2.830J / 6.780J / ESD.63J Control of Manufacturing Processes (SMA 6303)
Spring 2008

Control of Manufacturing Processes

Subject 2.830/6.780/ESD.63

Spring 2008

Lecture #21

Case Study: Spatial Modeling

May 6, 2008

Case Study Reading

- J. C. Davis, R. S. Gyurcsik, J.-C. Lu, and J. M. Hughes-Oliver, "A Robust Metric for Measuring Within-Wafer Uniformity," *IEEE Trans. on Components, Packaging, and Manuf. Tech. - Part C,* vol.19, no. 4, pp. 283-289, Oct. 1996.
- P. K. Mozumder and L. M. Loewenstein, "Method for Semiconductor Process Optimization Using Functional Representations of Spatial Variations and Selectivity," *IEEE Trans. on Components, Hybrids, and Manuf. Tech.*, vol. 15, no. 3, pp. 311-316, June 1992.
- R.-S. Guo and E. Sachs, "Modeling, Optimization and Control of Spatial Uniformity in Manufacturing Processes," *IEEE Trans. on Semiconductor Manuf.*, vol. 6, no. 1, pp. 41-57, Feb. 1993.

Agenda

- Spatial Sampling
  - Example: impact of sampling plan on response regression
- Spatial Non-Uniformity Models
  - DOE/RSM with both process and spatial dependencies
  - “Multiple Response Surface” (MRS) vs. “Single Response Surface” (SRS) approaches

Spatial Trends

- In many manufacturing processes, a spatial trend in some response is observed
  - Wafer fabrication: "wafer scale" trends in film thicknesses, electrical properties, etc. resulting from inherent equipment/process asymmetries

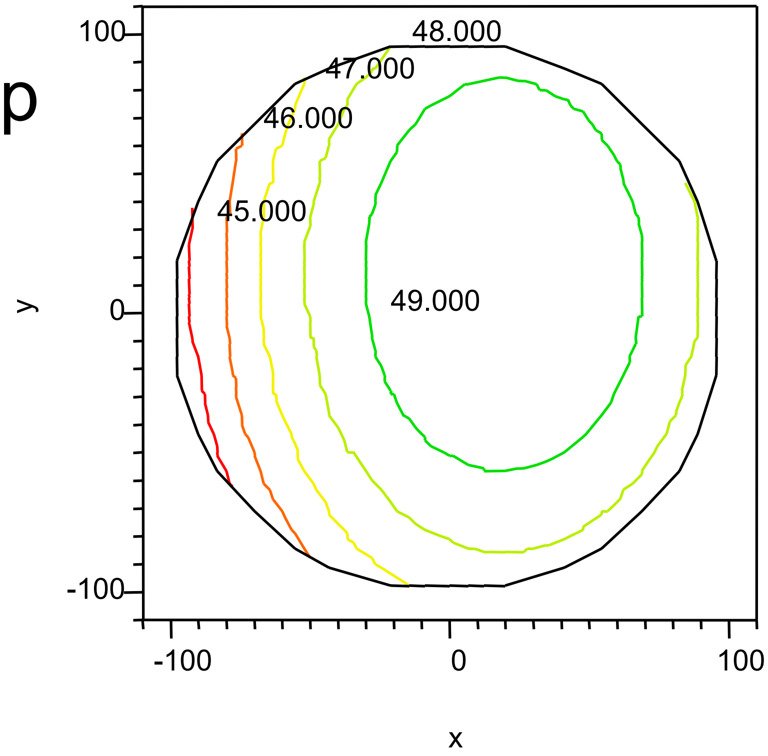
- Key questions:
  - How model?
  - How summarize (e.g. nonuniformity metric)?

Example

- Synthetic data
  - We construct a spatial response for some parameter (resistivity) so we know the "true" spatial dependency:

