APPLICATION OF DIMENSIONAL ANALYSIS TO STATISTICAL PROCESS MODELING

by

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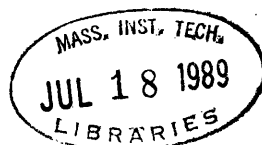## MASSACHUSETTS INSTITUTE OF TECHNOLOGY

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ABSTRACT

This work explores the use of Dimensional Analysis as a technique for combining the benefits of empirical modeling and analytical modeling for physical processes. Two processes in the semiconductor industry, Low Pressure Chemical Vapor Deposition (LPCVD) of Polysilicon and LPCVD of Low Temperature Oxide, are dimensionally analyzed and experimentally modeled. The grouped parameters that Dimensional Analysis yields are shown to be physically more significant than the primitive variables, that is, variables that are directly and independently controlled, and therefore model processes much better. Furthermore, the set of dimensionless, grouped parameters is smaller in number than the set of primitive variables, thereby reducing the total number of experiments needed to characterize a process. For each process, the "best" polynomial regression to experimental data is found for both the dimensionless parameters and the primitive variables. The average ratio of dimensionless parameter model F-tests to primitive variable model F-tests is 5:1 for polysilicon, and 2.25:1 for LTO. Also, an "Application" theorem, which measures the modeling and design of experiments gain yielded by Dimensional Analysis is presented. This "Application" theorem parallels the Pi theorem, but is adapted to fit the specific needs of manufacturing processes.

The experimental aspect of this work involved minimizing the wafer to wafer variance of the Low Temperature Oxide process. This was achieved by designing and performing an orthogonal array of eighteen experiments that characterized the growth rate of the process. Models of the film deposition for eleven evenly distributed wafers were created and evaluated using the L_{18} array. These models were then used to calculate the wafer to wafer variance. The variance was reduced from eleven percent to six percent.

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1.0   INTRODUCTION

1.1   Motivation

Modeling of physical processes has traditionally been either analytically or empirically based. The analytical approach centers on the solution of mathematical equations that describe the physical situation. Examples of this approach include finite difference and finite element solutions to stress-strain problems and fluid flow problems by Jensen [1] and Wahl [2]. Empirical solutions rely on curve fitting of data, a prime example being polynomial response surfaces commonly used for the modeling of chemical processes [3].

A principal strength of analytical modeling is the ability to extrapolate when predicting the response of a process far from the operating point currently being used. Other advantages of analytically based models include the generalization of the solution to other similar problems, an understanding of the process that comes with the solving of the problem, and the fact that analytical modeling does not require physical access to the process being modeled.

Two key strengths of experimental modeling are the high degree of accuracy within the interpolated region of experimentation and the ease of application to systems where the underlying physics is not thoroughly understood. One common concern about experimental methods is the large number of experimental runs often needed to characterize and improve the process. This concern stems from the fact that performing experiments with on-line equipment is an expensive proposition, many times resulting in scrapped product and down-time.

1.2   Goal of current work

This effort sets out to determine if analytical modeling and experimental modeling can be combined so that the resultant models would have high interpolative and extrapolative accuracy with few experimental points. Working along this line, Prueger [4] used a few (nine) experiments to calibrate a finite-difference model giving both the accuracy of experimental methods, and the extrapolative power of mechanistic models. This paper explores the use of Dimensional Analysis as a method for combining physical and experimental modeling.

2.0   DIMENSIONAL ANALYSIS

2.1   History and Example

Dimensional analysis is a technique commonly used to simplify the analysis of complex multivariable problems in fields such as fluid mechanics and heat transfer [5] [6]. Dimensional analysis starts with a list of the primitive variables that describe a physical process. Based on their dimensions, the list of primitive variables is transformed into a set of dimensionless parameters. The set of dimensionless parameters is smaller in number than the original list of basic variables. In addition, these dimensionless variables have greater physical meaning than the primitive variables. Therefore, it is often found that physical processes may be represented by simple functions of the dimensionless groups.

A classic example of the use of dimensional analysis is the development of the Reynolds number for describing fluid flow. The Reynolds number [5] [6],

$$R_e = \frac{\rho V D}{\mu} \tag{1}$$

is a single dimensionless quantity which relates the fluid density ρ, the velocity of the fluid V, the fluid viscosity μ, and a characteristic system dimension D. If the Reynolds number is being used to simplify the analysis of the flow in pipes, the characteristic system dimension is taken to be the pipe diameter D. As an example, it has been found that a Reynolds number of approximately 2300 [5] [6] defines the boundary between laminar and turbulent fluid flow in pipes.

2.2   Basis for Pi Theorem

The cornerstone of dimensional analysis is the Pi Theorem [7], developed by E. Buckingham in 1914. The Pi theorem provides a step by step approach to the development of dimensionless groups, such as the Reynolds number, which characterize a problem. The derivation of the Pi theorem is based on the principle of dimensional homogeneity, which states that solutions for physical processes are made up of additive terms which must have

the same dimensions. For instance, all the terms in the equation of motion for a uniformly accelerating object,

$$X = X_0 + V_0 T + \frac{1}{2} g T^2 \qquad (2)$$

have dimensions of length. By placing the necessary condition of dimensional homogeneity on a physical system the ways in which variables may be combined to form a solution have been limited. It is this limitation which results in the aforementioned transformation of the original set of variables to a smaller and more physically meaningful set of dimensionless parameters.

The principle of dimensional homogeneity is not a physically based axiom. Rather, it is derived from a more fundamental truth that deals with systems of units and measurements. The underlying concept is that physical quantities do not change simply because of a change in the units in which that quantity is measured. For example, if a board is cut to be one foot long, saying the board is twelve inches long does not change the length of the board. It is therefore a basic principle to say that any equation that truly describes a physical relationship between variables must yield correct results regardless of the fundamental units used to measure the variables.

The only way in which equation (2) can meet the requirement that physical quantities do not change if the yardstick that measures them changes is to have additive terms of the same dimensions. For instance, suppose the numerical values (with the dimensions of the terms below the numbers) of the terms of equation (2) are

$$8 = 2 + 5 + 1 \qquad (3)$$

$$L = L + L + M \qquad (4)$$

where length (L) is measured in units of meters, and mass (M) in units of kilograms. Now

let length be measured in units of centimeters or .01 meters, and mass be measured in grams or .001 kilograms. Equation (3) now reads,

$$800 = 200 + 500 + 100 \tag{5}$$

which is not a correct result. However, if the dimensions of each term in equation (4) would have been the same, our results would be:

$$8R = 2R + 5R + 1R \tag{6}$$

which is completely consistent, where R is the ratio of the new unit of measure to the old unit of measure. For instance, if the terms in equation (2) were originally measured in kilometers, and the unit of measurement for length changed to meters, R = 1000.

As this simple example demonstrates, if equations are to be independent of the system of units their variables are measured by, they must be composed of additive terms which have the same dimensions. That is, equations must obey the principle of dimensional homogeneity.

The Pi theorem provides a step by step procedure for transforming a primitive set of variables into a group of dimensionless parameters that always conforms to the principle of dimensional homogeneity. The Pi theorem is shown below. The interested reader may find the derivation in the literature [7].

2.3   The Pi Theorem

The first part of the Pi theorem determines how many parameters will affect the process after dimensional analysis is performed, while the second part of the Pi theorem describes the steps necessary to generate these dimensionless parameters.

Part I:

Any functional relationship between N variables can be reduced to a functional relationship between N-K dimensionless parameters, where K is the maximum number of dimensionally independent variables, that is variables that cannot be "power grouped" such that they form a dimensionless parameter among themselves. The dimensionless parameters referred to are of the form:

$$\text{Dimensionless Parameter} = (V_1)^{\alpha}(V_2)^{\beta}(V_3)^{\delta} \dots \tag{7}$$

where alpha, beta, and gamma are real exponents, and V_1, V_2, and V_3 are some of the N variables.

Part II:

The dimensionless groups that govern a process can be generated by adhering to the following procedure:

Step 1.

List all the variables that affect the process and their dimensions.

Step 2.

Choose K variables that are dimensionally independent, where K is defined as in Part I of the Pi Theorem.

Step 3.

Use the K chosen variables to form one dimensionless parameter for each of the N-K unchosen variables by grouping each unchosen variable with whatever powers of the K chosen variables is necessary. The dimensionless parameters should be of the form specified in equation (7).

These "power groups" are the new dimensionless variables that describe the process.

2.4   Application of Dimensional Analysis to Pipe Flow

Determining the pressure drop down a length of tube in which fluid is flowing is a common problem in the field of fluid mechanics. The variables affecting the process are the density (ρ) of the fluid, the diameter (D) and length (L) of the pipe, the velocity (V) of the fluid, and the viscosity (μ) of the fluid.

Dimensional Analysis of the pipe system, begins by listing the variables and dimensions that affect the pressure drop, as in figure (1), columns 1 and 2. Next the maximum number of variables that do not form a dimensionless parameter among themselves are chosen to "group" the remaining variables, as is done in column 3. Finally, using the chosen variables, each unchosen variable is grouped to form a dimensionless parameter, as in column 4. The result is three dimensionless quantities, one of which is the Reynolds number of equation (1).

Variable step 1	Dimensions step 1	Choose step 2	Parameter step 3
ΔP	M/LT^2		$\dfrac{\Delta P}{\rho V^2}$
D	L	✓	
ρ	M/L^3	✓	
μ	M/LT		$\dfrac{VD\rho}{\mu}$
L	L		$\dfrac{L}{D}$
V	L/T	✓	

Figure 1: Dimensional Analysis for flow in a pipe.

Since the five primitive variables that describe the process were related to one another in the form,

$$g(\Delta P, D, L, V, \rho, \mu) = 0 \qquad (8)$$

and now are known to appear only in the groups found in column 4, we may say that equation (8) is of the form,

$$g(\frac{\Delta P}{\rho V^2}, \frac{VD\rho}{\mu}, \frac{L}{D}) = 0 \qquad (9)$$

This equation may be changed to the explicit form simply by solving for the dimensionless output parameter, leaving the following functional relationship,

$$\frac{\Delta P}{\rho V^2} = f(\frac{VD\rho}{\mu}, \frac{L}{D}) \qquad (10)$$

It is of interest to note that linear regression to these parameters obeys the principle of dimensional homogeneity, as the dimensions of any term that is composed of the three dimensionless parameters is itself dimensionless. Furthermore, note that the full linear regression,

$$\Delta P = C_0 + C_1 V + C_2 D + C_3 \rho + C_4 \mu + C_5 L \qquad (11)$$

is dimensionally incorrect, as only the diameter of the tube and length of the tube have the same dimension, length. Note that a polynomial regression in primitive variables, such as the one above, can be physically correct only if each primitive variable has the same dimensions, since true constants may not have dimensions.

3.0   APPLICATION TO STATISTICAL MODELING

3.1   Modeling and Experimental Design

Once the dimensionless parameters that govern a process have been determined, it is still necessary to postulate a model and design experiments to evaluate the model. The designing of effective experimental efforts for manufacturing processes usually comes down to a trade-off between the number of experiments necessary to gain a given amount of knowledge about the system and the cost of experiments and down-time. Though the techniques of designing the most efficient experimental effort are important, it is not the goal of this work to explore this field. Instead, this work analyzes techniques for better modeling.

3.2   Gains due to use of Dimensional Analysis

The application of Dimensional Analysis to a given system creates gains related to both the design of experiments and the modeling of the process. The gain related to the design of experiments is principally due to the reduction of the number of parameters which govern a process. The gain related to the modeling of the process is due to the more physically meaningful nature of the dimensionless parameters.

As an example of how the reduction in the number of variables is transformed into a measurable experimental gain, suppose that a given process is affected by five variables, but that upon the application of Dimensional Analysis, the process is found to be affected by only three dimensionless parameters. If, at some point in time, the experimental plan called for the use of Box-Behnken [8] three level designs, a reduction from 46 experiments to 15 experiments would have been achieved.

The gain in process modeling ability due to Dimensional Analysis stems from the grouping of the primitive variables into physically meaningful dimensionless parameters. Recall that regressions of the form taken by equation (11) are in violation of the principle of dimensional homogeneity. Therefore, equation (11) could never truly reflect the process being analyzed. However, a regression comprised of dimensionless parameters, it is suspected, has a much stronger chance of describing the physical process at hand. This paper will explore whether or not this hypothesis is true.

