Method for Semiconductor Process Optimization Using Functional Representations of Spatial Variations and Selectivity

Purnendu K. Mozumder, Member, IEEE, and Lee M. Loewenstein

Abstract — We present a methodology for determining the optimal equipment settings for a processing step based on experiment designs and model-based optimization. Traditional techniques suffer from the choice of optimization metrics that fail to take into account the spatial effects on the wafer. The process yield becomes increasingly sensitive to spatial variations as the size of the wafer and processing complexity increase and the ratio of the size of the process chamber to the wafer decreases. Furthermore, some of the metrics like nonuniformity and selectivity, as defined today, cannot be modeled with the desired accuracy. In this article we present a set of alternate metrics to alleviate the above-mentioned problems. We include the results of our study of a plasma-assisted silicon nitride etch step.

I. INTRODUCTION

The development of a small lot, quick turnaround application specific integrated circuit factory offers additional challenges over the conventional high volume production. Among these is a need for a large increase in knowledge about the individual process steps used in a manufacturing flow over that at hand today. In a largely computer-controlled factory we will have both the luxury and burden of dealing with processes with far more flexibility than we have presently. Sophisticated scientific approaches to process development and manufacturing are warranted to fully leverage the flexibility. This will mean that we need more detailed process models. These models must predict the responses of interest accurately while preserving information about the gradient (trends) in the responses with respect to the input variables. The development of these models is time consuming and material intensive. Therefore careful consideration must go to the choice of an experimental design procedure and to the specification of metrics for quality factors.

Two important issues for the development of etching processes in semiconductor manufacturing are how to best model process uniformity and selectivity. In developing etching processes, we strive for high uniformity—that is, minimum variability—across a wafer. We usually work to maximize the selectivity of the process so that underlying films are not attacked once they are exposed. We must define uniformity and selectivity carefully, particularly when developing process models with predictive capability.

Today’s methods of describing etch uniformity fail to consider spatial information. How the process development engineer goes about minimizing spatial variation may very well depend on its type—for instance, radial versus azimuthal variations. Similarly, selectivity, when defined as a ratio of experimental etch rates for different films, is difficult to model when processes become very selective. When the underlying material is barely etched, and its change in thickness contains a significant error due to measurement uncertainty, the etch rate ratio becomes a very noisy function, which is hard to model with any accuracy.

To deal with these issues we have developed functional representations of uniformity (that is, spatial variations) and selectivity. For uniformity we have fitted a low-order polynomial to the data for each wafer. For selectivity, we first obtained polynomial fits to the etch rate data for each material. We then calculated the selectivity from a ratio of the two functions.

The problem studied is a process which isotropically etches silicon nitride, Si$_3$N$_4$, films, stopping on a thin, underlying pad silicon dioxide, SiO$_2$, film. In the following sections, we will describe the equipment and chemistry pertaining to the etch process and the proposed modeling methodology. We will present the results obtained by applying the proposed methodology to the etch process.