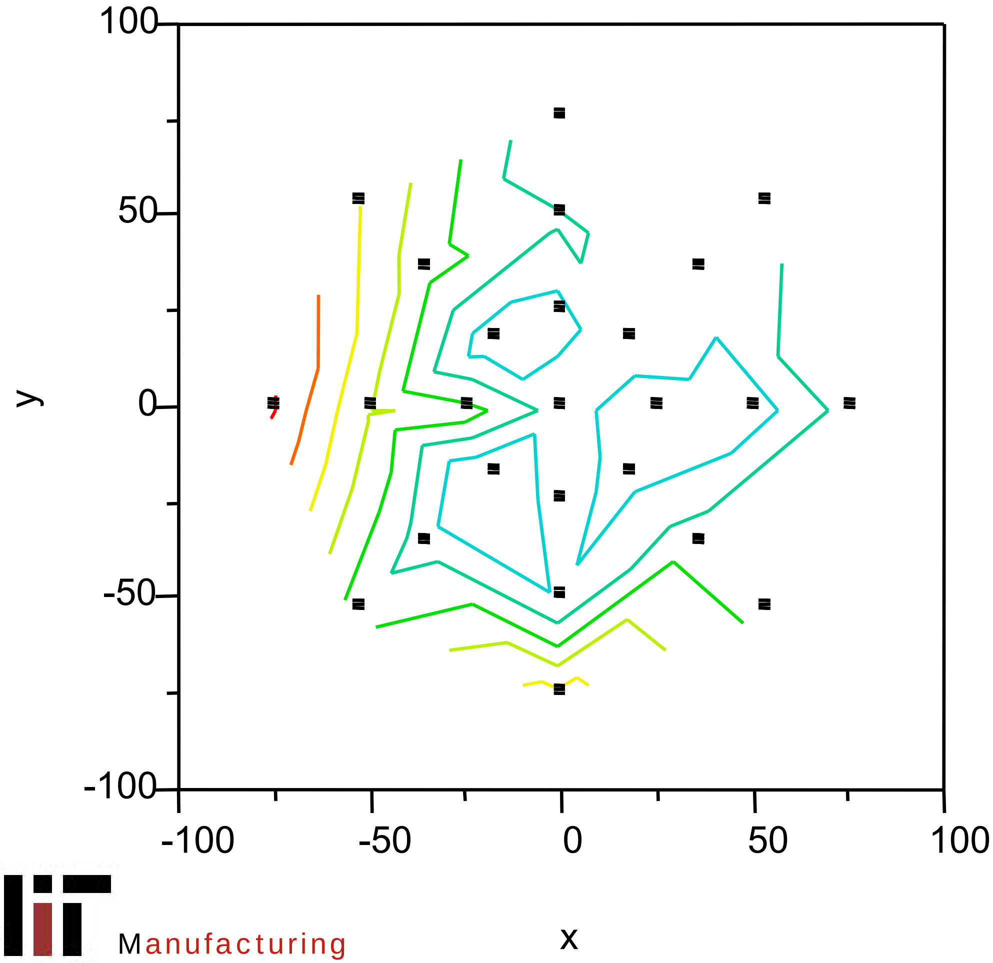
$$\rho = 50 - \frac{(x-20)^2}{50^2} - \frac{(y-15)^2}{70^2} + N(0, 0.49)$$

- Generate data sets
  - Common "circular" wafer map
  - Rectangular grid
- Calculate:
  - Response surface model
  - Non-uniformity metric, e.g. **σ/μ**



1. Radial Sampling Plan

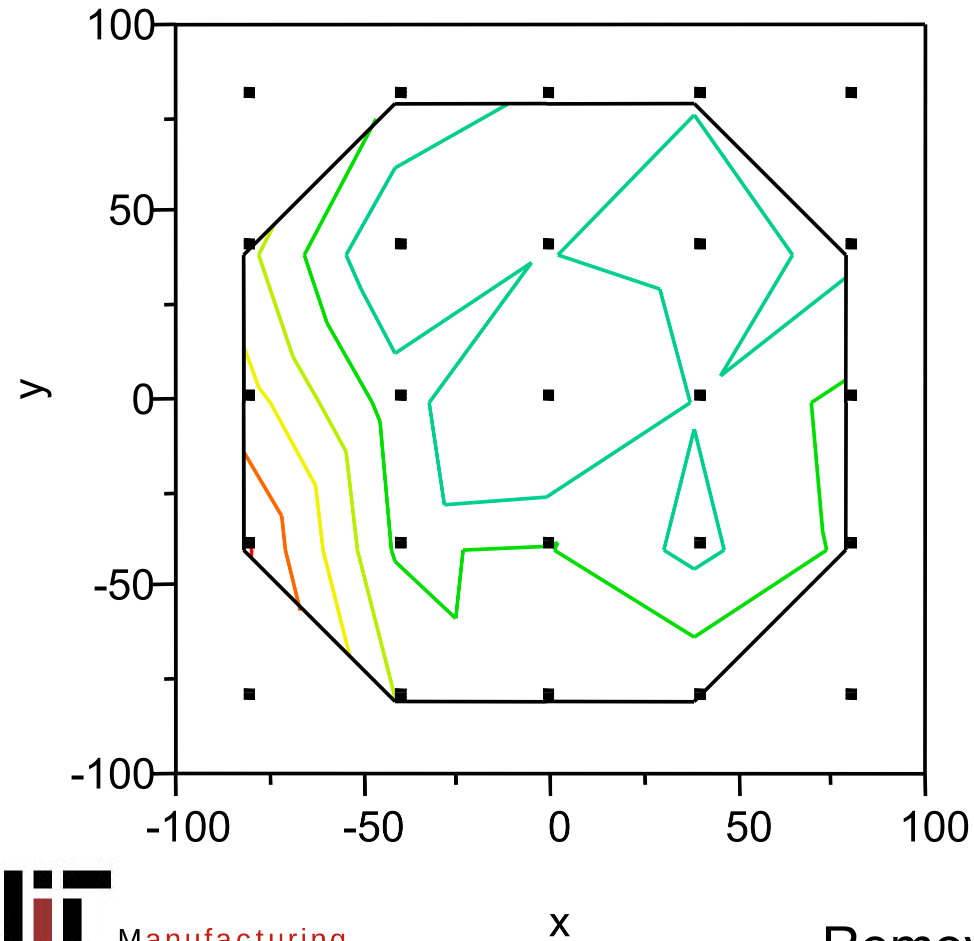
- 8 points at a radius of 75 mm
- 8 points at a radius of 50 mm
- 8 points at 25 mm radius
- 1 point at the center of the wafer