Some measure of the two benefits is needed. To quantify how much better, if at all, processes are modeled by using regression based on dimensionless parameters instead of primtive variables, one may rely on statistical measures such as the overall F-test (See appendix D), and the individual coefficient T-tests (See appendix D). Also, one may check to see that the results given by a regression make intuitive sense.

For simple problems, Part I of the Pi theorem predicts the reduction of variables, and therefore the gain for design of experiments. However, the Pi theorem is not well suited to the more complex processes typical of manufacturing, where all the variables that affect a process are not experimented upon. It will be shown that these variables, which will be called baseline variables, drastically alter the effects of dimensional analysis, and that there is a need for an alternative theorem.

3.3   Application Theorem

As an example, suppose that one decided to experiment with the pipe flow system just analyzed. One might choose to keep D constant, since to change D would require the purchasing of a new pipe. This type of variable will be called a baseline variable, as opposed to an experimental variable, which is altered throughout the experiment. When there are baseline variables present that affect the process, the following theorem is helpful:

Application theorem

There are N - (K-k) dimensionless experimental parameters that affect a process, where:

N is the total number of experimental variables. K is the maximum number of experimental and baseline variables that cannot be grouped into a dimensionless parameter (i.e. the K variables are dimensionally independent). k is the maximum number of baseline variables that cannot be grouped into a dimensionless parameter.

Application Corollary

When choosing "grouping" variables for the Pi theorem (Part II), choose k baseline variables and (K-k) experimental variables that cannot form a dimensionless parameter among themselves. This is the cleanest way to achieve the minimum number of parameters that affect a process.

Use of the Application theorem and the accompanying corollary will be demonstrated in the following examples.

4.0   MODEL FORMULATION USING DIMENSIONAL ANALYSIS

4.1   Introduction

The processes that are analyzed in this work are used in the fabrication of integrated circuits. Both are low pressure chemical vapor deposition (LPCVD) processes, one being the Low Temperature Oxide (LTO) deposition process [9], and the other being the polysilicon deposition process [4] [10]. These processes are very similar as far as the necessary equipment is concerned, but their physical mechanisms differ extensively, and therefore, so do the form of their models.

The low pressure chemical vapor deposition process is used to deposit a thin film on a silicon wafer. In order to create the thin films, the silicon wafers, which resemble in size and surface finish compact discs, are placed in holders that are in turn placed in a quartz tube as shown in Figure 2. The pressure in the tube is pumped down to about 300 mTorr, and gases (silane, oxygen, and phosphine are some of the most common) are sprayed into the tube, via injectors found in the bottom of the tube. These gases travel down the tube toward the pump end, flowing over and adsorbing on the wafers. The adsorbed gas then reacts on the wafer surface, creating a thin layer of the desired material (Polysilicon, silicon dioxide, and doped polysilicon are some of the most common). The duration of the reaction is controlled to determine the thickness of the layer. The wafers are then sent to other steps in the integrated circuits process.
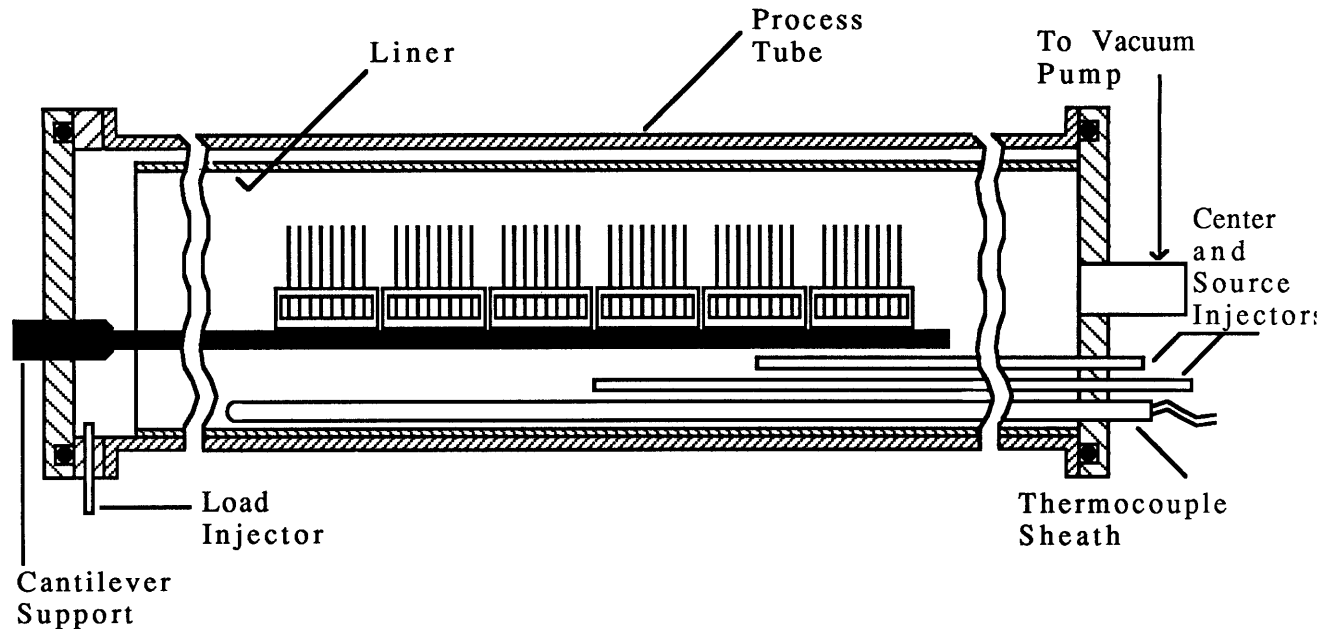
Figure 2: Deposition tube for polysilicon process. This figure is correct for the polysilicon process, for the LTO process, one more injector, the oxygen injector, is present near the load injector.

It is important that film thickness uniformity be maintained. For instance, if a film that is to be etched does not have a uniform thickness, over-etching of the thin areas will result in damage to the underlying surface and potential losses of product.

Film deposition can vary in two ways. First, the thickness can be different at the center of the wafer than at the edge of the wafer. This type of film variance is called within wafer non-uniformity. Secondly, the average film deposition on any given wafer may not be be the same as that of another wafer. This type of variance is called wafer-to-wafer non-uniformity. The principal variance for both the LTO and the polysilicon process is the wafer-to-wafer non-uniformity.

The wafer to wafer variance is due to the uneven concentrations of gases above the wafers. The gas concentration begins to become uneven when the gas first reacts on the wafer surfaces, producng a hydrogen byproduct. Both the injected gases and the hydrogen byproduct flow down the tube. The concentration of the injected gases decreases down the tube as the surface adsorption removes reactive gas molecules, and the concentration of the

hydrogen gas increases down the tube as the byproduct desorbs off of the wafer surfaces and joins the bulk flow of gas.

The increase in concentration of the byproduct near the pump end causes increased adsorption of hydrogen on the wafers in that vicinity. The adsorption of hydrogen molecules on those wafers slows the surface reaction by preventing adsorption of the injected gases onto the wafer surface, causing reduced depositon of the thin layer.

To combat the slowdown of the reaction on wafers near the pump end of the tube, process gases are injected near the pump end of the tube. The injection of process gases near the pump end increases their concentration in that area and reduces the buildup of hydrogen gases to some extent. By balancing the hydrogen buildup with an increase in the concentration of the process gases, the wafer to wafer non-uniformity can be reduced.

A more complete description of the physics behind the LTO process is presented in appendix E, as the experimental effort of this thesis is performed on the LTO process. The goal of the current modeling effort is to characterize the growth rate of LTO as a function of the experimental variables. The more accurately one can model the growth rate, the more confident one can be that a predicted, uniform profile will, in fact, turn out to be uniform. Both systems will be dimensionally analyzed, and the linear regression based on the dimensionless parameters will be compared to the linear regression based on the primitive variables.

4.2   Dimensional Analysis of the Polysilicon System

Dimensional Analysis will be applied to the modeling of the LPCVD of polysilicon in two ways. The first will be a straightforward application of the Pi theorem which will result in no gain. Then the application theorem will show that physical assumptions need to be made about the polysilicon system if Dimensional Analysis is to lead to a reduction of variables.

The polysilicon layer is created by spraying silane into the tube, and the other common gases, such as oxygen and phosphine, are left out of this process. The deposition is commonly carried out at a temperature of 625 °C and a pressure of 250 mTorr. The thickness of a typical layer is approximately 5000 angstroms.

The variables that affect the process are listed below (See figure 2).

Gr Growth rate of the polysilicon film (the output)

P Pressure in the tube

Q_1 Flow rate of silane at the front of tube

Q_2 Flow rate of silane in the middle of tube

Q_3 Flow rate of silane at the pump end of the tube

X Positon of Q3 injector

L_i Fixed geometry of tube, such as tube length

$\#$ Number of wafers

Ea_i Activation energies of various reactions (i.e. surface reactions).

RT Temperature as defined by molecular energy

M_i Molecular mass of each gas or thin film

$\%_i$ Ratios of various reaction coefficients. For example, the ratio of silane adsorption to oxygen adsorption.

The application of the Pi theorem begins by listing the variables and their dimensions, as in columns 1 and 2 of figure 3. If the variable is a baseline variable, it is labeled as such in column 1.

Variables	Dimensions	Choose	Parameters
Gr	L/T		$Gr\sqrt{M_i}/\sqrt{RT}$
P	M/LT^2		PL_i^3/RT
Q_1	M/T		$Q_1 L_i/\sqrt{M_i RT}$
Q_2	M/T		$Q_2 L_i/\sqrt{M_i RT}$
Q_3	M/T		$Q_3 L_i/\sqrt{M_i RT}$
X	L		X/L_i
L_i (baseline)	L	✓	
M_i (baseline)	M	✓	
$\%_i$ (baseline)	-0-		$\%_i$
# (baseline)	-0-		#
Ea_i (baseline)	ML^2/T^2		Ea_i/RT
RT (baseline)	ML^2/T^2	✓	

Figure 3: Failed Dimensional Analysis of polysilicon system.

Next, the maximum number (3) of variables which cannot form a dimensionless parameter by themselves is chosen, as in column 3.

Finally, each unchosen variable is grouped with as many of the chosen variables as necessary to form a dimensionless parameter, as in column 4. The dimensionless groups of column 4 are the new parameters of the problem.

Note that no reduction of variables has been achieved, as the number of experimental primitive variables (six, including growth rate) is the same as the number of experimental dimensionless parameters (six including dimensionless growth rate). Further, note that the dimensionless parameters are composed of one experimental variable, and a group of baseline variables. Since the baseline variables do not change value, the dimensionless parameters are equivalent to the primitive variables for the purpose of modeling and experimentation. Therefore, there is no experimental gain in this case.

The lack of gain in this case is due to the fact that all of the variables chosen in column 3 are baseline variables. Alternatively, one might have selected one experimental and two baseline variables. For example, Q_1, M_i, and L_i could be chosen as the dimensionally independent variables. The result would have been a different set of six dimensionless parameters,

$$\frac{GrM_i}{Q_1L_i}, \frac{Q_1}{\sqrt{PM_iL_i}}, \frac{Q_1}{Q_2}, \frac{Q_1}{Q_3}, \frac{X}{L_i}, \frac{Q_1L_i}{\sqrt{M_iRT}}, \frac{Q_1L_i}{\sqrt{M_iEa_i}} \qquad (12)$$

with the first five containing more than one experimental variable. Note that although there are seven dimensionless parameters above, the last two are the same as far as experimental variables are concerned. Therefore, there are only six experimental, dimensionless parameters. While there is clearly no gain due to a reduction in the number of variables in this case, there may be a gain due to the transformation of experimental variables. This can only be determined by comparing regression models founded on primitive variables and models founded on the dimensionless parameters.

The fact that there is no gain in variable reduction for this formulation of the LPCVD problem may be formally understood by utilizing the application theorem. In this case, K = 3, and k = 3, therefore the reduction of variables given by

$$\text{Reduction} = K - k \qquad (13)$$

is zero.