II. DESIGN METHODOLOGY

Our aim was to develop response surface models for the etch rate of Si$_3$N$_4$, nonuniformity of the Si$_3$N$_4$ etch, and the selectivity of Si$_3$N$_4$ over SiO$_2$. For notational convenience we will denote the etch rates and uniformities by the symbols $R(n)$ and $U(n)$, respectively, where $n = $ Si$_3$N$_4$, SiO$_2$. Similarly, we will represent the selectivity as $S$(Si$_3$N$_4$/SiO$_2$). The goal of the design was to maximize $U(Si_3N_4)$ and minimize $S(Si_3N_4)$ and maximize the mean of $R(Si_3N_4)$ over the wafer. Common definitions of $U(n)$ are either ($R(n, \text{max}) - R(n, \text{min}) / (2 \cdot R(n, \mu))$ or $R(n, \sigma)/R(n, \mu)$ over each wafer, where $R(n, \text{max})$ is the maximum $R(n)$, and the other $R(n, p)$ are defined similarly, where $p$ is a metric (e.g., max, min, standard deviation, mean, etc.) for $R(n)$. Both of these measures (especially the first) give rise to unstable models due to a high sensitivity of both measures to outliers and shape of the spatial distribution of etch rates across the wafers. An
example of this effect is evidenced in Fig. 1, where most of the wafer has an uniform etch rate except for a single outlier that skews both uniformity measures. A similar problem exists for the selectivity, $S(Si_3N_4 : SiO_2)$ is defined as $R(Si_3N_4, p)/R(SiO_2, p)$ on each wafer. Since $R(SiO_2, p)$ is much smaller than $R(Si_3N_4, p)$, the error variance in the measurement and the spatial error variance are comparable to the $R(SiO_2, p)$ on the wafer. Taking the inverse of $R(SiO_2)$ magnifies the contribution of the error variance of $R(SiO_2)$ to the error variance of the selectivity. Moreover, the near-normal distribution of errors for $R(SiO_2)$ translates to a cumbersome distribution of the error in selectivity. These factors make the modeling of the selectivity difficult and the resulting model unstable. The literature suggests various remedies, such as the use of logarithmic transforms, but these do not work well [5].

Our approach to solving these problems was to create twolayered models. The first layer is a spatial model of $R(Si_3N_4)$ and $R(SiO_2)$ over the wafer. The second layer consists of the process models: mappings of the equipment settings to the coefficients that parameterize the spatial variations. The advantage of such a model is that we did not need to determine the metric of nonuniformity a priori. Since the two-layered models carry the spatial information, the experimenter can define any metric of the nonuniformity as well as the mean using the model coefficients. We modeled $S(Si_3N_4 : SiO_2)$ as a ratio of two polynomials, instead of a single polynomial representing a ratio of data points. This ratio of polynomials led to a more robust model and fits the data better than a single polynomial.

Finally, we used the equipment models as inputs to an optimizer, together with the desired quality characteristics, to determine the optimal operating point. In addition, we included in the optimization scheme as constraints or penalties both the engineer's knowledge and additional criteria not expressed in the models. For example, we had to include the stability of the equipment in a certain range of operations. We will show how the choice of $R(Si_3N_4)$ and $R(SiO_2)$, instead of $S(Si_3N_4 : SiO_2)$, as objectives leads to a more robust optimization.

Creation of the models, or response surfaces, required the use of efficient experiment design. We performed our experimental design using the method of Latin hypercube sampling (LHS) [4, 2]. The LHS technique tries to lessen the problems associated with traditional experiment design strategies such as fractional factorials, central composites, and alphabet $(O$, $G$, $I)$ optimal [1]. LHS can be looked upon as a stratified Monte Carlo sampling where the pairwise correlations can be minimized to a small value (which is essential for uncorrelated parameter estimates) or else set to a desired value [6]. The sampling technique is not specifically suited to any model, and the design points generated are spread through the interior of the region of interest, unless otherwise specified [6]. Moreover, if one suspects during the modeling that the process can be best represented by two or more models instead of a single one, the LHS can be split into multiple parts without destroying the essential features of the design other than reducing the sample size for each regression. This is not possible for traditional designs.

III. PROCESSING METHOD

We used 150-mm diameter Si ($p$-type, $\{100\}$) wafers coated with films of Si$_3$N$_4$, SiO$_2$ or polycrystalline Si (poly-Si). We formed the Si$_3$N$_4$ and poly-Si films by low pressure chemical vapor deposition onto a base film of thermal SiO$_2$. We grew the SiO$_2$ films by furnace oxidation of Si. The gases, CF$_4$ and N$_2$, passed through a remote microwave discharge, while H$_2$ bypassed the discharge. Mass flow controllers maintained gas flows. An MKS throttle valve controller regulated the total pressure. Further details on the reactor may be found in [3]. We determined $R(n)$ for each material by subtracting the film thickness after etching from the film thickness before etching, then dividing by the process time of 60 s.

