********************************************************************
! do loops for r and theta
**********************************************************************
!
do j1=1,ircells
do j2=1,ithetacells
  !
  !****************************************************************
  ! specify poly-Si film thickness for cell [micrometers]
  ! Notes:
  ! 1) the variable film has units of [nm]
  !****************************************************************
  
d2=film(j1,j2)/1.0d3 ! poly-Si film
!
**********************************************************************
! vary the incident polar angle of radiation from [0-90 deg.] in
! 1 degree increments.
**********************************************************************
!
do iangle=0,89
  theta1=iangle/180.0d0*Pi ! incident angle [rad]
  !
  !****************************************************************
  ! Snell's Law
  !****************************************************************
  
  theta2=dasin(n1*dsin(theta1)/n2) ! angle film 2 [rad]
  theta3=dasin(n1*dsin(theta1)/n3) ! angle film 3 [rad]
  theta4=dasin(n1*dsin(theta1)/n4) ! angle wafer [rad]
!
Appendix A

!****************************
! beta
!****************************
!
beta2=n2*k0*cos(theta2)
beta3=n3*k0*cos(theta3)
!
!****************************
! Y coefficients
!****************************
!
Y1pi=n1/cos(theta1)
Y1sigma=n1*cos(theta1)
Y2pi=n2/cos(theta2)
Y2sigma=n2*cos(theta2)
Y3pi=n3/cos(theta3)
Y3sigma=n3*cos(theta3)
Y4pi=n4/cos(theta4)
Y4sigma=n4*cos(theta4)
!
!****************************
! M matrices
!****************************
!
t1=beta2*d2
t2=cos(t1)
t3=beta3*d3
t4=cos(t3)
t5=t2*t4
t6=1.D0/Y2pi
t7=sin(t1)
t9=sin(t3)
t10=Y3pi*t9
t13=cmplx(0.D0,1.D0)
t14=t13*t2
t16=1.D0/Y3pi*t9
t19=t7*t4
Mpi(1,1)=t5-t6*t7*t10
Mpi(1,2)=-t13*Y2pi*t19-t14*t10
Mpi(2,1)=-Y2pi*t7*t16+t5
Mpi(2,2)=-Y2pi*t7*t16+t5

t1=beta2*d2
t2=cos(t1)
t3=beta3*d3
t4=cos(t3)
t5=t2*t4
t6=1.D0/Y2sigma
t7=sin(t1)
t9=sin(t3)
t10=Y3sigma*t9
t13=complx(0.D0,1.D0)
t14=t13*t2
t16=1.D0/Y3sigma*t9
t19=t7*t4
Msigma(1,1)=t5-t6*t7*t10
Msigma(1,2)=-t14*t16-t13*t6*t19
Msigma(2,1)=-t13*Y2sigma*t19-t14*t10
Msigma(2,2)=-Y2sigma*t7*t16+t5

! reflection coefficients

rpi=(t20-Mpi(1,1)-Mpi(1,2)*Y4pi)*Y1pi
rpi=abs(rpi)**2

rsigma=(t20-Msigma(1,1)+Msigma(1,2)*Y4sigma)*Y1sigma
rsigma=abs(rsigma)**2

R=(rpi+rsigma)/2

eps(iangle)=1-R
Appendix A

*calculate spectral, hemispherical emissivity: epslambda.*
*radiation is assumed to vary directionally with polar angle.*
*using Simpson's 1/3 & 3/8 rules to complete calculation.*

epslambda=0.0d0
dangle=1.0d0/180.0d0*Pi ! 1 deg. [rad]
do iangle=0,82,2 ! Simpson's 1/3 rule
  anglerad=iangle/180.0d0*Pi ! incident angle [rad]
  t1=anglerad+dangle
  t2=anglerad+2.0d0*dangle
  f0=eps(iangle)*cos(anglerad)* &
     & sin(anglerad)
  f1=eps(iangle+1)*cos(t1)*sin(t1)
  f2=eps(iangle+2)*cos(t2)*sin(t2)
  epslambda=epslambda+dangle/3.0d0* &
     & (f0+4.0d0*f1+f2)
end do

do iangle=84,87,3 ! Simpson's 3/8 rule
  anglerad=iangle/180.0d0*Pi
  t1=anglerad+dangle
  t2=anglerad+2.0d0*dangle
  t3=anglerad+3.0d0*dangle
  f0=eps(iangle)*cos(anglerad)* &
     & sin(anglerad)
  f1=eps(iangle+1)*cos(t1)*sin(t1)
  f2=eps(iangle+2)*cos(t2)*sin(t2)
  f3=eps(iangle+3)*cos(t3)*sin(t3)
  epslambda=epslambda+dangle/3.0d0* &
     & 8.0d0*(f0+3.0d0*f1+3.0d0*f2+f3)
enddo

!****************************************************************
! copy epslambda to emissivity of a specific cell
!****************************************************************
emissivity(j1,j2)=2.0d0*epslambda
end do
end do