In order to maximize the potential gain through the use of Dimensional Analysis, the problem must be reformulated in a way that leads to a reduction of variables when Dimensional Analysis is applied. The reformulation is based on a physical understanding of the process and the way in which the variables affect the process. For instance, it is known that the term RT only appears in two groups. The dimensionless parameters are Ea/RT and PL_i^3/RT. Ea/RT is always constant, and thus does not affect the process, and PL_i^3/RT, for reasons dealing with the process physics, can be understood to have only a small effect upon the process.

The molecular density of the gas, P/RT, affects the process in two ways. First, the molecular density affects the concentration of the individual species above the surface. However, increasing the amount of all species does not change the growth rate. This is due to the fact that the surface is saturated. Therefore, only changes in the ratio of concentrations will result in a change of growth rate. Second P/RT affects the diffusion of the gases, but since temperature is constant, the diffusion varies as $1/P$. Also, velocity down the tube increases as $1/P$, since the same amount of gas being sprayed into the tube

expands to fill more volume. Thus, though the gases are able to diffuse at a faster rate, they face an equivalently stronger resistance.

Thus, RT and Ea may be discarded from the analysis, as they only appear in the terms Ea/RT and PL_i^3/RT. Pressure, however is known to affect the process in ways other than through PL_i^3/RT, and therefore must not be removed. For example, pressure influences the distribution of gas as it flows from the injectors. Now the dimensional analysis may be redone, and the application theorem gives assurance that there will be a reduction of one variable (K - k = 1).

The new list of variables that affects the polysilicon deposition process is listed in column 1 of figure 4 and each variable's dimensions are listed in column 2.

Variables	Dimensions	Choose	Parameters
Gr	L/T		$Gr\sqrt{M_i}/\sqrt{PL_i^3}$
P	M/LT^2	✓	
Q_1	M/T		$Q_1 L_i/\sqrt{PM_iL_i}$
Q_2	M/T		$Q_2 L_i/\sqrt{PM_iL_i}$
Q_3	M/T		$Q_3 L_i/\sqrt{PM_iL_i}$
X	L		X/L_i
L_i (baseline)	L	✓	
M_i (baseline)	M	✓	
$\%_i$ (baseline)	-0-		$\%_i$
# (baseline)	-0-		#

Figure 4: Successful Dimensional Analysis of polysilicon system.

The use of the Application Corollary leads to the choice of P (pressure), M_i (molecular masses), and L_i (geometric lengths) as the three variables that will group the remaining, unchosen variables (See column 3 of figure 4). Note that there is no way to form a dimensionless parameter by power grouping the three variables among themselves.

In figure 4, the notation L_i refers to all fixed tube geometry. These include diameter of the wafers, length of the tube, spacing of the wafers, and diameter of the tube. Note that by

choosing any constant length as a "grouping" variable, all other constant lengths are bound to be grouped as a ratio of two constant lengths. Since these grouped quantities are dimensionless and constant, they may be eliminated from further consideration. Thus, it is not necessary to consider all the baseline variables having the dimensions of length, one baseline variable having dimensions of length is sufficient.

As usual, the unchosen variables are "power grouped" with some exponential combination of the three variables chosen in column 3. The "power grouping" is achieved by trial and error and typically no algorithm is needed to group the variables. The experimental, dimensionless parameters in functional form are:

$$\frac{Gr\sqrt{M_i}}{\sqrt{PL_i^3}} = f\left(\frac{Q_1}{\sqrt{PM_iL_i}}, \frac{Q_2}{\sqrt{PM_iL_i}}, \frac{Q_3}{\sqrt{PM_iL_i}}, \frac{X}{L_i}\right) \tag{14}$$

Note that, consistent with application theorem (Part I), there was a reduction of one parameter, from the six experimental, primitive variables to the five experimental, dimensionless parameters.

4.3   Choice of models for Polysilicon

Due to constraints caused by the experimental budget, only nine experimental runs were available to calibrate any model which might be used. In order to maintain a sufficient number of degrees of freedom, it was decided that both the primitive variable model and the dimensionless parameter model would be allotted only six coefficients each in a linear model. Both models were initially chosen based on physical understanding about the form of the response. The dimensionless parameter model was chosen to be the first model formulated, that is, no trial and error improvement was allowed. However, the primitive variable model was improved by trial and error, and represents the model with the best least squares fit chosen from six trials. In this manner, all possible advantages are given to the primitive variable model.

The primitive variable model having the minimum least squares fit is:

$$Gr = C_0 + C_1X + C_2P + C_3Q_1 + C_4Q_2 + C_5XQ_3 \tag{15}$$

The dimensionless parameter model is:

$$\frac{Gr}{\sqrt{P}} = C_0 + C_1 X + C_2 \frac{Q_1}{\sqrt{P}} + C_3 \frac{Q_2}{\sqrt{P}} + C_4 \frac{Q_3}{\sqrt{P}} + C_5 \frac{Q_3}{\sqrt{P}} X \tag{16}$$

4.4   Dimensional Analysis for the LTO System

For the Low Temperature Oxide deposition process, both silane and oxygen are injected into the tube, with oxygen being sprayed into the front of the tube, and silane being sprayed into the front, middle, and back of the tube. The typical operating setpoints are a temperature of 400 °C and a pressure of 300 mTorr.

The dimensional analysis of this process is almost exactly the same as that of the polysilicon process just analyzed. The derivation of the dimensionless parameters for chemical vapor deposition of Low Temperature Oxide is as follows:

The list of variables that affect the process is:

Gr	Growth rate of Silicon dioxide (the output)
P	Pressure in the tube
Q_{ox}	Flow rate of oxygen at the front of tube
Q_1	Silane flow rate in the front of tube
Q_{sc}	Total Silane flow rate in the middle and end of tube
X	Positon of Qsc injector
L_i	Fixed geometry of tube, such as length
M_i	Mass of various molecules
Ea_i	Activation energy of various reactions (i.e. surface reactions)
#	Number of wafers
RT	Temperature as defined by molecular energy.
$\%_i$	Ratios of various reaction coefficients. For instance, the ratio of adsorption coefficients of hydrogen and oxygen.

The same logic that was applied to the polysilicon system to remove the variables Ea and RT can be applied to the LTO system. The resultant variable list is given by column 1 of figure 5. The dimensions of each variable are listed in column 2, as usual.

Variables		Dimensions	Choose	Parameters
Gr		L/T		$GrM_i/Q_{ox}L_i$
P		M/LT^2		$Q_{ox}/\sqrt{PM_iL_i}$
Q_{ox}		M/T	✓	
Q_1		M/T		Q_{ox}/Q_{sc}
Q_{sc}		M/T		Q_{ox}/Q_1
X		L		X/L_i
L_i	(baseline)	L	✓	
M_i	(baseline)	M	✓	
$\%_i$	(baseline)	-0-		$\%_i$
#	(baseline)	-0-		#

Figure 5: Dimensional Analysis of LTO system.

Using the Application corollary as a guide, one selects two baseline variables and one experimental variable. M_i, L_i, and Q_{ox} are the variables chosen based on physical knowledge about the reaction mechanism. Q_{ox} was chosen because it is known that the flow rate ratios are probably the most important parameters for this process. The reaction mechanism, Langmuir-Hinshelwood adsorption with bimolecular reaction, implies that growth rate is dependent upon the ratio of oxygen and silane concentrations above the wafer. The concentrations above the surface are closely related to the flow rates (See appendix E).

The unchosen variables are then grouped into dimensionless parameters by using exponents of the chosen variables, as in column 4 of figure 5. The dimensionless parameters, in functional form are:

$$\frac{GrM_i}{Q_{ox}L_i} = f(\frac{Q_{ox}}{\sqrt{PM_iL_i}}, \frac{Q_{ox}}{Q_{sc}}, \frac{Q_{ox}}{Q_1}, \frac{X}{L_i})$$ (17)

Once again, there has been a reduction from six experimental, primitive variables, to five experimental, dimensionless parameters, as per the Application theorem.

4.5 Choice of LTO Model

The number of experiments performed was limited to 18 for the LTO system, due to experimental budget constraints. In light of this restriction, and having a strong desire to have a high ratio of experiments to coefficients, both the primitive variable model and the dimensionless parameter model were limited to nine terms. However, the best (defined as largest F-test) regressions were given by models with seven terms. As with the polysilicon process, the dimensionless parameter model was not altered from the first intuitive model that was derived. Similarly, the primitive variable model is the best (for maximum overall F-test) of all the various regressions attempted (about 6 or 7).

The dimensionless parameter model is :

$$\frac{Gr}{\sqrt{P}} = C_0 + C_1 X + C_2 \frac{Q_{ox}}{Q_l} + C_3 \frac{Q_{ox}}{Q_{sc}} + C_4 \frac{Q_{ox}}{\sqrt{P}} + C_5 \frac{Q_{ox}}{Q_{sc}} X + C_6 \left[\frac{Q_{ox}}{Q_{sc}}\right]^2 \qquad (18)$$

The best primitive variable model is:

$$Gr = C_0 + C_1 X + C_2 P + C_3 Q_{ox} + C_4 Q_l + C_5 Q_{sc} + C_6 X Q_{sc} \qquad (19)$$

These two models were evaluated using 18 experiments. Once again, the comparison was based primarily on the results for the overall F-test, with some consideration given to the physical sensibility of the results.

5.0 EXPERIMENTS, RESULTS, AND DISCUSSION

5.1 Experimental Array for Polysilicon

The experimental work for this process was carried out by Prueger [4]. The array used for the evaluation of the two polysilicon models is the nine experiment orthogonal array, shown in figure 6 [11]. The experiments were carried out in primitive variables, so that the primitive variable model would have the advantage of being evaluated with very little correlation among the dependent variables (only the last term in the model is not orthogonal to the other parameters). The levels of the variables were chosen through experience and centered around the previous operating point, producing the following experimental array:

run #	X (inches)	Q1 (sccm)	Q2 (sccm)	P (mTorr)
1	6.875	30	40	200
2	8.875	45	55	200
3	10.875	60	70	200
4	10.875	30	55	250
5	6.875	45	70	250
6	8.875	60	40	250
7	8.875	30	70	350
8	10.875	45	40	350
9	6.875	60	55	350

Figure 6: L_9 array for polysilicon process

Where Q3 is given by the constraint Q3 = 150 - Q2 - Q1. This linear relationship means that regressions involving the linear Q1, Q2, and Q3 will experience multicollinearity effects.

The average film thickness on the wafers was about 5000 Angstroms. Two typical profiles for the L_9 array are shown in figure 8.
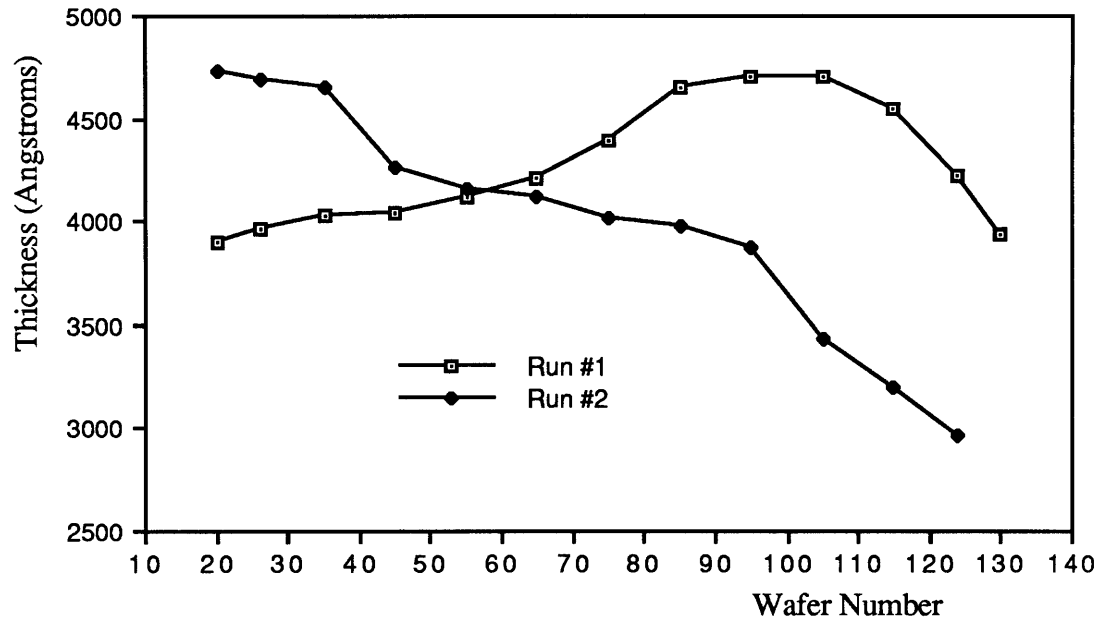
Figure 8: Typical growth rate profiles for polysilicon.