IV. EXPERIMENT DESIGN

In our experiment design we used a two-step experiment strategy. First, we used a linear screening experiment to determine the subset of important variables (those significantly affecting the responses). In our case these are $R(Si_3N_4)$, $R(SiO_2)$, $U(Si_3N_4)$, and $U(SiO_2)$. Then we used a LHS experiment, in the reduced set of variables, to estimate the response surface models. While a linear screening experiment
may not be an adequate method of determining the subset of influential variables, in this case the process engineer knew that none of the equipment or process variables exhibited strong periodicity that would “hide” its effect from the linear experiment.

We started with seven parameters as inputs and performed a linear screening experiment using ECHIP [7]. The result showed five significant parameters that affected the output. Table I shows the parameters, symbols, units, and the ranges used.

We designed a 35-point LHS experiment using software developed at the Sandia National Laboratories. We chose 35 points as a compromise between the number of wafers and the number of terms we could possibly need to estimate if the models were between quadratic and cubic. Five of the 35 points were replicates corresponding to five different experiment runs. We used the replicates to determine the pure experimental error. The analysis of variance (ANOVA) uses the pure error to determine the lack of fit (LOF) for the models. In our model building effort we tried to reduce the LOF without overfitting to the data. We discretized the sampling distributions for the temperature and power since the equipment knobs for these parameters did not allow continuous settings. We discretized the temperature in 20°C steps, and the power in 100-W steps. Since the experiment allowed setting the parameters independently, we did not specify correlation coefficients to the program. The program minimized the correlation coefficients: the largest correlation and rank correlations among the independent parameters were $-0.081$ and $-0.085$, respectively.

For each condition, we etched two wafers (both Si$_3$N$_4$ and SiO$_2$). On each wafer, we made 19 thickness measurements in two concentric hexagons and at a center point both before and after the etch.

V. RESULTS AND DISCUSSIONS

A. Models

To model the spatial variation across the wafers, we tried both Cartesian and polar coordinates. The Cartesian coordinates with quadratic models fitted very well. The polar coordinates showed significantly worse fits. This is because, some of the wafers had pronounced lack of radial symmetry (especially for SiO$_2$). For others, there were axial symmetry, the symmetry was about tilted axes. Therefore, higher order polar models would be necessary. Another possibility was to use the $\sin n\theta$ and $\cos n\theta$. That would, however, decrease the spatial smoothness of the models, making them hard to interpret.

For the models, the center point was chosen as (0, 0). Therefore, the constant in the spatial models corresponds to the etch rate at the center. Most of the $R^2$ for the spatial models were greater than or equal to 0.9. For the wafers with $R^2 < 0.9$, especially SiO$_2$, isolated “islands” (Fig. 2) on the wafer maps are the reason for bad fit. The results of the spatial models are summarized in Table II. We observed that the fits for $R(SiO_2)$ are slightly worse than $R(Si_3N_4)$. This is expected since $R(SiO_2)$ is much smaller than $R(Si_3N_4)$, while the measurement errors are the same for both. This phenomenon worsens the signal-to-noise for $R(SiO_2)$ compared to $R(Si_3N_4)$, which adversely affects the $R^2$. Since we were to use the models for design and optimization rather than process control, we did not apply outlier rejection. We observed, by applying outlier rejection on a few wafers, that rejection of 1 or 2 points significantly increased the model fits.