return
end subroutine optics
Fortran Subroutine: Output

subroutine output(i1,irowA,isec)
use global_data, only: A, emissivity, film, &
 & key_data, ircells, izcells, u
!
!
!**********************************************************************
! Subroutine Name: output
!
! Subroutine Overview:
! Fortran subroutine that saves key process data at 1 second
! intervals. The data is saved to disk when the program ends.
!
! Author: Robert M. Smith
! Project: PhD research
!
! Last Revision: 3/5/98
!**********************************************************************
!
!**********************************************************************
! descriptions of variables passed to the master program
!**********************************************************************
!
! i1                  - index of analog time loop
! irowA               - last row of analog data
! isec               - time [s]
!
!**********************************************************************
! descriptions of variables used in this subroutine
!**********************************************************************
!
! A                   - Labview data
! emissivity          - emissivity of wafer per cell
! film                - deposited film [nm]
! key_data            - process data saved to disk
! ircells            - No. radial cells (j1 index)
! izcells             - No. z cells (j3 index)
! j1                 - index for r direction
! j4                 - 2nd index for key_data
! j5                 - 3rd index for key_data
! u                  - temperature of each cell [K]
!**********************************************************************
! variable declarations
!**********************************************************************
!
implicit none
!
integer:: i1,irowA,isec,j1,j4,j5
!
!**********************************************************************
! identify 1 second intervals & record key_data
! Notes:
! 1) time [s]
! 2) temperature [deg. C]
! 3) emissivity
! 4) film thickness [Angstroms]
!**********************************************************************
!
if (A(i1,1) >= isec) then
  do j1=1,ircells
    key_data(j1,1,isec)=A(i1,1) ! time
    key_data(j1,2,isec)=j1 ! cell
    key_data(j1,3,isec)=u(j1,1,izcells)- & ! wafer temperature
                           & 273.0d0
    key_data(j1,4,isec)=emissivity(j1,1) ! wafer emissivity
    key_data(j1,5,isec)=film(j1,1)*10.0d0 ! film thickness
  end do
  isec=isec+1
end if
!
!**********************************************************************
! write process data to disk after process has terminated
!**********************************************************************
!
if (i1 == irowA) then
  open(unit=10,file='c:\bsmith\solution.txt', &
       status='unknown')
  write(unit=10,fmt=201) ! file header
  do j5=1,200
    do j1=1,ircells
      write(unit=10,fmt=202) &
                         (key_data(j1,j4,j5),j4=1,5)
    end do
  end do
  close(10)
endif
201 format(' time[s] cell temp.[deg.C] emissivity film[Ang.]')
202 format(f6.2,x,f3.0,x,f6.1,x,f5.3,x,f6.1)
!
!
return
end subroutine output
APPENDIX B
LabVIEW® Program: DAQ.vi

Front Panel

### Board 1: Serial Communications
- **Elapsed Time of Experiment**
- **Transistor Name**
- **Channel**
- **Serial Communications**
  - **Serial Port**
  - **Link**
  - **Baud Rate**

### Board 2: Analog Signals
- **Error Message (Data Acq.)**
  - **No error has occurred**
- **Timestamp[s]**
- **5.00 Vdc**
- **ion-gauge (m-spec)**

### File Header
- **Stop Date Acquisition**
- **Target Film Thickness [Å]**
- **Target Temp. [deg. C]**
- **Target Pressure [torr]**

### Channels
- **Display Channel**
- **Channels Acquired**
  - #0: 5.00 Vdc (default on, power supply)
  - #1: ion gauge (m-spec)
  - #2: ion gauge (m-spec)
  - #3: ion gauge (m-spec)
  - #4: ion gauge (m-spec)
  - #5: ion gauge (m-spec)
  - #6: ion gauge (m-spec)
  - #7: ion gauge (m-spec)

### Random Scan Parameters
- **DAQ Interval [ms]**
  - 0 - 10 V
- **Range**
  - 0 - 10 V

### Display Channel
- **Emission**
- **Electron Multiplier**
- **EM Voltage**

### DAQ Interval [ms]
- 0 - 10 V

### Random Scan Parameters
- **No Error**
- **Source**

### Error Message (File R & W)
- **Sensor1**
- **Name**
  - **Sensor2**
  - **Name**

### Link Parameters
- **Mass [AMU]**
- **Dwell [ms]**
- **Upper limit**
- **Lower limit**
  - **SP Noise**

### Random Scan Parameters
- **No Error**
- **Source**

### Stop Data Acquisition
- **EM Voltage**
  - 0.00 E+0

### Deposition Prediction
- **Target Film Thickness [Å]**
- **Target Temp. [deg. C]**
- **Target Pressure [torr]**

### Deposition Started (yes/no)
- **Deposition Finished (yes/no)**

### Random Scan Parameters
- **RTCD Pressure [torr]**
- **H₂ Background**
- **H₂ Signal**
- **H₂ Total**
- **Wafer Temp. [deg. C]**
- **Wafer Diameter [mm]**
- **H₂ Flow [cc/min]**
Sequence 0: initiate communication with the mass spec.

Open communications with mass spec and start instrument.

Note: for this program to operate in its intended manner, the emission of the mass spec must already be on. To accomplish this run the VI titled Startup.vi.

Program Note: code is intended to start here and does some initialization work. Flow of the program then proceeds to Sequence 1 where two While Loops concurrently acquire data from both the fibers using the A/D board and the mass spec using the serial card at different frequencies. Control is then passed to the second sequence where the data is bundled and written to a file.
Sequence 3: Save data to file.

Comments:
1) data in matrix form is received from Sequence 2 using a Sequence Local
2) data matrix transposed
3) data then converted to string with exponential format
4) while data is being prepared for file, a new file is opened and a header written to the file
5) next the data, in string format, is written to file
6) finally the file is closed
7) an error routine is used to output any errors associated with writing the file to the panel window
Appendix B

Acquire analog signals

H₂⁺ background signal started (yes/no)
Block Diagram
This program is designed to determine the repeatability of the mass spec by sampling Nitrogen. It records the mass spec pressure before and after sampling.