Measurements were made on thirteen of the 150 wafers in the tube, giving thirteen independent sets of data. Separate models were created for each of the thirteen sets of data, with all models being of the same form as equations (18) and (19), with only the coefficients differing.

5.2   Results and Discussion for Polysilicon

The overall F-test comparisons for each of the thirteen regressions are:

Wafer #	F-test (D.A.)	F-test (Prim.)
20	167.850	94.129
26	131.421	59.531
35	90.586	27.840
45	46.495	9.389
55	42.995	3.841
65	60.378	3.163
75	32.363	2.409
85	19.524	2.395
95	52.308	15.338
105	204.983	83.546
115	100.276	35.818
124	125.963	48.602
130	265.960	70.964

Figure 9: F-test results for polysilicon system.

For each wafer, the dimensionless parameter regression is superior to the primitive variable regression. The average ratio of F-tests is approximately 5:1. Not only is the dimensionless model better statistically, it also makes more physical sense. For instance, the average T-test for C_o is smaller by a factor of 2.0 in the dimensionless model than it is in the primitive variable model. This is intuitively reasonable; if the flow rates are set equal to zero, then the growth rate should be zero.

Based on the higher overall F-test, and the more physically sensible results, the dimensionless parameter model apparently allows for superior modeling of physical processes, as suspected. Regardless of the advantages given the primitive variable model, such as experimentation in primitive variable space and multiple models from which to choose the best primitive variable model, the dimensionless model was always more significant, and intuitively more sensible.

The average residual for the polysilicon is 85 angstroms, which is on order of the replicate error. For this reason, it is felt that both models are estimating their outputs as well as possible.

Future work (see the conclusions section) will explore whether or not an improved F-test means that there is practical improvement (as defined by the ability to optimize and control with a model).

5.3 Experimental Array for LTO

The reasons for choosing the 18 experiment orthogonal array [12] for the LTO process were much the same as those for choosing the nine experiment array for the polysilicon process. There was an experimental budget constraint which limited us to 18 experiments. Once again, the experiments were performed in primitive variable space, thereby giving any advantages that originated from designed experiments to the primitive variable model. The levels were chosen with the help of an experienced operater such that the minimum wafer-to-wafer variance would fall within the experimental array. Thus, the array used for evaluation of the LTO linear models is:

Run #	X	P	Q_{load}	Q_{sc}	Q_{ox}
1	0.0	300	38.8	46.4	130
2	0.0	375	48.5	58.0	130
3	0.0	450	58.2	69.6	130
4	0.0	300	58.2	69.6	155
5	0.0	375	38.8	46.4	155
6	0.0	450	48.5	58.0	155
7	2.5	300	38.8	58.0	130
8	2.5	375	48.5	69.6	130
9	2.5	450	58.2	46.4	130
10	2.5	300	48.5	69.6	155
11	2.5	375	58.2	46.4	155
12	2.5	450	38.8	58.0	155
13	5.0	300	48.5	46.4	130
14	5.0	375	58.2	58.0	130
15	5.0	450	38.8	69.6	130
16	5.0	300	58.2	58.0	155
17	5.0	375	38.8	69.6	155
18	5.0	450	48.5	46.4	155

Figure 10: L_{18} array for LTO process

Two typical profiles for this array are shown in figure 11. Replicate data is shown in figure 12. Additional profiles are shown in appendix A. As can be seen, the variation between runs is much larger than the variation between replicates.
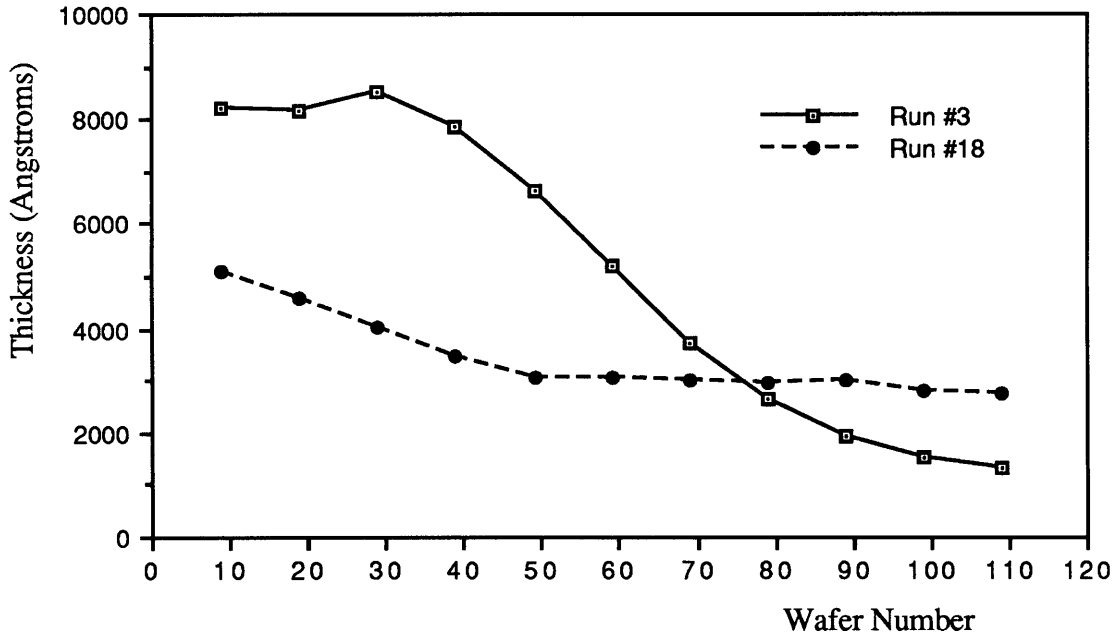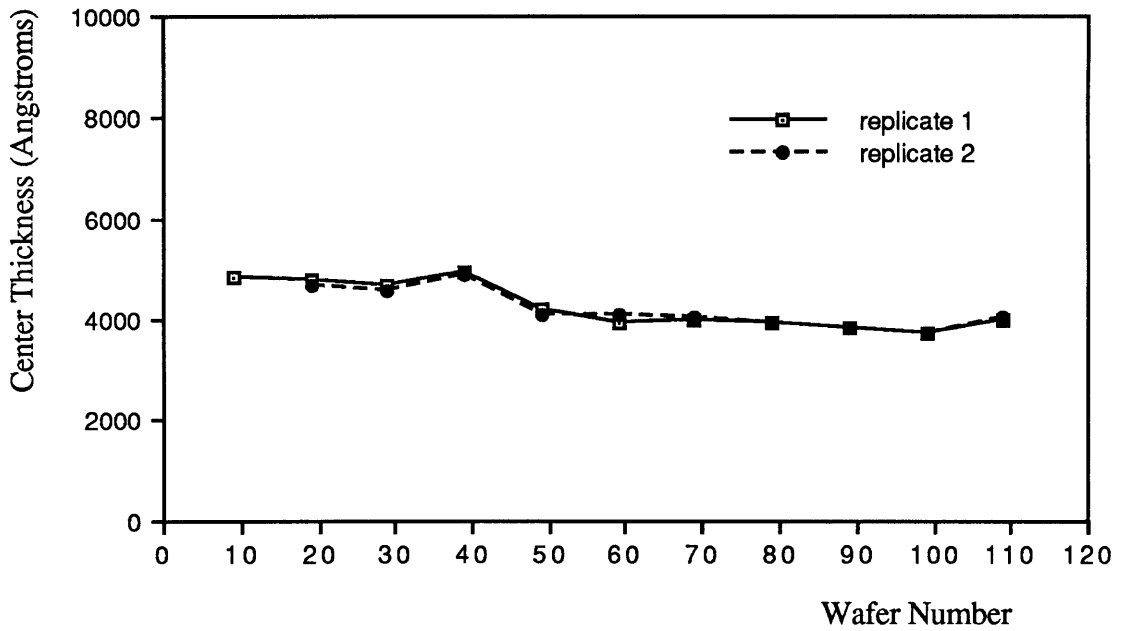

Figure 11: Typical growth rate profiles for LTO.

Figure 12: Replicate data for LTO.

Due to time constraints, the replicates were run after the experiments. No alteration of equipment, such as maintenance, was done during the L_{18} array experiments or during the replicate experiments, although maintenance was done between the completion of the array and the start of the replicates.

For the LTO system, eleven sets of data were created, one set for each of the eleven wafers of interest. The primitive regression model given by equation (19), and the dimensionless parameter model given by equation (18) were used for all eleven wafers, with only the individual coefficients differing.

5.4   Results for LTO

The overall F-test for each regression is:

Wafer #	F-test (D.A.)	F-test (Prim.)
9	80.48	36.40
19	52.79	26.07
29	29.54	12.62
39	38.21	23.14
49	40.50	43.60
59	27.95	12.98
69	17.76	5.09
79	12.82	3.34
89	14.36	4.08
99	14.32	6.41
109	10.27	5.73

Figure 13: F-test results for LTO system.

Here, as for the polysilicon process, the dimensionless parameter model is better than for the primitive variable model, having a larger F-test for 10 of the 11 models (wafers). The average ratio of the F-tests for the two models is about 2.25:1.

For some applications, the sum of squares of residuals may be the quantity of interest. Therefore, regressions using both dimensionless parameters and primitive variables were formulated and compared based on that criterion. The results are listed in appendix C.

6.0   MODELING AND OPTIMIZATION TECHNIQUE

6.1   Modeling and Optimization

As stated before, the wafer to wafer standard deviation,

$$\sigma = \sqrt{\frac{1}{11}\sum_{i=1}^{11} (Gr_i - \overline{Gr})^2} \tag{20}$$

is one of the principal reasons for failure of the LTO deposition process (See figures in appendix A). The practical goal of this project is to minimize the wafer to wafer variance, while achieving a specified target thickness. The eleven models (one model for each wafer) that were calibrated with the data of the L_{18} array may be used for exactly this purpose.

Since the growth rate on each of the eleven wafers is expressed by equation (18) , the standard deviation (which is simply a function of the eleven growth rates) is only a function of the parameters in equation (17). The standard deviation was calculated through the use of equation (20), with Gr_i given by the eleven dimensional analysis regression models for growth rate. The process parameters found to give the minimum standard deviation are:

$$X = 5.0 \text{ in.}, Q_{ox} = 155 \text{ sccm}, Q_l = 38.8 \text{ sccm}, Q_{sc} = 69.6 \text{ sccm}, P = 300 \text{ mTorr} \tag{21}$$