X	Y	rho
25	0	49.9601097
17.68	17.68	49.1136113
0	25	49.7359187
-17.68	17.68	49.8140025
-25	0	48.2246087
-17.68	-17.68	50.1927006
0	-25	49.2427469
17.68	-17.68	49.6791275
50	0	49.8336576
35.36	35.36	49.2292189
0	50	48.9286926
-35.36	35.36	48.2485797
-50	0	47.8966527
-35.36	-35.36	49.2351389
0	-50	49.426475
35.36	-35.36	48.6728475
75	0	48.8338909
53.03	53.03	49.0658809
0	75	49.4461394
-53.03	53.03	47.4035767
-75	0	46.4175911
-53.03	-53.03	48.6600647
0	-75	47.278698
53.03	-53.03	48.6137312
0	0	49.187609

2. Square Sampling Plan

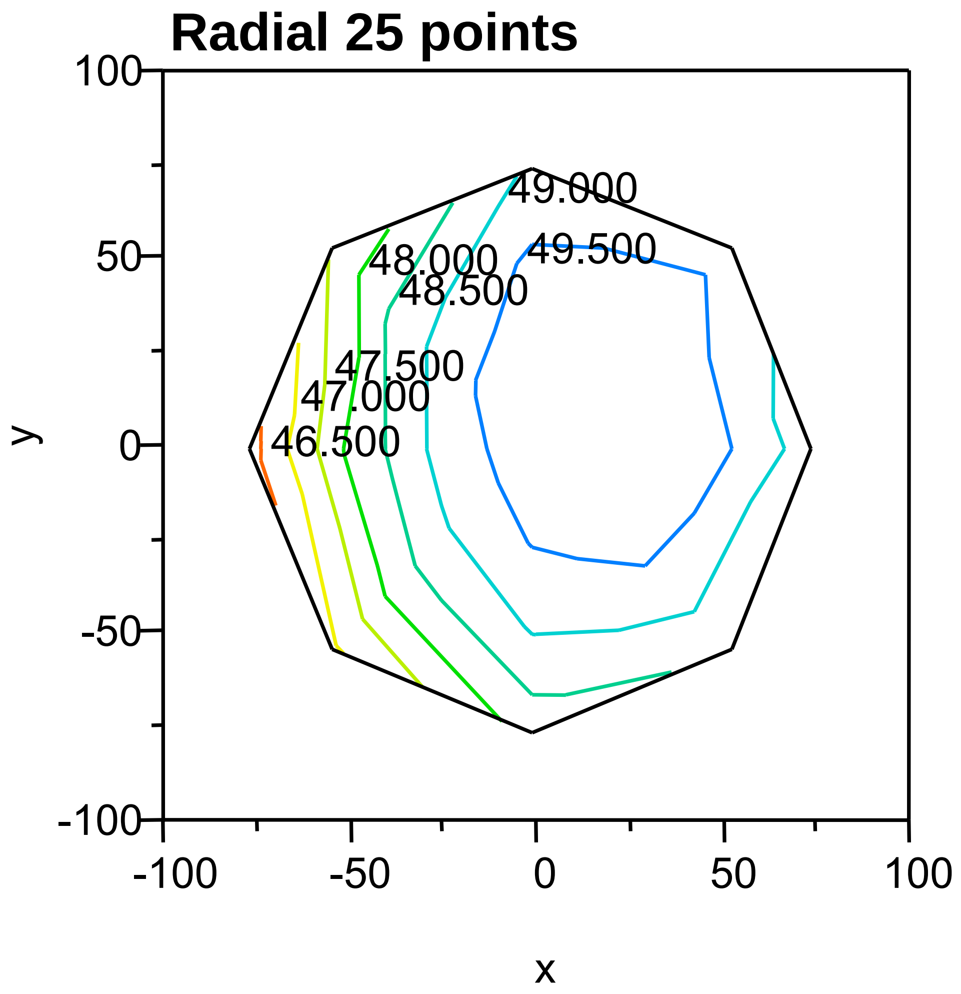
- 5 x 5 pattern of evenly spaced points, at 0, ±40 mm, and ±80 mm