- **Read System Information from Instrument**
  - **Link Parameters**
  - **Error Out (System Info)**

- **Set Status Lights to Default Off**
  - **default: off**
  - **Electron Multiplier**
  - **Emission**

- **scanning EM setting #0**

- **MS scan #**
  - **p1 [torr]**
  - **p2 [torr]**
  - **AMU intensity [A]**

- **Statistics mean / st dev.**
  - **Y Maximum**
  - **Y Minimum**
  - **Y Precision**
  - **Y Format**

- **X Maximum**
- **X Minimum**
- **X Precision**
- **X Format**
- **XY Chart**

- **Turn emission and electron multiplier on and check that both attributes are turned on**

- **Electron Multiplier**
  - **Emult**
  - **HDW**

- **Emission**
  - **Emission**
  - **Turn emission and electron multiplier on and check that both attributes are turned on**

- **F21 Emis OFF**
- **F22 EM ON**
- **F23 EM OFF**
- **F20 Emis ON**
Appendix B

EM settings

Acquires mass spec pressure signal after mass spec data is acquired.

- Board #
- Low channel
- High channel
- Rate
- ConvertData
- Mode
- Formula Node: D/A conversion
- Index Array

Formula Node: calculate pressure in torr

\[ p_2 \text{ [torr]} = \frac{20(x - \text{floor}(x)) - 10 \cdot \text{floor}(2(x - \text{floor}(x)))}{10^{11 + \text{floor}(2x)}}; \]

Acquires mass spec pressure signal before mass spec data is acquired.

- Board #
- Low channel
- High channel
- Rate
- ConvertData
- Mode
- Formula Node: D/A conversion
- Index Array

Formula Node: calculate pressure in torr

\[ p_1 \text{ [torr]} = \frac{20(x - \text{floor}(x)) - 10 \cdot \text{floor}(2(x - \text{floor}(x)))}{10^{11 + \text{floor}(2x)}}; \]

Range

2 [torr]
Appendix B

Random Scan Parameters

- Error Out (Scan Para.)
- AMU intensity [A]
- EM Voltage

Mass spec scans

7500 ms wait mass spec data acquisition

File Header

- Error Out (File R & W)

write data to disk

- function
- new file
- File Header
LabVIEW® Program: Startup.vi

Front Panel

Block Diagram
Error Message: Degas

Error Message: Sequential Scan 3
LabVIEW® Program: Timer2.vi

Front Panel

Block Diagram
# Maple program: Emissivity
#
# author: Robert M. Smith
# Interference of optical wave in polysilicon,
# SiO2 film & Si wafer. Program includes
# variable incident polar angle [0-pi/2]
#
# variables
#
# d2 - thickness of polysilicon film [Å]
# d3 - thickness of SiO2 film [Å]
# f0-3 - parts of Simpson's rule
# Isimpson - results from Simpson's rule
# k0 - parameter involving wavelength [1/μm]
# lambda - wavelength [μm]
# Mpi - coefficient matrix M2pi*M3pi
# Msigma - coefficient matrix M2sigma*M3sigma
# M2pi - coefficient matrix for polysilicon film
# M2sigma - coefficient matrix for polysilicon film
# M3pi - coefficient matrix for SiO2 film
# M3sigma - coefficient matrix for SiO2 film
# n1 - real refractive index of Ar/SiH4 gas
# n2 - real refractive index of poly-Si
# n3 - real refractive index of SiO2
# n4 - real refractive index of Si wafer
# t1-4 - temp. variables used in Simpson's rule
# Y2pi - film coefficient
# Y2sigma - film coefficient
# Y3pi - film coefficient
# Y3sigma - film coefficient
# beta2 - constant for polysilicon film
# beta3 - constant for SiO2 film
# lambda - wavelength [μm]
# theta1 - incident angle of radiation at gas poly-Si interface [rad]
# theta2 - incident angle of radiation at poly-Si SiO2 interface [rad]
# theta3 - incident angle of radiation at SiO2 Si wafer interface [rad]
# theta4 - transmission angle of radiation in Si wafer
#
# defining refractive index data
n1:=1.000259:
n2:=3.43:
n3:=1.46:
n4:=3.43:

# defining wavelength & constant
lambda:=0.966;
k0:=evalf(2*Pi/lambda):

# defining film thickness of SiO2
d3:=1000:

d3:=d3/1e4:

# vary incident angle of radiation over polar angles
# from [0-pi/2]. 1 deg. increments.
for j from 0 by 1 to 30 do
  # update film thickness
  d2[j]:=j*100:
  print(j,d2[j]);
  d2a:=d2[j]/1e4:

  for i from 0 by 1 to 90 do
    # incident angle of radiation on poly-Si film
    theta1:=evalf(i/180*Pi):

    # Snell's Law
    theta2:=evalf(arcsin(n1*sin(theta1)/n2));
    theta3:=evalf(arcsin(n1*sin(theta1)/n3));
    theta4:=evalf(arcsin(n1*sin(theta1)/n4));

    # Beta

beta2 := n2 * k0 * cos(theta2);
beta3 := n3 * k0 * cos(theta3);

# Y coefficients

Y1pi := n1 / cos(theta1);
Y1sigma := n1 * cos(theta1);
Y2pi := n2 / cos(theta2);
Y2sigma := n2 * cos(theta2);
Y3pi := n3 / cos(theta3);
Y3sigma := n3 * cos(theta3);
Y4pi := n4 / cos(theta4);
Y4sigma := n4 * cos(theta4);