The optimization was performed after maintenance had changed the machine setup. This change degraded the performance of both the previous setting (baseline setting) and the predicted optimum. After the maintenance, the standard deviation of the baseline setting was about 11 percent of the mean. After the maintenance, the standard deviation of the optimized setting was about six percent of the mean. The growth rate profile for the parameters in equation (21) is:
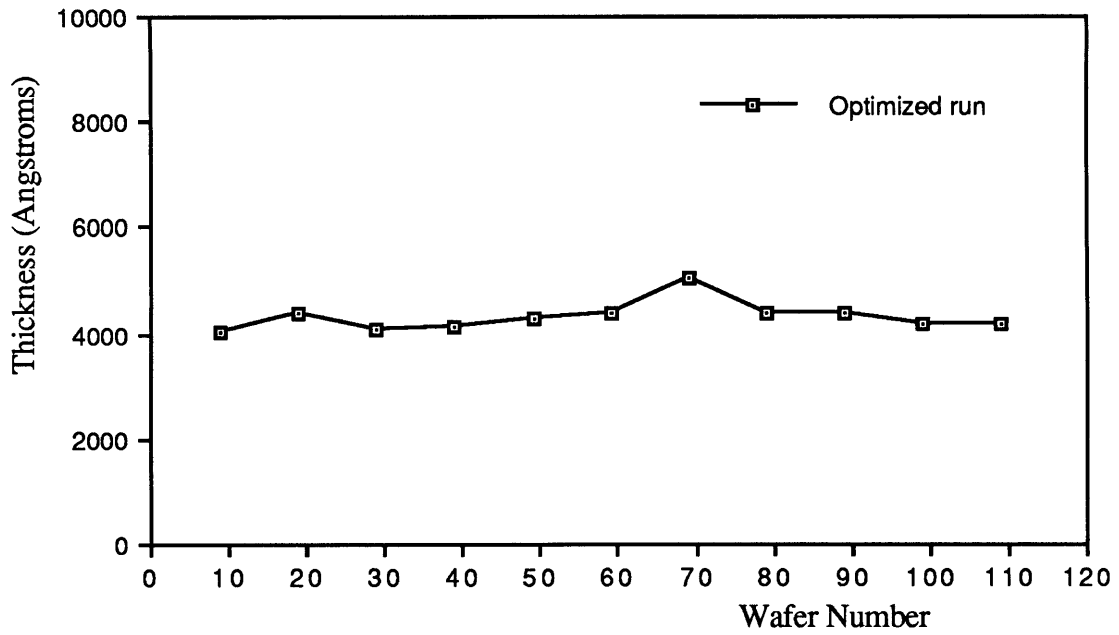
Figure 14: Optimum profile for LTO.
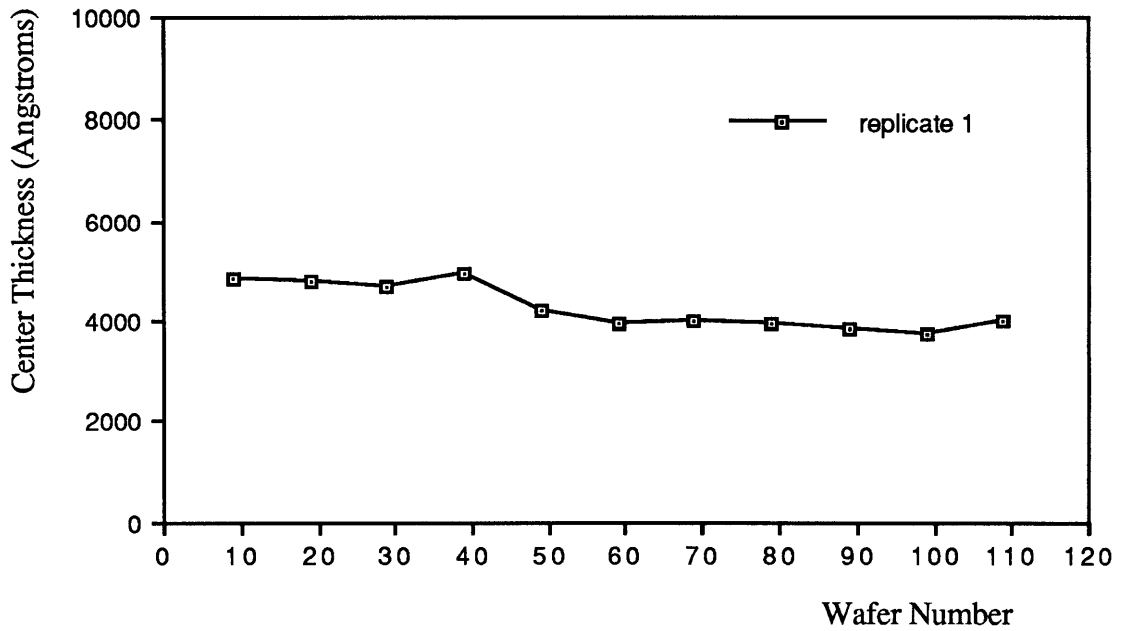
The baseline profile is:

Figure 14: Baseline profile for LTO.

7.0   CONCLUSIONS

7.1   Summary

With the goal of developing models that have high interpolative and extrapolative accuracy with few data points required, this work has combined essential elements of physical modeling with the design of experiments.

Dimensional Analysis, a technique commonly used in the physical sciences to simplify the analysis of complex multivariable problems, has been applied to the formulation of models for processes. While the primary emphasis of this work has been to understand the beneficial impact of Dimensional Analysis on modeling, positive impacts on the design of experiments that might accompany this modeling have been observed.

The benefits resulting from the application of Dimensional Analysis to process modeling are twofold in nature. First, it may be possible to realize a reduction in the number of parameters needed to describe many process. Second, the dimensionless groupings of the variables resulting from the Pi theorem contain physical information that often leads to higher modeling accuracy than is obtained with ungrouped variables. Indeed, regression analysis using dimensionless parameters is guaranteed to satisfy the principle of dimensional homogeneity. It should be noted that few regressions based on ungrouped variables satisfy the principle of dimensional homogeneity.

To non-dimensionalize simple problems, the Pi theorem may be applied directly, but for more complicated systems, the Application theorem is needed. The Application theorem parallels the Pi theorem in that it predicts the reduction of parameters. However, the Application theorem takes into account the practical fact that all variables that affect a process do not necessarily change value.

These variables are present in both of the systems that are analyzed in this paper, the Low Pressure Chemical Vapor Deposition (LPCVD) of polysilicon and the LPCVD of low temperature oxide (LTO), two processes used in the manufacturing of integrated circuits. The Application theorem predicts that no reduction of variables will occur from the Dimensional Analysis. However, using knowledge of the process physics, some variables

can be transformed so that there is a reduction of variables. Following this transformation, the Pi theorem is applied to each process, and dimensionless parameters are defined.

Using knowledge of the process physics, models are formulated based on the primitive variables and on the dimensionless parameters. The primitive variable model is improved via trial and error, while the dimensionless parameter model is not.

Both models for the polysilicon process are evaluated using an L_9 orthogonal array designed in primitive variable space. Similarly, both models for the LTO process are evaluated using an L_{18} orthogonal array based upon primitive variable space. The L_9 array was performed earlier by Prueger []. The L_{18} array was performed during the course of this investigation as a means of studying the effects of Dimensional Analysis and as a means of improving the LTO process. The L_{18} array most suited the dual purposes of this work.

The models are compared based on the overall F-test. The average ratio of F-tests for the polysilicon process is 5:1 in favor of the dimensionless parameter model. The average ratio of F-tests for the LTO process is 2.25:1 in favor of the dimensionless parameter model. Also, the model coefficients are more sensible for the dimensionless parameter model for each process.

One goal of this work was to minimize the wafer to wafer variance of the LTO process. The Dimensional Analysis models were used to calculate the wafer to wafer variance, and this quantity was minimized. An experiment was run at the predicted process parameters and the minimum wafer to wafer standard deviation was found to be six percent of the mean, as opposed to the previous best setting, which was 11 percent of the mean. It should be noted that both of these values deteriorated due to recent part replacements in the tube.

7.2   Related work:

Two theses, one by Storm [13] and one by Chaddha [14] deal directly with the use of dimensional analysis as a method for transforming primitive variables to a more advantageous set of parameters.

The thesis by Storm outlines the development of a sequential optimizer. The sequential optimizer takes an output of a process, such as the yield of a chemical reaction, and

incrementally improves it. The size of the increment depends upon the goodness of fit of the underlying statistical model for the process of interest. Storm compared the number of increments necessary to optimize a process for a dimensionless model and a primitive variable model.

Chaddha used dimensionless parameters to successfully model the LPCVD doped polysilicon process. Comparison was made with a primitive variable model.

7.3   Future work

There are many processes for which no reduction of variables occurs after application of the Pi theorem. Additionally, many of these processes cannot be reasoned with physically so that some variables are excluded, as was done for the two process in this paper.

Even when this is so, the Pi theorem can be used to generate sets of transformed variables which are equal in number to the set of primitive variables, but not in substance. This can be achieved by choosing one or more experimental variables with which to group unchosen variables (column 3). Note that by choosing different experimental variables, different dimensionless parameters are formed. It is proposed that some or all of these transformations may be successful from a modeling point of view, even if they are not from a design of experiments point of view.

Note that for every dimensionless transformation, there are many possible model combinations. Software is being developed that explores these transformations.

This software is comprised of data entry, and four loops which find the best dimensinless regression possible. The first loop specifies the reduction of variables (from 0 to 4), and makes assumptions regarding the dimensions that appear in the baseline variables. The second loop decides which experimental variables will be chosen to non-dimensionalize the remaining variables. The third loop specifies the number of terms in the model. The fourth loop determines the form of the model. Each model is evaluated, and the best (various criterion) selected.

APPENDIX A: GROWTH RATE MEASUREMENTS AND RESULTS

Measurement

The wafers used for the Low Temperature Oxide experiments were 100 millimeter in diameter, and 475 to 575 microns thick. The wafers are P type with boron dopant, and a resistivity of 5 to 30 ohms. The lattice orientation was 100.

A nanospec was used to measure the film thickness. The replicability of the nanospec measurement was solely dependent upon how accurately the wafer could be placed on the nanospec stand. That is, if the wafer was measured in exactly the same position, the nanospec would measure the same thickness within five angstroms.

The growth rate on a wafer was characterized by measuring film thickness at the center of the wafer, the only point that could be consistently placed on the nanospec stand. The entire wafer may be characterized by the measurement at one point, since the variance on a wafer is neglible.