For the process models, we first tried a quadratic fit. The fits, however, were mediocre. The $R^2$ ranged from 0.4 to 0.8. Attempting to fit a full cubic would make the model overfit in 35 points, since the number of coefficients to be estimated would be greater than 31 (the number of distinct experiment design points). So we tried a cubic additive model. An additive model is where linear, quadratic, and cubic terms exists for each variable but no interactions exist. The models are of the

### Table I

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Temperature</th>
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<th>Pressure</th>
<th>$N_2$</th>
<th>$H_2$</th>
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<td>scem</td>
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<tr>
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### Table II

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<th>$R^2 &gt; 0.90$</th>
<th>$R^2 &gt; 0.80$</th>
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<tr>
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<td>6</td>
<td>6</td>
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TABLE III
GOODNESS OF FITS FOR SPATIAL COEFFICIENTS FOR $R(Si_{3}N_{4})$ AND $R(SiO_{2})$

<table>
<thead>
<tr>
<th>Term</th>
<th>1 - $R^2$</th>
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<th>$x^2$</th>
<th>$xy$</th>
<th>$y$</th>
<th>$y^2$</th>
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<td>0.95</td>
<td>0.98</td>
<td>0.90</td>
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<tr>
<td>$R^2$ - $R(SiO_{2})$</td>
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<td>0.90</td>
<td>0.93</td>
<td>0.94</td>
<td>0.93</td>
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</table>

where $y$ represents the response of interest (viz., $R(Si_{3}N_{4})$), $x_i$ represents the $i$th input variable, and $a_{ik}$ represents the coefficient of the $k$th power of $x_i$.

We estimated 16 coefficients (compared to 21 for a full quadratic). Although the fit improved significantly for wafers with lower $R^2$, there was no improvement for the models with $R^2$ close to 0.8. We introduced a set of second-order cross terms in the model. We then had 26 to estimate. Models were of the form:

$$y = a_0 + \sum_{i=1}^{5} a_{i1}x_i + a_{i2}x_i^2 + a_{i3}x_i^3 + \sum_{i=1,j>i}^{5} b_{ij}x_ix_j$$

where, in addition to (1), the term $b_{ij}$ represents the mixed quadratic coefficient of $x_i x_j$. The models were adequate, both in terms of $R^2$ and ANOVA of errors. We list the results in Table III. We trimmed down the models using Student’s $t$-test for significance on the regression coefficients. We rejected the coefficients that we did not find to be significant ($\alpha = 0.05$). The need for cubic terms arose due to the rapid change from etch to deposition for relatively small changes in the process conditions, particularly the H$_2$ flow rate, and the large region of operation chosen for the models.

The final response surface model of the etch rate on a given position on a wafer subjected to a set of process conditions within the defined region of operation is expressed in a matrix form as

$$R(n) = [1 \ x \ x^2 \ xy \ y \ y^2] M [\begin{array}{c} T \\ H^2 \\ TP \end{array}$$

$$= \begin{bmatrix} a_0 & a_{11} & \cdots & a_{53} & b_{1,2} & \cdots & b_{1,5} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ a_0 & a_{6,1} & \cdots & a_{10,3} & b_{2,1} & \cdots & b_{2,5} \end{bmatrix}$$

A graphical representation of the two-layered model expressed in 3 is presented in Fig. 3.

### B. Optimization

In this section we will explain the use of the models to define metrics for nonuniformity and selectivity. Furthermore, we will discuss the process of optimization used to determine the optimal process conditions for the strip.

For the $Si_{3}N_{4}$ strip process there are three important quality characteristics. In order of importance, they are:

1. maximum $S(Si_{3}N_{4} : SiO_{2})$;
2. minimum $U(Si_{3}N_{4})$ across individual wafers;
3. maximum $R(Si_{3}N_{4}, \mu)$.