# define M matrices

with(linalg):
M2pi := linalg[ matrix ](2, 2, [cos(beta2 * d2a), -I / Y2pi * sin(beta2 * d2a),
                          -I * Y2pi * sin(beta2 * d2a), cos(beta2 * d2a)]):
M2sigma := linalg[ matrix ](2, 2, [cos(beta2 * d2a), -I / Y2sigma * sin(beta2 * d2a),
                                 -I * Y2sigma * sin(beta2 * d2a), cos(beta2 * d2a)]):
M3pi := linalg[ matrix ](2, 2, [cos(beta3 * d3), -I / Y3pi * sin(beta3 * d3),
                                -I * Y3pi * sin(beta3 * d3), cos(beta3 * d3)]):
M3sigma := linalg[ matrix ](2, 2, [cos(beta3 * d3), -I / Y3sigma * sin(beta3 * d3),
                                  -I * Y3sigma * sin(beta3 * d3), cos(beta3 * d3)]):
Mpi := evalm(M2pi &* M3pi):
Msigma := evalm(M2sigma &* M3sigma):

# calculate reflection coefficients

rpi := abs(rpi)^2:
rsigma := ((Msigma[1, 1] + Msigma[1, 2] * Y4sigma) * Y1sigma -
           (Msigma[2, 1] + Msigma[2, 2] * Y4sigma)) / ((Msigma[1, 1] + Msigma[1, 2] * Y4sigma) * Y1sigma +
           (Msigma[2, 1] + Msigma[2, 2] * Y4sigma)):
rsigma := abs(rsigma)^2:

# calculate reflection
# R := (rpi + rsigma) / 2:

# calculate the spectral, directional emissivity
# epsilon[i,j]:=1-R:
# print(i,epsilon[i,j]);
od:
od:
#
# calculate the spectral, hemispherical emissivity
#
Isimpson:=0:
t1:=1/180*Pi:
for j from 0 by 1 to 30 do
  for i from 0 by 2 to 82 do
    t2:=i/180*Pi:
    f0:=epsilon[i,j]*cos(t2)*sin(t2):
    t3:=t2+t1:
    f1:=epsilon[i+1,j]*cos(t3)*sin(t3):
    t4:=t3+t1:
    f2:=epsilon[i+2,j]*cos(t4)*sin(t4):
    Isimpson:=Isimpson+evalf(2*(t1/3*(f0+4*f1+f2)));
    # print(i,Isimpson);
  od:
  for i from 84 by 3 to 87 do
    t2:=i/180*Pi:
    f0:=epsilon[i,j]*cos(t2)*sin(t2):
    t3:=t2+t1:
    f1:=epsilon[i+1,j]*cos(t3)*sin(t3):
    t4:=t3+t1:
    f2:=epsilon[i+2,j]*cos(t4)*sin(t4):
    t5:=t4+t1:
    f3:=epsilon[i+3,j]*cos(t5)*sin(t5):
    Isimpson:=Isimpson+evalf(2*(3*t1/8*(f0+3*f1+3*f2+f3))):
  od:
  print(j,Isimpson);
  Isimpson:=0:
od:
APPENDIX D
Matlab Program: Insight.m

%***************************************************************************
% Program Name: insight.m
%
% Program Overview:
% Matlab program for reading files containing
data acquired by the real-time data
% acquisition system. Digital data is
% converted to physical data and plotted.
%
% author: Robert M. Smith
% project: PhD research
% last revision: 7/8/98
%***************************************************************************
%***************************************************************************
% variables
%***************************************************************************
%
% A - matrix of numerical data from data file
% B - matrix of temperature in [C]
% fid - file identifier used for opening data files
% file - name of data file without extension
% header - text header of data file
% header2 - header variable with data reformatted
% h1-5 - handle for figures 1-5
% i - indice used for parsing data file header
% k1 - temporary variable used for parsing data file header
% k2 - temporary variable used for parsing data file header
% r0 - row number where mass spec data ends
% r - rows of variable header2
% sp - location of spaces in variable header
% sp1 - numerical representation of variable header
%
%***************************************************************************
% house keeping
%***************************************************************************
%
clear % removes all variables
clc % clears command window
close all % close all figure windows
%
% ********************************************************
% reading data file
%********************************************************
%
file = input('data file name (w/o .txt)- ','s'); % get data file name
[header,A]=hdrload([file,'.txt']); % reading data file
%
%********************************************************
% parse variable header & display on screen
%********************************************************
%
sp=findstr(header,','); % location of spaces
sp1=abs(header); % convert to numerical data
header2(1,1:sp(1))=header(1:sp(1)); % start of column header
imax=length(sp);
for i=2:imax
    k1=sp(i-1)+1; % end of column header
    k2=sp(i);
    header2(i,1:k2-k1+1)=sp1(k1:k2); % composing column headers
end
header2(imax+1,1:length(sp1)-k2)... % adding last column header
    =sp1(k2+1:length(sp1));
header2=setstr(header2); % convert number to ascii
r=size(header2,1); % number of rows in header2
fprintf(1,'

column headers (%0.0f)

',r) % number of columns
disp(header2) % column headers from file
%
%********************************************************
% calibration data & conversion of digital data
% to physical data
%
% DAQ board calibrated 10/15/96
% calibration results
% A/D signals [0, 2048, 4090]
% voltage [0, 4.998, 9.985V]
%
% constant 5 Vdc from power supply used to check
Appendix D

% A/D board is operating correctly
%******************************************************************************%

% A(:,2)=A(:,2)*9.985/4090; % power supply voltage
%******************************************************************************%

% pressure of ion gauge on mass spec vacuum system
%******************************************************************************%

% A(:,3)=A(:,3)*9.985/4090; % A/D data to voltage
A(:,3)=(20*(A(:,3)-floor(A(:,3)))-10*floor(2*(A(:,3)-floor(A(:,3))))).*10.^(11-floor(2*A(:,3)));
%******************************************************************************%

% pressure of Convectron gauge on mass spec vacuum system
%******************************************************************************%