Results

The profiles for all 18 runs of the LTO experimentation are:
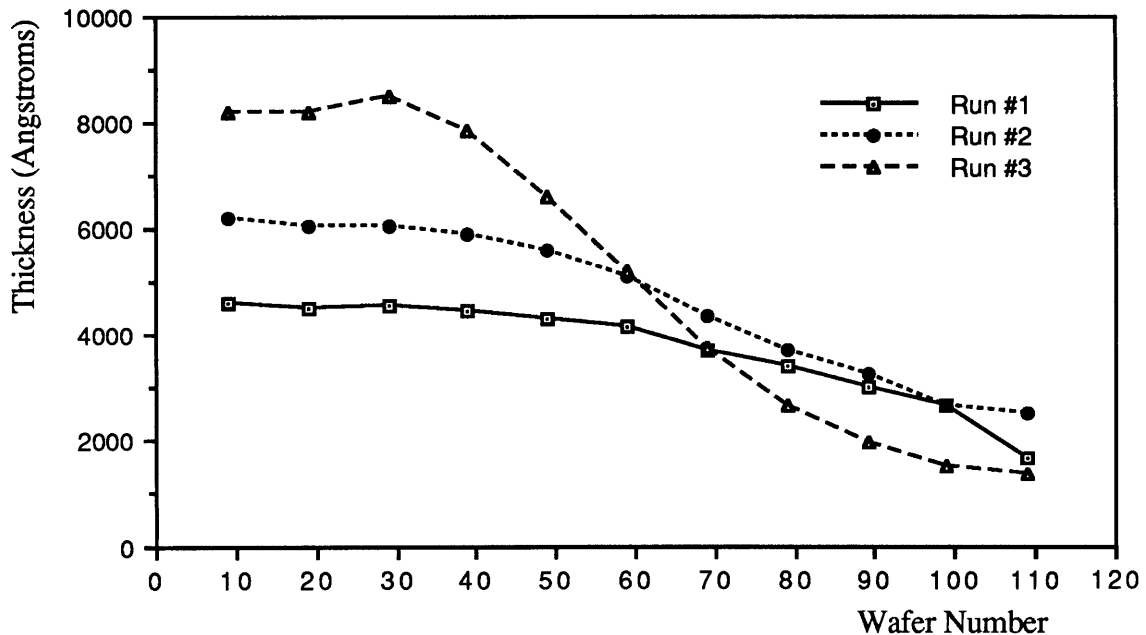
Figure A1: Profile for LTO runs 1-3
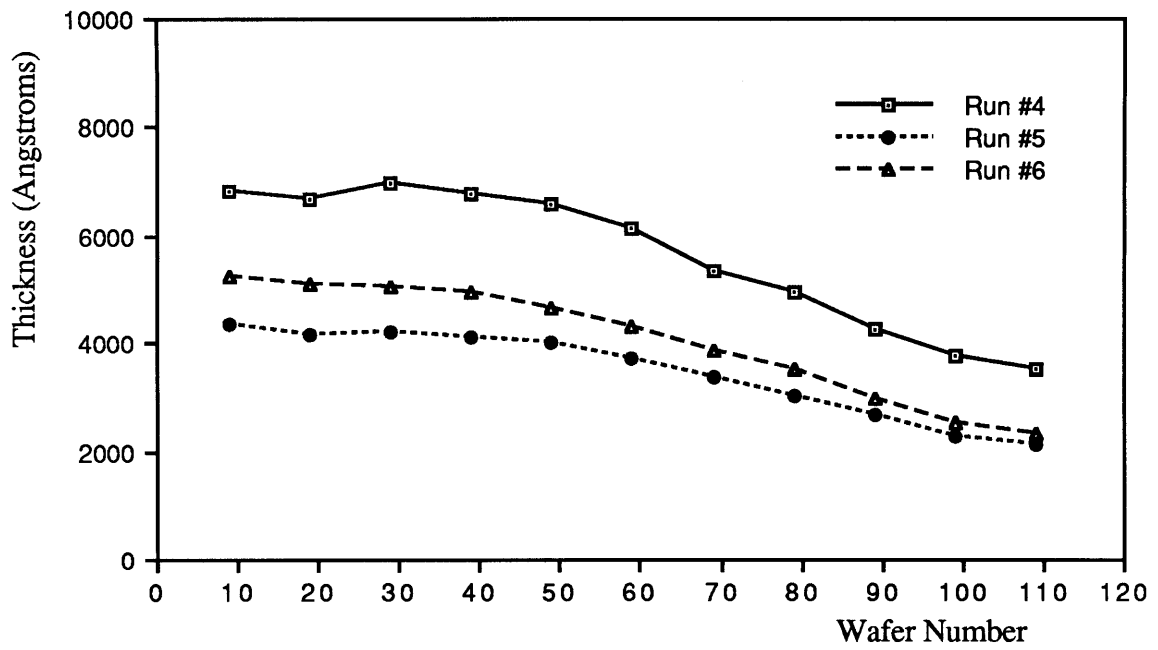
Figure A2: Profile for LTO runs 4-6
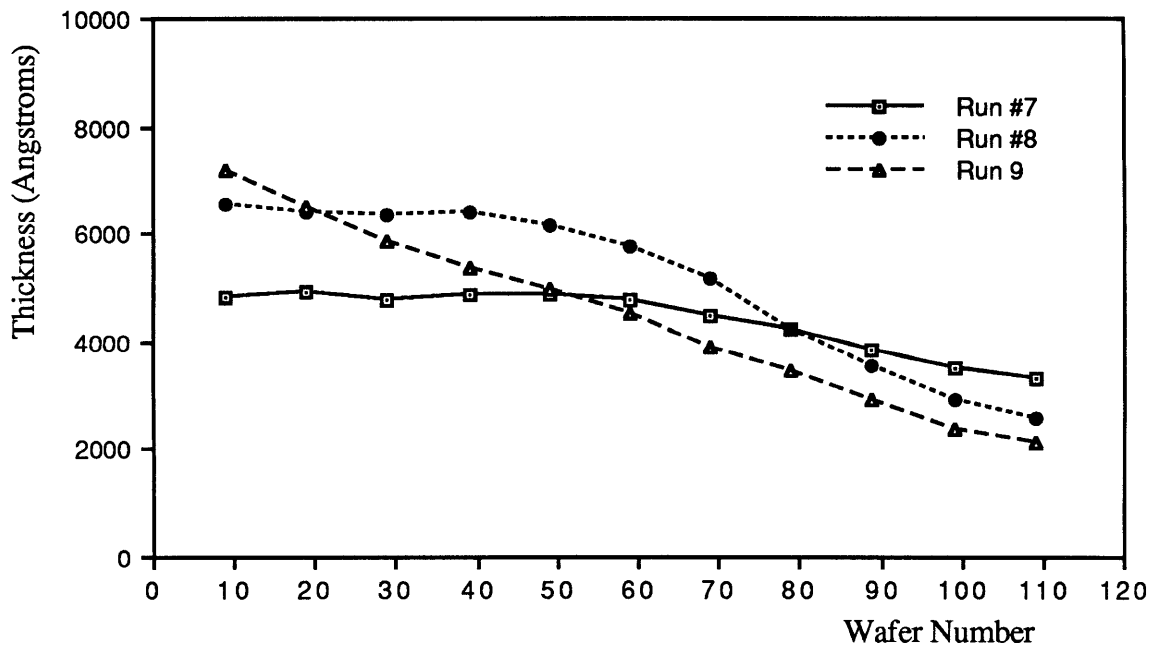
Figure A3: Profile for LTO runs 7-9.
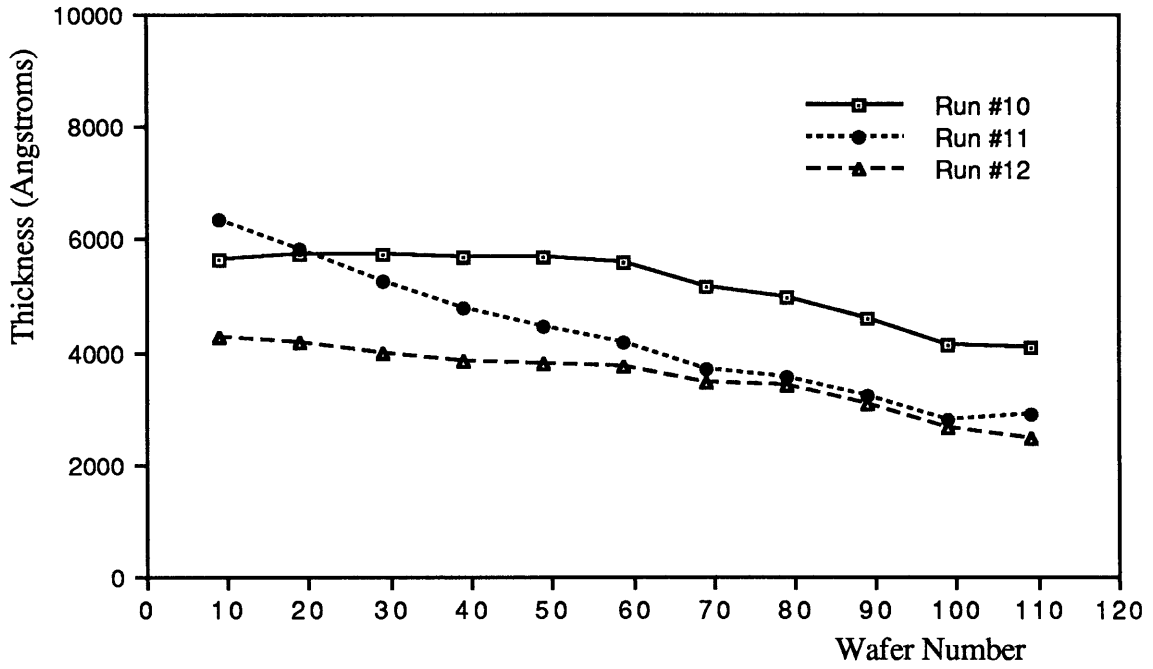
Figure A4: Profile for LTO runs 10-12.
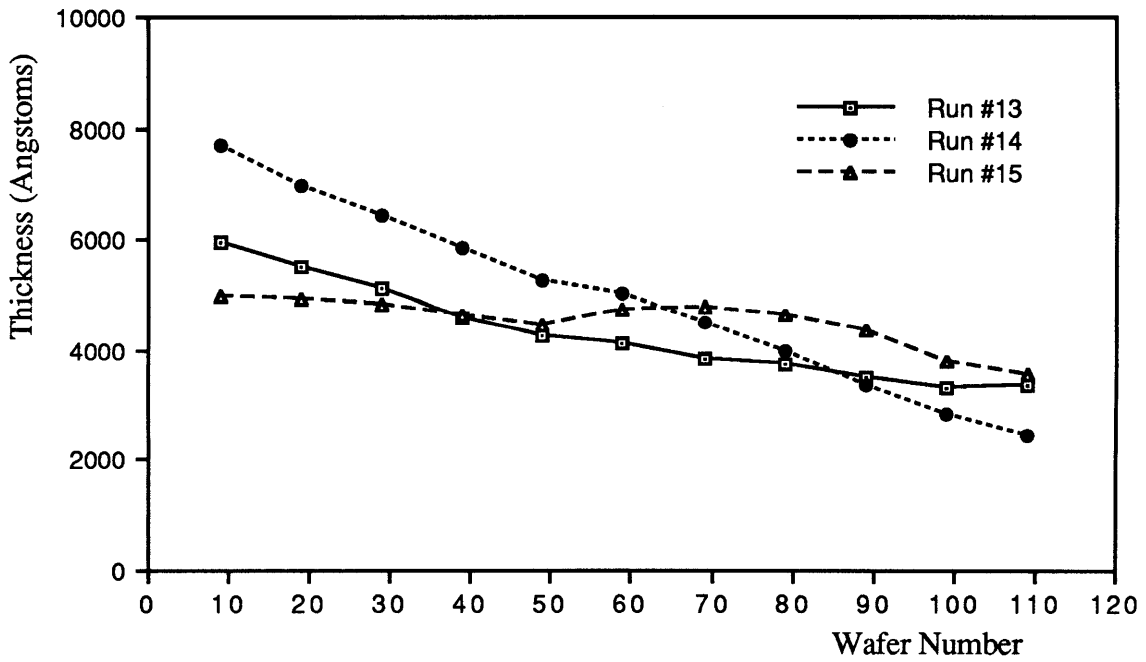
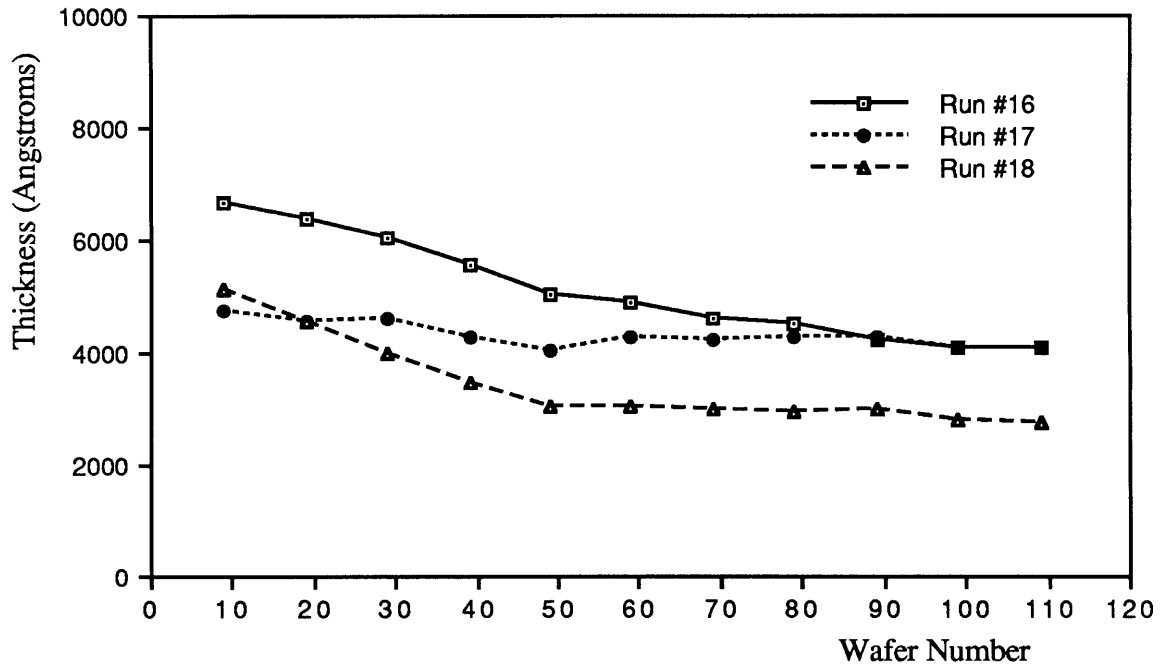Figure A5: Profile of LTO runs 13-15.

Figure A6: Profile of runs 16-18.