To carry out a multicriteria optimization, we weighted the quality characteristics by their relative importance. However, the process and spatial models that we developed did not directly relate the quality characteristics to the process parameters. We had to perform appropriate transformations before we could input the models to an optimizer. For both $Si_{3}N_{4}$ and $SiO_{2}$, six coefficients (quadratic models) characterize the spatial distributions of the etch rate across the wafer. For $Si_{3}N_{4}$, we expressed the etch rate as a function of the spatial coordinates:

$$R(Si_{3}N_{4}) = c_0^N + c_1^N x + c_2^N y + c_2^N x^2 + c_3^N xy + c_4^N y^2.$$  (5)

We expressed $R(SiO_{2})$ similarly. We represented the selectivities as ratio of polynomials. Each of the 12 coefficients is a function (pure cubic + mixed quadratic) of 5 process parameters. We aimed the optimization toward manipulating the process parameters to generate a set of coefficients that optimize the quality characteristics. To perform the optimization the quality characteristics had to be defined in terms of the spatial model coefficients. As an example, let us first look at the formulation of the average etch rate and the nonuniformity. If the uniformity is specified as $U(n) = R(n, \sigma)/R(n, \mu)$, and assuming that the wafer is circular with radius $r$ (75 mm in our case): the simplification (neglecting the superscripts) leads to

$$R(n) = c_0 + \frac{(c_{2x} + c_{2y})r^2}{4},$$

$$U(n) = \frac{[(6r^2c_{1x} + 3r^4c_{2x}) + 6r^2c_{1y} + 2r^4c_{2y}c_0 + 3r^4c_{2y} + 12r^2c_{2y}c_0 + 2r^4c_{2y}c_0 + 24r^2c_{2y} + 24r^2c_{2y}^2/24R(n, \mu)^2} - 1]^{1/2}.$$  (7)

The exact formulation of $U(Si_{3}N_{4})$ depends on the definition of the uniformity. In general, if all the coefficients, except
$c_0^N$, are identically zero, the wafer will have a totally uniform etch rate, i.e., the nonuniformity will be zero. Therefore, one may look upon the minimization of nonuniformity as the minimization of the linear and quadratic coefficients.

A problem arises with the weighting the coefficients appropriately for the optimization. There are two possibilities.

1) Use maximum values of $x$ and $y$ in the linear and quadratic parts of the equation. Change the values of the coefficients to their absolute values. This will be the worst-case deviation.

2) Use the exact equation of the spatial variation of the etch rate and then sample spatially over the wafer to estimate the nonuniformity (variance, max–min, etc.).

In our formulation of the problem, we chose approach 1 for two reasons. 1) Approach 1) leads to fewer computation cycles within each iteration (sampling) of the optimizer. Moreover, there is no foreseeable advantage in choosing approach 2) in terms of the algorithm for minimizing $U(Si_3N_4)$. 2) The objective function for approach 1 has a smoother functionality with respect to the process conditions, helping the already complex optimization. However, either approach will serve the purpose of minimizing $U(Si_3N_4)$ equally well: the optimization procedure may have to be adapted for nonsmooth behavior or local minima.

Expression of the selectivity as the ratio of the mean etch rates is inaccurate. While the exact expression for the mean of the selectivity is mathematically cumbersome, in the limiting case of the nonuniformity tending to zero the average selectivity will reduce to the ratio of the average etch rates. Where the nonuniformity is small, the errors introduced in the mean of the selectivity are also small. The advantage of specifying the selectivity as the ratio of polynomials stems from each polynomial having an excellent goodness of fit compared to a single polynomial model for the ratio of mean etch rates. The residuals for $R(Si_3N_4)$, $R(Sio_2)$, a single polynomial for $S(Si_3N_4 : SiO_2)$ and the ratio of two polynomials are plotted in Fig. 4. It is evident that the ratio of two polynomials results in a superior fit compared to a single polynomial. Not only is the error variance lower for the ratio of polynomials, but the marked “cone” shape of the error variance observed in the single polynomial is greatly reduced. This is expected since the ratio of polynomials can fit a larger family of functions compared to a single polynomial. Moreover, no additional cost is incurred in estimating the coefficients of the polynomials since the coefficients are determined while fitting $R(Si_3N_4)$ and $R(Sio_2)$.