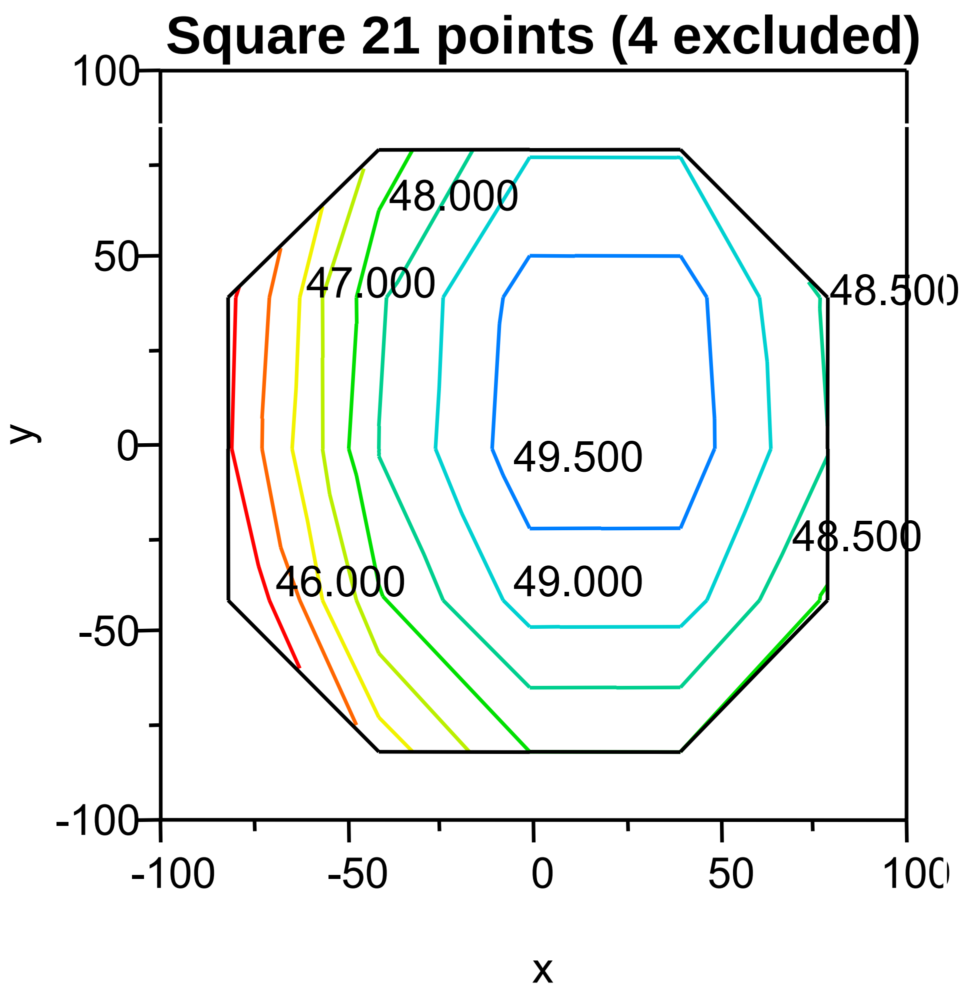


X	Y	rho	radius
-80	**-80**	**43.0470061**	**113.137085**
-80	-40	43.8235773	89.4427191
-80	0	45.5348185	80
-80	40	46.7131975	89.4427191
-80	**80**	**44.4409087**	**113.137085**
-40	-80	46.9708298	89.4427191
-40	-40	48.0724036	56.5685425
-40	0	48.4718544	40
-40	40	50.0468027	56.5685425
-40	80	48.1854786	89.4427191
0	-80	47.8974197	80
0	-40	47.9125541	40
0	0	50.8052758	0
0	40	49.0474654	40
0	80	49.2586326	80
40	-80	47.0922886	89.4427191
40	-40	49.2927422	56.5685425
40	0	48.9410342	40
40	40	48.4946369	56.5685425
40	80	49.0316954	89.4427191
80	**-80**	**46.2385337**	**113.137085**
80	-40	47.8303103	89.4427191
80	0	47.7426285	80
80	40	49.2722787	89.4427191
80	**80**	**48.1145491**	**113.137085**

Remove bolded data – outside wafer boundary.

Underlying Patterns (Noise Free)





- Noise-free interpolation of surfaces, based on JMP contouring algorithm.

Surface Regression – Radial Pattern

- Model form: $\hat{\rho} = a + bx + cy + dxy + ex^2 + fy^2$

Radial Pattern

Summary of Fit

Rsquare	0.654747
RSquare Adj	0.563891
Root Mean Square Error	0.602697
Mean of Response	48.89365
Observations (or Sum Wgts)	25

- **Correctly rejects *xy* term**
- **Incorrectly rejects *y* term**
- **R^2 appears poor at 0.65**

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	5	13.088445	2.61769	7.2064
Error	19	6.901635	0.36324	Prob > F
C. Total	24	19.990080		0.0006

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	49.572542	0.200911	246.74	<.0001
X	0.0114423	0.003222	3.55	0.0021
Y	0.0021554	0.003222	0.67	0.5115
x*y	0.0001744	0.000097	1.79	0.0894
x*x	-0.00031	0.000075	-4.12	0.0006
y*y	-0.000175	0.000075	-2.32	0.0314

Surface Regression – Square Pattern

- Model form: $\hat{\rho} = a + bx + cy + dxy + ex^2 + fy^2$

Rectangular Pattern

Summary of Fit