% A(:,4)=A(:,4)*9.985/4090; % A/D data to voltage
A(:,4)=(20*(A(:,4)-floor(A(:,4)))-10*floor(2*(A(:,4)-floor(A(:,4))))).*10.^(11-floor(2*A(:,4))); % torr -> mtorr
A(:,4)=A(:,4)*1000; %******************************************************************************%

% temperature of optical probe #1
% data recorded over the temp range [400,700 C]
% calibration curve for voltage >=0.33V
% calibration curve computes temps. in Celcius
%******************************************************************************%

% A(:,5)=A(:,5)*9.985/4090; % convert A/D data to voltage
for i=1:length(A(:,5))
    if A(i,5)>=0.33
        A(i,5)=-286.89+2121.5*A(i,5); % deg. C
        A(i,5)=A(i,5)+273.15; % deg. K
    else
        A(i,5)=0; % no calibration for V<0.33V
    end
end
%******************************************************************************%

% temperature for optical probe #2
no probe present at this time
%***********************************************************************
A(:,6)=A(:,6)*0;
%***********************************************************************
temperature for pyrometer
% no pyrometer signal captured at this time
% [0-5V] --> [0-1000C]
%***********************************************************************
A(:,7)=A(:,7)*9.985/4090*1000/5+273.15; % convert A/D data to voltage
%***********************************************************************
butterfly valve position
% [0-10V] --> [0-100% open]
%***********************************************************************
A(:,8)=A(:,8)*9.985/4090*100/10;
%***********************************************************************
RTP pressure
% [0-10V] --> [0-10 torr]
%***********************************************************************
A(:,9)=A(:,9)*9.985/4090;
%***********************************************************************
plotting data
%***********************************************************************
set(0,'DefaultAxesFontName','Times') % set default font for session
h1=figure; % 1st figure window
subplot(2,1,1) % creating subplot 1
plot(A(:,1),A(:,2)) % creating plot
legend('constant 5.00 Vdc signal') % adding legend
axis([0,inf,0,10]) % autoscaling axes
title('Test Signal Checking A/D Board') % labeling title
xlabel('time [s]') % labeling x axis
ylabel('voltage [Vdc]') % labeling y axis

subplot(2,1,2) % creating subplot 2
plot(A(:,1),A(:,8)) % creating plot
axis([0,inf,0,100]) % autoscaling axes
title('RTP Butterfly Valve Position') % labeling title
xlabel('time [s]') % labeling x axis
ylabel('valve position [% open]') % labeling y axis
%
%********************************************************
% pressure signals
%********************************************************
%
h2=figure; % 2nd figure window

subplot(3,1,1) % creating subplot 1
semilogy(A(:,1),A(:,3) % creating plot
legend('Stableion (mass spec, Ar)') % adding legend
axis([0,inf,1e-7,1e-4]) % autoscaling axes
title('Pressure') % labeling title
ylabel('pressure [torr]') % labeling y axis

subplot(3,1,2) % creating subplot 2
plot(A(:,1),A(:,4)) % creating plot
legend('Conveutron (mass spec), Ar') % adding legend
axis([0,inf,0,250]) % autoscaling axes
ylabel('pressure [mtorr]') % labeling y axis

subplot(3,1,3) % creating subplot 3
plot(A(:,1),A(:,9)) % creating plot
legend('Baratron manometer (RTP)') % adding legend
axis([0,inf,0,10]) % autoscaling axes
xlabel('time [s]') % labeling x axis
ylabel('pressure [torr]') % labeling y axis
%
%********************************************************
% temperature
%********************************************************
%
h3=figure; % 3rd figure window

subplot(3,1,1) % creating subplot 1

plot(A(:,1),A(:,[5,7])) % creating plot
legend('probe#1','pyrometer') % adding legend
axis([0,inf,0,1500]) % autoscaling axes
title('Wafer Temperature') % labeling title
ylabel('temperature [K]') % labeling y axis

subplot(3,1,2) % creating subplot 2
plot(A(:,1),A(:,[5,7])) % creating plot
legend('probe#1','pyrometer') % adding legend
axis([0,inf,900,1050]) % autoscaling axes
ylabel('temperature [K]') % labeling y axis

subplot(3,1,3) % creating subplot 3
B(:,[1,2,3])=A(:,[5,6,7])-273.15; % convert temperature to [C]
plot(A(:,1),B(:,[1,3])) % creating plot
legend('probe#1','pyrometer') % adding legend
axis([0,inf,0,1000]) % autoscaling axes
xlabel('time [s]') % labeling x axis
ylabel('temperature [K]') % labeling y axis

%********************************************************
% mass spectrometer data
% Si, N2, SiH+, SiH2+, SiH3+, SiH4+
%********************************************************

h4=figure; % 4th figure window
r0=find(A(:,11)==0); % locate zeroes in data
r0=r0(1)-1; % last row of data
subplot(2,1,1) % creating subplot 1
semilogy(A(1:r0,10),A(1:r0,14),'-',... % creating plot
A(1:r0,10),A(1:r0,15),'-',...
A(1:r0,10),A(1:r0,16),'-',...
A(1:r0,10),A(1:r0,17),'.w',...
A(1:r0,10),A(1:r0,18),':g')
legend('Si+ with N2+ purge','SiH+','SiH2+','SiH3+','SiH4+') % adding legend

% In data file, columns of mass spec data are
% buffered with zeroes because less mass spec
% than analog signals are acquired. The next
% two lines of code find the end of the mass
% spec data so the zeroes are not plotted
%********************************************************