The within wafer variance was also characterized using five points on each wafer. Four points were at the wafer edge, at 12 o'clock, 3 o'clock, 6 o'clock and 9 o'clock. The fifth point is in the center, and sigma is calculated by

$$S = \sqrt{\frac{1}{4}\sum_{i=1}^{5} (Gr_i - \overline{Gr})^2}$$ (A1)

A typical within wafer variance profile is shown in figure A7. The error bars indicate plus or minus one sigma.
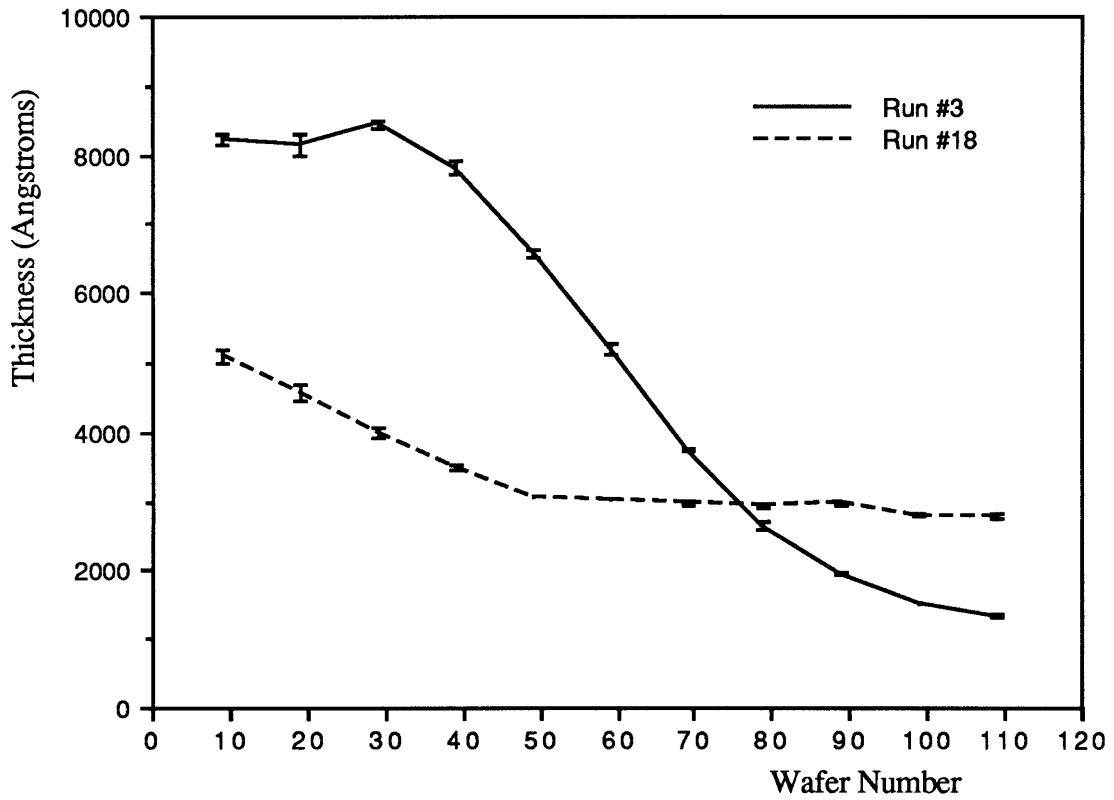
Figure A7: Typical within wafer variance for LTO.

APPENDIX B: STEP COVERAGE AND STRESS

In each of the eighteen runs, three patterned wafers were placed in the deposition tube at wafer positions 25, 50, and 75. The patterns were placed on these wafers so that step coverage for the LTO system could be analyzed, if needed. The line spacing of interest is shown in figure (B1). The height of the pattern is 5000 angstroms.
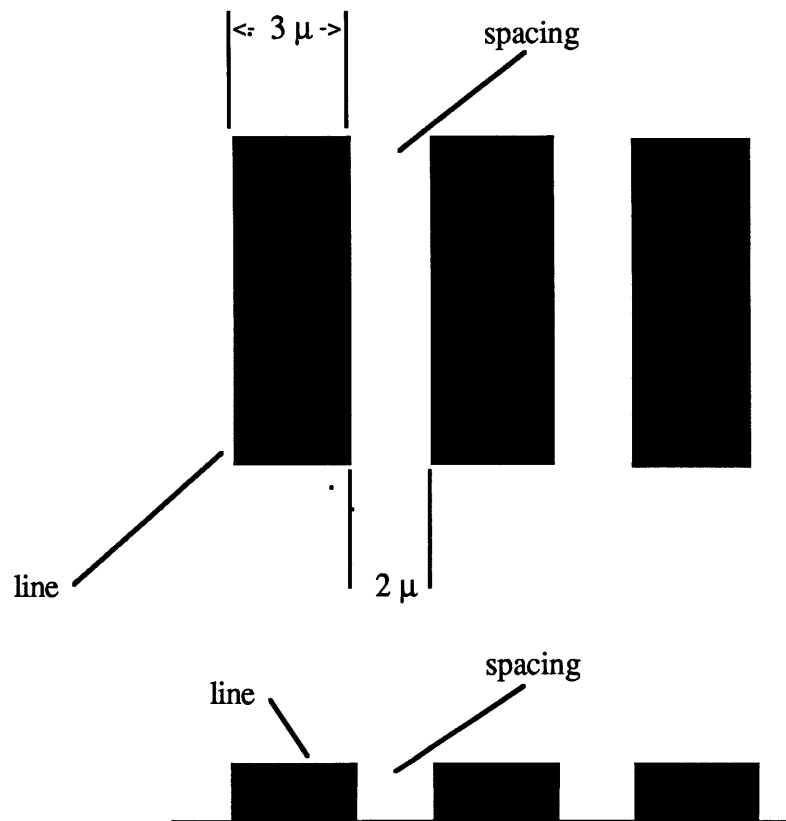
Figure B1: Pattern on wafers.

Also placed in the tube during each run are three prime wafers at wafer positions 29, 59, and 89. These three wafers may be used to characterize the average stress on each wafer. These wafers have no prior treatment and are bare silicon.

APPENDIX C: ALTERNATE CRITERION FOR MODEL COMPARISON

Another measure of the practical utility of a model is the residuals of the output. The residuals of the output are likely to be critical for some interpolating applications, and in some applications involving confidence limits. Thus, two different models, one based on primitive variables and the other based on dimensionless parameters, were evaluated in terms of this quantity. Since the proposed test is the smallest residuals, 15 terms were used for each model. No additional terms were allowed since some degrees of freedom are required. The primitive variable model is:

$$Gr = C_0 + C_1X + C_2P + C_3Q_l + C_4Q_{sc} + C_5Q_{ox} + C_6X^2 + C_7P^2 + C_8Q_l^2 \qquad (C1)$$
$$+ C_9Q_{sc}^2 + C_{10}Q_{ox}^2 + C_{11}Q_{sc}Q_{ox} + C_{12}Q_{ox}Q_l + C_{13}Q_{sc}Q_l + C_{14}XQ_{sc}$$

The dimensionless parameter model is:

$$\frac{Gr}{\sqrt{P}} = C_o + C_1X + C_2\frac{Q_{ox}}{Q_l} + C_3\frac{Q_{ox}}{Q_{sc}} + C_4\frac{Q_{ox}}{\sqrt{P}} + C_5X^2$$
$$+ C_6X\frac{Q_{ox}}{Q_l} + C_7X\frac{Q_{ox}}{Q_{sc}} + C_8X\frac{Q_{ox}}{\sqrt{P}} + C_9(\frac{Q_{ox}}{Q_l})^2 + C_{10}\frac{Q_{ox}Q_{ox}}{Q_l\ Q_{sc}} \qquad (C2)$$
$$+ C_{11}\frac{Q_{ox}Q_{ox}}{Q_l\ \sqrt{P}} + C_{12}(\frac{Q_{ox}}{Q_{sc}})^2 + C_{13}\frac{Q_{ox}Q_{ox}}{Q_{sc}\ \sqrt{P}} + C_{14}(\frac{Q_{ox}}{\sqrt{P}})^2$$

The dimensionless parameter model is the full quadratic of dimensionless parameters, while the primitive variable model contains all the lnear and squared primitive variable terms plus the best possible two factor interactions.

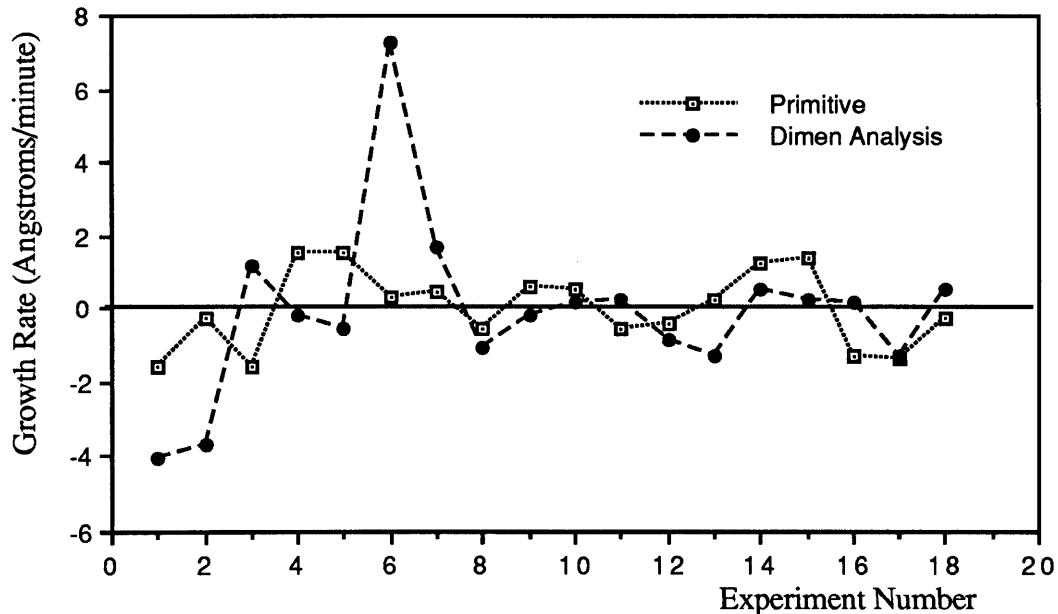The residual plots for every other wafer are:
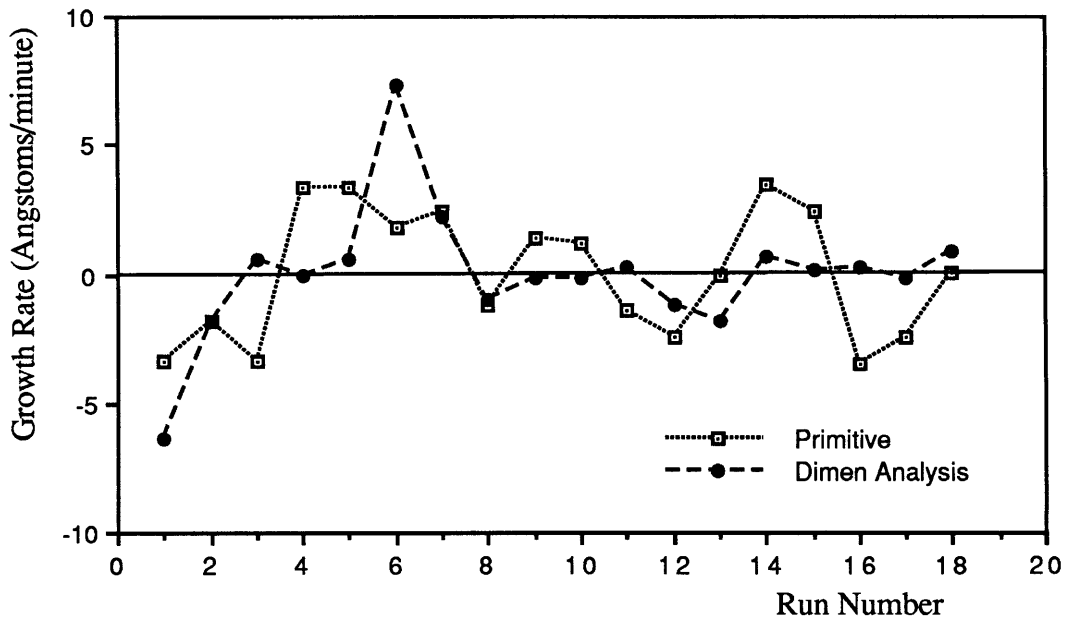

Figure C1: Residuals for LTO wafer #9.