Examination of Fig. 4 and the preceding analysis lead us to believe that using $R(SiO_2)$ as an metric for optimization rather than $S(Si_3N_4 : SiO_2)$ could lead to a more stable optimization. Mathematically this can be justified for two reasons.

1. The error variance for $R(SiO_2)$ is smaller compared to that of the ratio of polynomials representing $S(Si_3N_4 : SiO_2)$.

2. The model for $R(SiO_2)$ is smoother (has fewer modes) compared to that of $S(Si_3N_4 : SiO_2)$. This enhances the probability of the optimizer converging to the global extremum in a complex optimization scheme.

We can now map the problem of process optimization as a multicriteria optimization of the form:

$$\min_{T,F,E,N} w_{R0} R(SiO_2, \mu)$$

$$\min_{T,F,E,N} w_{U1} U(Si_3N_4)$$

$$\max_{T,F,E,N} w_{RX} R(Si_3N_4, \mu)$$

where the $w$'s represent the specific weights applied to each objective. These weights are based on the process engineer's judgment.

We used the optimizer MACH1 for the optimization. This optimizer uses a combination of Gauss–Newton and variable metric methods. We chose the initial weights for $R(SiO_2, \mu)$, $U(Si_3N_4)$ and $R(Si_3N_4, \mu)$ as 5, 3, and 2, respectively.

The first results from the optimizer were unsatisfactory: $R(Si_3N_4, \mu)$ was high but $S(Si_3N_4 : SiO_2)$ was mediocre. Furthermore, the H2 flow rate was too high, which indicated possible instability. Also, there were regions in the design space where $R(SiO_2, \mu)$ was negative. We noted that a negative etch rate means a deposition and effectively results in an infinite selectivity. We incorporated this into the optimization in the form of a further objective stating that the difference of the $R(SiO_2, \mu)$ and $U(SiO_2)$ should be kept close to zero.

Addition of the constraint led to a much better optimum, with desirable input conditions at the optimal point. By altering the objectives it was found that the transformed problem behaved better than the original problem. We estimated that the cubic models account for local optima, which get smoothed out by the addition of the new objective function, enabling MACH to reach a “better minimum.” The novel method of representing selectivity enabled us to decouple the problem and attain a stable solution. As a further experiment, we ran both the unconstrained and the constrained problems from many different starting points. The results showed that for the unconstrained case several local minima were found, which was greatly reduced for the transformed problem. Tables
TABLE IV
OPTIMAL VALUES OF INPUT PARAMETERS

<table>
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<tr>
<th>Parameters</th>
<th>Temperature</th>
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<th>Pressure</th>
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TABLE V
OPTIMAL VALUES OF OUTPUT PARAMETERS

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<tr>
<th>Parameters</th>
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IV and V contain the final results of the optimization. We calculated the worst-case selectivity by adding/subtracting the 2σ values of the model residuals to/from the optimized values of R(Si₂N₂, µ) and R(SiO₂, µ). For our results the worst-case S(Si₂N₂ : SiO₂) is given by (33.1 – 1.94/0.07 + 0.99) ≈ 15. To complete our analysis we used the traditional method of defining selectivity and mean etch rates and performed the same optimizations. The results were found to be inferior to that of the new approach. Due to the large variance in the models for the quality characteristics, especially the selectivity, the mean selectivity as well as the worst case was found to be significantly lower compared to the results from the new approach.

VI. CONCLUSIONS

We have described a method for semiconductor process optimization, which uses two-layered models. The first layer involves creating a spatial model—one for each film of interest—of the etch results. The second layer maps the coefficients of the spatial models to equipment settings. All this is done before any optimization scheme is employed. The process engineer then may optimize the etch process by maximizing coefficients which contribute to the desired maximum etch rate, while minimizing coefficients which contribute to nonuniformity. He also may minimize coefficients which represent undesired etches, and thus obtain etch selectivity. This method may be used for other process optimization needs such as for thin film depositions and patterned etches.

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REFERENCES


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