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
axis([0,inf,1e-10,1e-8]) % autoscaling end of x axis
title('Reaction products') % labeling title
xlabel('time [s]') % labeling x axis
ylabel('intensity [A]') % labeling y axis

subplot(2,1,2)
semilogy(A(1:r0,10),A(1:r0,12)) % creating plot
legend('AMU 18') % adding legend
axis([0,inf,1e-11,1e-9]) % autoscaling end of x axis
title('Reaction products') % labeling title
xlabel('time [s]') % labeling x axis
ylabel('intensity [A]') % labeling y axis

%********************************************************
% mass spectrometer data
% H2+
% Ar++, Ar+
% ********************************************************
% h5=figure; % 5th figure window

subplot(2,1,1) % creating subplot 1
semilogy(A(1:r0,10),A(1:r0,11)) % creating plot
legend('H2+') % adding legend
axis([0,inf,1e-9,1e-7]) % autoscaling end of x axis
title('Reaction products') % labeling title
xlabel('time [s]') % labeling x axis
ylabel('intensity [A]') % labeling y axis

subplot(2,1,2) % creating subplot 2
semilogy(A(1:r0,10),A(1:r0,13),'-',... % creating plot
    A(1:r0,10),A(1:r0,19),'--') % adding legend
legend('Ar++','Ar+') % autoscaling end of x axis
title('Reaction products') % labeling title
xlabel('time [s]') % labeling x axis
ylabel('intensity [A]') % labeling y axis

%********************************************************
% data plotted is assumed to be in the following format
% column #1  time stamp for analog signals
% column #2  5.00Vdc signal from power supply
% column #3  ion guage (mass spec)
% column #4  convectron guage (mass spec)
% column #5  fiber optic probe #1
% column #6  fiber optic probe #2
% column #7  pyrometer (RTP)
% column #8  butterfly valve position (RTP)
% column #9  pressure guage (RTP)
% column #10 time stamp for mass spec signals
% column #11 H2+  signal (AMU=2)
% column #12 H2O+  signal (AMU=18)
% column #13 Ar++  signal (AMU=20)
% column #14 Si+   signal (AMU=28)
% column #15 SiH+  signal (AMU=29)
% column #16 SiH2+ signal (AMU=30)
% column #17 SiH3+ signal (AMU=31)
% column #18 SiH4+ signal (AMU=32)
% column #19 Ar+   signal (AMU=40)

%******************************************************************************
%
%******************************************************************************
%
% end of program
Matlab Subroutine: Hdrload.m

function [header, data] = hdrload(file)

% HDRLOAD Load data from an ASCII file containing a text header.
% [header, data] = HDRLOAD('filename.ext') reads a data file
% called 'filename.ext', which contains a text header. There
% is no default extension; any extensions must be explicitly
% supplied.
%
% The first output, HEADER, is the header information, returned
% as a text array.
% The second output, DATA, is the data matrix. This data matrix
% has the same dimensions as the data in the file, one row per
% line of ASCII data in the file. If the data is not regularly
% spaced (i.e., each line of ASCII data does not contain the same
% number of points), the data is returned as a column vector.
%
% Limitations: No line of the text header can begin with
% a number. Only one header and data set will be read,
% and the header must come before the data.
%
% See also LOAD, SAVE, SPCONVERT, FSCANF, FPRINTF, STR2MAT.
% See also the IOFUN directory.
%
% check number and type of arguments
%
if nargin <1
    error('Function requires one input argument');
elseif ~isstr(file)
    error('Input argument must be a string representing a filename');
end
%
% Open the file. If this returns a -1, we did not open the file
% successfully.
%
fid = fopen(file);
if fid== -1
    error('File not found or permission denied');
end
%
% Initialize loop variables
% We store the number of lines in the header, and the maximum length
% of any one line in the header. These are used later in assigning
% the 'header' output variable.
% no_lines=0;
% max_line=0;

% We also store the number of columns in the data we read. This way
% we can compute the size of the output based on the number of
% columns and the total number of data points.
% ncols=0;

% Finally, we initialize the data to [].
% data=[];

% Start processing.
% line=fgetl(fid);
if ~isstr(line)
disp('Warning: file contains no header and no data')
end;
[data,ncols,errmsg,nxtindex]=sscanf(line,'%f');

% One slight problem, pointed out by Peter vanderWal: If the first
% character of the line is 'e', then this will scan as 0.00e+00.
% We can trap this case specifically by using the 'next index'
% output: in the case of a stripped 'e' the next index is one,
% indicating zero characters read. See the help entry for 'sscanf'
% for more information on this output parameter.
% We loop through the file one line at a time until we find some
% data. After that point we stop checking for header information.
% This part of the program takes most of the processing time, because
% fgetl is relatively slow (compared to fscanf, which we will use
% later).
%
while isempty(data)|(nxtindex==1)
    no_lines=no_lines+1;
    max_line=max([max_line, length(line)]);
%
% Create unique variable to hold this line of text information.
% Store the last-read line in this variable.
% eval(['line',num2str(no_lines),'=',strcat('line',num2str(no_lines),')]);
% line=fgetl(fid);
if ~isstr(line)
    disp('Warning: file contains no data')
    break
end;
[data,ncols,errmsg,nxtindex]=sscanf(line,'%f');
end % while

% Now that we have read in the first line of data, we can skip the
% processing that stores header information, and just read in the
% rest of the data.
% data=[data; fscanf(fid, '%f')];
fclose(fid);

% Create header output from line information. The number of lines and
% the maximum line length are stored explicitly, and each line is
% stored in a unique variable using the 'eval' statement within the
% loop. Note that, if we knew a priori that the headers were 10 lines
% or less, we could use the STR2MAT function and save some work.
% First, initialize the header to an array of spaces.
% header=setstr(' '*ones(no_lines, max_line));
for i=1:no_lines
    varname=['line' num2str(i)];
    % Note that we only assign this line variable to a subset of this
    % row of the header array. We thus ensure that the matrix sizes in
    % the assignment are equal.
    eval(['header(i,1:length(' varname '))=' varname '];');
end

% Resize output data, base on the number of columns (as returned
% from the sscanf of the first line of data) and the total number of
% data elements. Since the data was read in row-wise, and MATLAB
% stores data in columnwise format, we have to reverse the size
% arguments and then transpose the data. If we read in irregularly
% spaced data, then the division we are about to do will work.
% Therefore, we will trap the error with and EVAL call; if the reshape
% fails, we will just return the data as is.
% eval('data=reshape(data,ncols,length(data)/ncols)'';', '');
Matlab Program: Massspec.m

% Program Name: massspec.m

% Program Overview:
% Matlab program for computing when events occur during an experiment. Program also calculates the amount of Hydrogen generated during deposition-- see variable H2area.