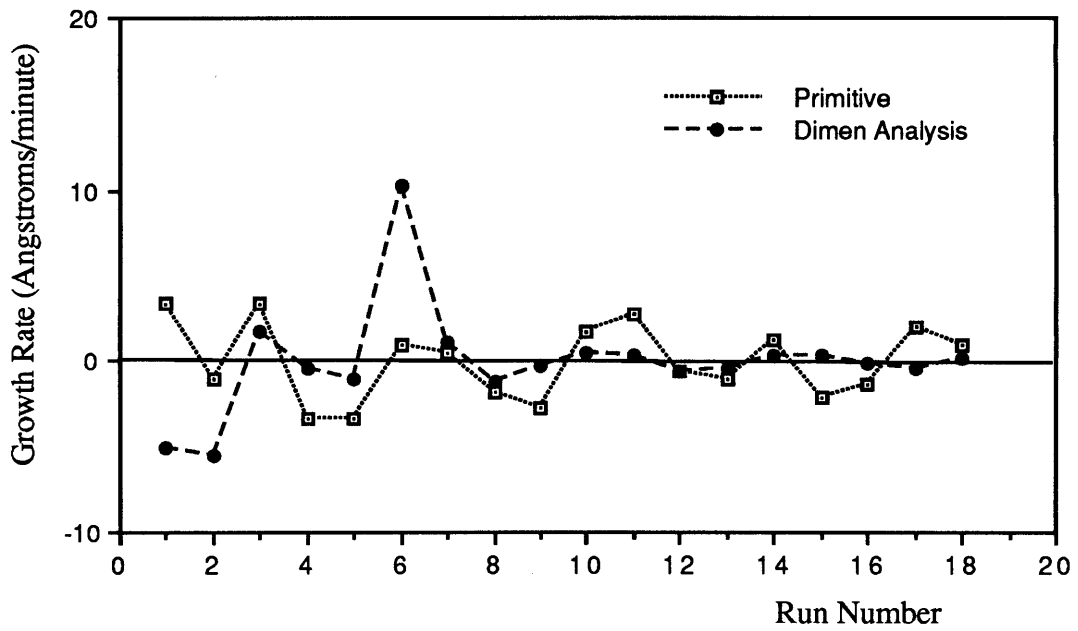Figure C2: Residuals for LTO wafer #29.

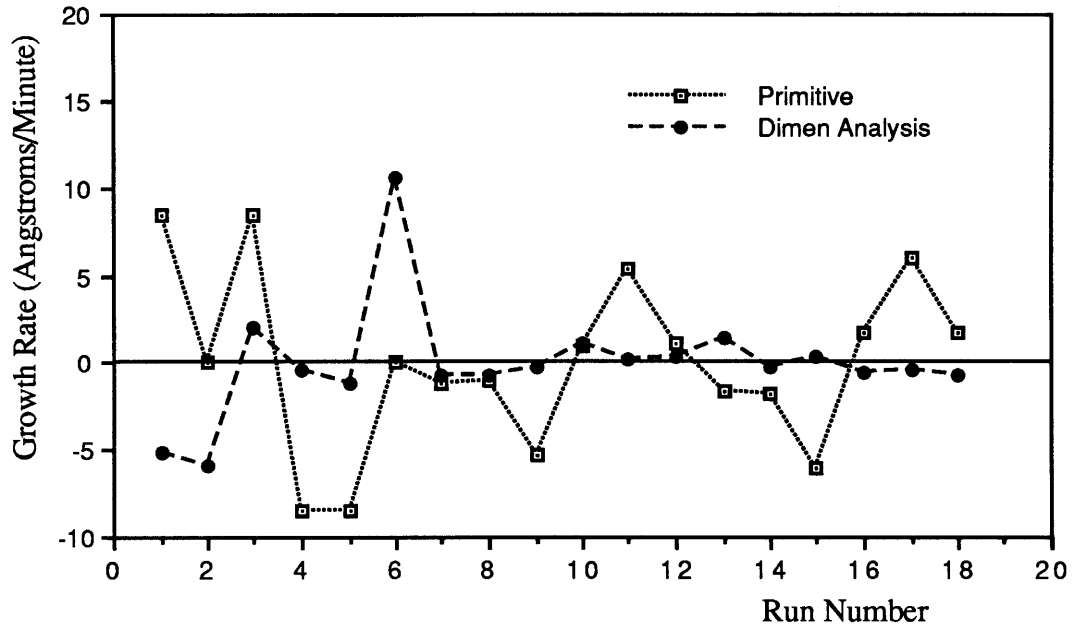

Figure C3: Residuals for LTO wafer #49.
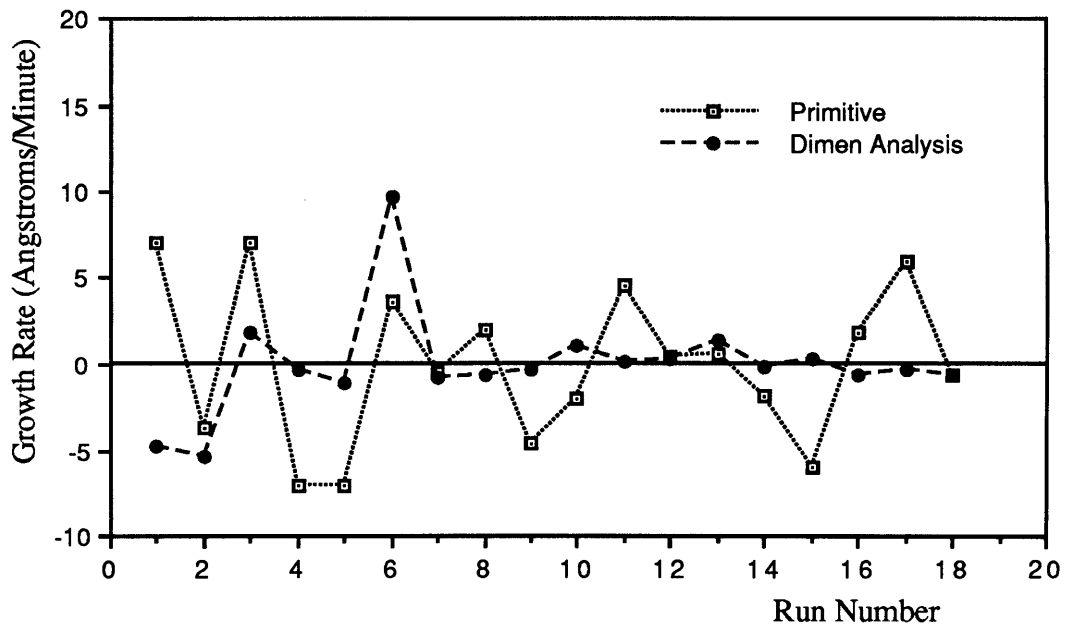
Figure C4: Residuals for LTO wafer #69.

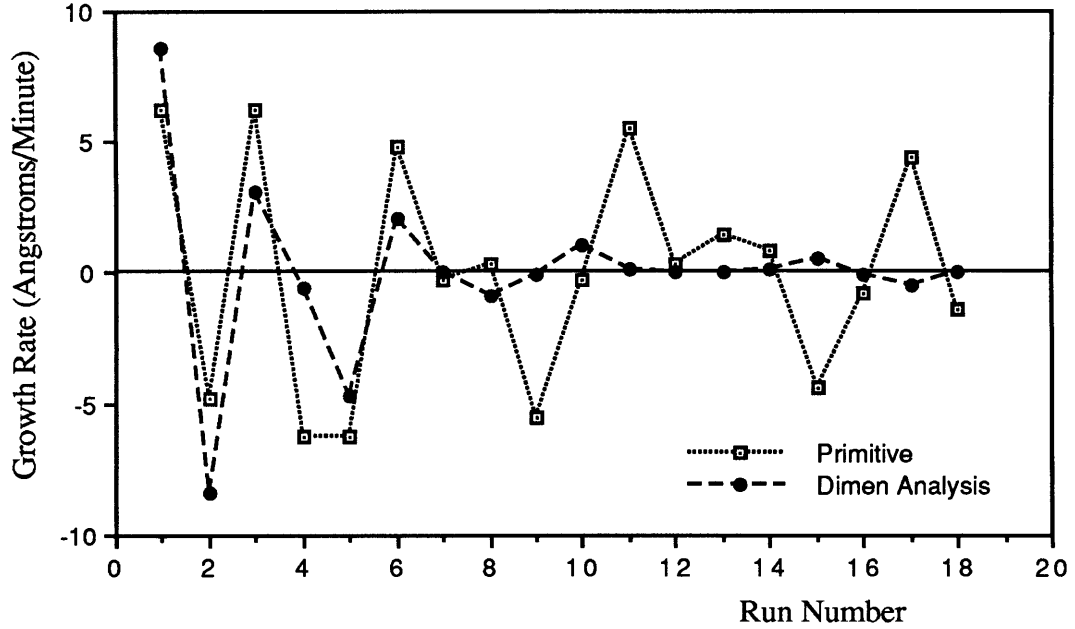Figure C5: Residuals for LTO wafer #89.

Figure C6: Residuals for LTO wafer #109.

Note that the average residual for the dimensionlesss parameter model is always smaller than the average residual of the primitive variable model. Further, note that the dimensionless parameter model does better down the tube, comparitively speaking. Run #6 is an exception, and is felt to be a result of inadequate design of experiments.

APPENDIX D: F-TESTS AND T-TESTS

The F-test is defined as the average square of the predicted experimental values about their mean divided by the average squared error at each experimental data point,

$$\text{F-test} = \frac{\dfrac{1}{P}\sum\limits_{1}^{N}(Y_i - \overline{Y})^2}{\dfrac{1}{N\text{-}P}\sum\limits_{1}^{n} E_i^2} \tag{D1}$$

where N is the number of data points and P+1 is the number of coefficients in the regression model.

Intuitively, the F-test is a test that at least one coefficient in the model is not equal to zero. The higher the F-test, the less the chance that all coefficients in the model are zero [15].

The T-test is harder to define qualitatively, but in essence the T-test is used to measure whether or not a specific coefficient is non-zero. The higher the T-test, the less the chance that the coefficient is zero [15].

APPENDIX E: PROCESS PHYSICS OF LTO

The deposition thickness of the Low Temperature Oxide film is dependent upon the ratio of silane to oxygen, rather than the absolute amount of either. Minimization of wafer to wafer variance is achieved, qualitatively speaking, by injecting an excess amount of oxygen into the front of the tube and varying amounts of silane into the front, center, and end of the tube.

Both gases diffuse rapidly from the injector nozzles and begin to flow toward the pump end of the tube. The gases begin to adsorb onto the wafer sites in a competitive arrangement. That is, either gas alone would cover the entire wafer surface via adsorption. Since the area of the wafers is limited, the oxygen and silane gases must compete for the surface. Hydrogen gas, which is not injected into the tube, but is produced by the reaction, also competes for surface area. The decimal percentage of the oxygen covered surface is given by the Langmuir - Hinshelwood mechanism,

$$\theta_{ox} = \frac{K_{ox}C_{ox}}{1 + K_{ox}C_{ox} + K_{si}C_{si} + K_H\sqrt{C_H}} \tag{E1}$$

The decimal percentage of silane covering the surface is,

$$\theta_{si} = \frac{K_{si}C_{si}}{1 + K_{ox}C_{ox} + K_{si}C_{si} + K_H\sqrt{C_H}} \tag{E2}$$

K_{si} is the adsorption coefficient of silane, K_{ox} is the adsorption coefficient of oxygen, C_{si} is the molecular concentration of silane above the wafer surface, C_{ox} is the molecular concentration of oxygen above the wafer surface. K_H is the desorption coefficient of hydrogen, and C_H is the concentration of hydrogen above the surface.

Various reaction mechanisms have been proposed, but the bi-molecular surface reaction explains most of the experimental phenomenon. This mechanism proposes that the growth rate of the SiO2 film is proportional to the probability of finding one oxygen molecule adjacent to two silane molecules. Thus the proposed reaction mechanism is,

$$Gr = K\theta_{ox}^2\theta_{si} \tag{E3}$$

or, by substituting equations (A1) and (A2),

$$Gr_{S_iO_2} = \frac{K_{React}K_{ox}^2K_{si}C_{si}C_{ox}^2}{(1 + K_{ox}C_{ox} + K_{si}C_{si} + K_H\sqrt{C_H})^3} \tag{E4}$$

As the gas moves toward the pump end, hydrogen builds up. As equation (A4) suggests, the growth rate will begin to drop. Unlike the polysilicon process, the growth rate cannot be brought up simply by increasing the silane content in the back end of the tube. Rather, the more difficult task of adjusting the silane to oxygen ratio must be performed.

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