% Note: This program assumes insight has been run previously and the data is already memory.

% author: Robert M. Smith
% project: PhD research
% last revision: 5/20/98

% variables
% A - matrix of numerical data from data file
% c1 - number of columns of matrix A
% h2bckgrd - H2+ signal intensity when deposition starts
% h2step - H2+ generated per each time step during deposition [A]
% h2total - total H2+ generated during deposition [A]
% i1 - index of analog signals
% i2 - index of mass spec signals
% idepend - deposition over switch (0=off, 1=on)
% idepstart - Hydrogen background switch (0=off, 1=on)
% ipdep - target pressure switch (0=off, 1=on)
% itdep - target temperature switch (0=off, 1=on)
% ptarget - target deposition pressure in RTCVD chamber [Torr]
% ptol - allowable variation from pressure tolerance [Torr]
% tttarget - minimum wafer deposition temperature [K]

% house keeping
clc % clears command window
close all % close all figure windows

%***********************************************************************
% program assumes data is in the following order
% column #1  time stamp for analog signals
% column #2  5.00Vdc signal from power supply
% column #3  ion guage (mass spec)
% column #4  con vectron guage (mass spec)
% column #5  fiber optic probe #1
% column #6  fiber optic probe #2
% column #7  pyrometer (RTP)
% column #8  butterfly valve position (RTP)
% column #9  pressure guage (RTP)
% column #10 time stamp for mass spec signals
% column #11 H2+   signal (AMU=2)
% column #12 H20+  signal (AMU=18)
% column #13 Ar++  signal (AMU=20)
% column #14 Si+   signal (AMU=28)
% column #15 SiH+  signal (AMU=29)
% column #16 SiH2+ signal (AMU=30)
% column #17 SiH3+ signal (AMU=31)
% column #18 SiH4+ signal (AMU=32)
% column #19 Ar+   signal (AMU=40)
%***********************************************************************
%
%***********************************************************************
% display wafer# on screen
%***********************************************************************

disp(file)
fprintf(1,'n',file)

%***********************************************************************
% variable declaration
%***********************************************************************

h2step=0.0d0; % H2+ per time step
h2total=0.0d0; % total H2+
i2=1; % mass spec time index
idepend=0; % idepend off
idepstart=0; % idepstart off
ipdep=0; % ipdep off
iprofile=1; % temperature profile
itdep=0; % itedp off
ptarget=5.0d0; % target pressure
ptol=0.1d0; % pressure tolerance
ttarget=873.0d0; % 600 C
[r1,c1]=size(A); % size of data matrix A

% loop through analog signals
%**********************************************************************

% loop through analog signals
%**********************************************************************

for i1=1:r1

  %****************************************************
  % loop to find the massspec time that is equivalent
  % to the time stamp of the analog data
  %****************************************************
  
  while A(i2,10) < A(i1,1)
    i2=i2+1;
  end

  %****************************************************
  % the target pressure for deposition must be achieved
  % before deposition can begin
  %****************************************************
  
  if (ipdep == 0 & A(i1,9) >= ptarget - ptol &... 
    idepstart == 0)
    ipdep=1;
  end

  %****************************************************
  % the target temperature for deposition must be
  % achieved before deposition can begin
  %****************************************************
  
  if (itdep == 0 & A(i1,7) >= ttarget & idepstart == 0)
    itdep=1;
  end

  %****************************************************
  % deposition begins once both the target pressure and
  % target wafer temperature have been achieved
  %****************************************************

end

if (ipdep == 1 & itdep == 1 & idepstart == 0)
    idepstart=1;
    h2bckgrd=abs(sum(A(i2-2:i2+2,11))/5) % H2+ background
end

% Once deposition begins the amount of H2+ generated
% is computed. The H2+ generated that needs to be
% measured occurs after deposition begins but before
% deposition end.
%**************************************************************************

if (idepstart == 1 & idepend == 0)
    h2step=(A(i2,11)-h2bckgrd)*(A(i1,1)-A(i1-1,1));
    h2total=h2total+h2step;
end

% deposition ends after deposition has started, before
% deposition has ended, and the butterfly valve’s
% position exceeds 80% open
%**************************************************************************

if (idepstart == 1 & idepend == 0 & A(i1,8) > 80)
    idepend=1;
    h2total
end
end
Matlab Program: Polysurf.m

%******************************************************************************
% Program Name: polysurf.m
%
% Program Overview:
% Matlab program for creating a 3D plot of
% polysilicon & oxide films.
%
% author:  Robert M. Smith
% project:  PhD research
% last revision:  6/3/98
%******************************************************************************
% variables
%******************************************************************************
%
% D - diameter of wafer [mm]
% h1-2 - figure handles
% meanfilm - average thickness of the dep. film [Å]
% N - number of data points
% stps - grid width [mm]
% thick - film thickness [Å]
% t1 - temporary variable
% vol - volume of deposited film [mm^3]
% x - x location film measurement [mm]
% xi - x mesh location [mm]
% xp - same as x except used for plots
% x1-2 - x data used for plotting [mm]
% y - y location film measurement [mm]
% yi - y mesh location [mm]
% yp - same a y except used for plots
% y1-2 - y data used for plotting [mm]
% z - poly film thickness [Å]
% zi - z mesh film thickness [Å]
% z1-2 - z data used for plotting [mm]
%
%******************************************************************************
% house keeping
%******************************************************************************
%
clear % clears variables
clc % clears command window
close all % closes figure windows

%********************************************************
% reading data file
%********************************************************

file=input('data file name (ex: poly001)- ','s'); % get data file name
fid=fopen(fullfile(file,'.txt'),'rt');
thick=fscanf(fid,'%5f'); % reading data
fclose(fid);

thick=thick';
N=length(thick);

%********************************************************
% defining x and y position of data points for both computations & plotting.
%********************************************************

x=[-40 -20 0 20 40; ...  
   -40 -20 0 20 40;]  
   -40 -20 0 20 40;]  
   -40 -20 0 20 40;]  
   -40 -20 0 20 40];
y=[-40 -40 -40 -40 -40;]  
   -20 -20 -20 -20 -20;]  
   0 0 0 0 0;]  
   20 20 20 20 20;]  
   40 40 40 40 40];

xp=[NaN -20 0 20 NaN;]  
   -40 -20 0 20 40;]  
   -40 -20 0 20 40;]  
   -40 -20 0 20 40;]  
   NaN -20 0 20 NaN];
yp=[NaN -40 -40 -40 NaN;]  
   -20 -20 -20 -20 -20;]  
   0 0 0 0 0;]  
   20 20 20 20 20;]  
   NaN 40 40 40 NaN];

% converting thick (vector) to z (matrix)
Appendix D

%********************************************************
% z=zeros(5);
z(1,1)=(2*sum(thick([1 4]))-sum(thick([2 9])))/2;  % the following 7 lines
z(1,5)=(2*sum(thick([3 8]))-sum(thick([2 13])))/2;  % define the 4 boundary
z(5,1)=(2*sum(thick([14 19]))-sum(thick([9 20])))/2;  % nodes needed to
z(5,5)=(2*sum(thick([18 21]))-sum(thick([13 20])))/2;  % compete the 5x5
z(1,2:4)=thick([1:3]);  % matrix needed for use
z(2,1:5)=thick([4:8]);  % with the function
z(3,1:5)=thick([9:13]);
z(4,1:5)=thick([14:18]);
z(5,2:4)=thick([19:21]);
%
%********************************************************
% creating mesh over cartesian domain and computing
% zi at each node location
%********************************************************
%
sts=-40:1:40;
[xi,yi]=meshgrid(stps);
zi=interp2(x,y,z,xi,yi,'cubic');
%
%********************************************************
% creating 3D plot of data points
%********************************************************
%
h1=figure;  % create 1st figure
set(0,'DefaultAxesFontName','Times')  % set default font for session
colormap(jet)
mesh(xi,yi,zi)
zlabel('polysilicon film thickness [Å]')  % zlabel
colorbar('vert')
title(file)
xlabel('x-axis [mm]')
ylabel('y-axis [mm]')
hold on
%
%********************************************************
% plotting location of film thickness measurements
%********************************************************
%
zp=zeros(size(xp))+min(min(zi))-250; % raising plot from z=0
plot3(xp,yp,zp,'ko')

%**********************************************************************
% plotting flat of wafer
%**********************************************************************
%
y1=linspace(-31.75/2,31.75/2,100);
x1=zeros(1,length(y1))-47.4129;
z1=zeros(1,length(y1))+zp(1,1); % raising plot from z=0
plot3(x1,y1,z1,'k')

%**********************************************************************
% plotting circular edge of wafer
%**********************************************************************
%
x2=linspace(-47.4129,50,200);
y2=sqrt((zeros(size(x2))+50).^2-x2.^2);
z2=zeros(1,length(x2))+zp(1,1); % raising plot from z=0
plot3(x2,y2,z2,'k',x2,-y2,z2,'k')
hold off

%**********************************************************************
% integrate volume under surface
% Note: The volume is calculated by using the fact that each surface patch represents an area 1 mm² and zi denotes the height of the film on that patch. By averaging zi, the average film thickness can be calculated. Then the volume of material deposited can be computed for the surface area of the wafer.
%**********************************************************************

D=100;
vol=0;
t1=mean(zi);
meanfilm=mean(t1) % average film [Å]
vol=pi/4*D^2*meanfilm/1e7;
fprintf(1,\nvol. deposited = %6.4f mm^3\n',vol)

%**********************************************************************
% plot 2D film thickness profiles for x & y = 0
%**********************************************************************
%
h2=figure; % create 2nd figure
subplot(2,1,1) % creating subplot 1
plot(xi(41,1:81),zi(41,1:81)) % y=0
title('y=0')
xlabel('x-axis [mm]')
ylabel('film thickness [Å]')
subplot(2,1,2) % creating subplot 2
plot(yi(1:81,41),zi(1:81,41)) % x=0
title('x=0')
xlabel('y-axis [mm]')
ylabel('film thickness [Å]')

%********************************************************
% film thickness profile data for plotting with results
% predicted from fortran code. using y axis data
% for y=[0,40] because the minor flat is not in this
% direction. x axis data not considered because the
% flat adversely effects film uniformity
%********************************************************

filmprofile=zeros(41,2);
filmprofile(1:41,1)=yi(41:81,41);
filmprofile(1:41,2)=zi(41:81,41);

end