RSquare	0.766179
RSquare Adj	0.688239
Root Mean Square Error	0.859359
Mean of Response	48.11609
Observations (or Sum Wgts)	21

- **Correctly rejects *xy* term**
- **Keeps *y* term**
- **R^2 better at 0.77**

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	5	36.298420	7.25968	9.8303
Error	15	11.077466	0.73850	Prob > F
C. Total	20	47.375886		0.0003

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	49.606808	0.395623	125.39	<.0001
x	0.0137149	0.003684	3.72	0.0020
y	0.0115245	0.003684	3.13	0.0069
y*x	-0.000073	0.00009	-0.82	0.4261
x*x	-0.000404	0.000081	-4.98	0.0002
y*y	-0.000172	0.000081	-2.12	0.0514

Surface Regressions – Summary

$$\text{true}: \quad \rho = 49.794 + 0.016x + 0.0061y + 0xy - 0.0004x^2 - 0.0002y^2$$

$$\text{radial}: \quad \hat{\rho} = 49.572 + 0.0114x + 0.002y + 0.00017xy - 0.0003x^2 - 0.00017y^2$$

$$\text{square}: \quad \hat{\rho} = 49.607 + 0.0137x + 0.0115y - 0.000073xy - 0.0004x^2 - 0.00017y^2$$

- Radial:
  - Correctly rejects *xy* term
  - Incorrectly rejects *y* term
  - R^2 is poor at 0.65
- Square:
  - Correctly rejects *xy* term
  - Keeps *y* term
  - R^2 better at 0.77

Calculated Nonuniformity Metrics

Radial Sampling Plan

Mean	48.89365
Std Dev	0.91264
Std Err Mean	0.18253
Upper 95% Mean	49.27037
Lower 95% Mean	48.51693
N	25.00000

$NU = \sigma/\mu = 0.018666$

Rectangular Sampling Plan

Mean	48.11609
Std Dev	1.53909
Std Err Mean	0.33586
upper 95% Mean	48.81667
lower 95% Mean	47.41551
N	21.00000

$NU = \sigma/\mu = 0.031987$

- Very different apparent non-uniformities!
  - 1.9% vs. 3.2%
- Why?
  - May be sampling different portions of curvature
  - Data points are "representing" different amounts of the underlying wafer surface

Estimates from Dense 29 x 29 Spatial Sample

Moments

Mean	48.30429
Std Dev	1.52280
Std Err Mean	0.05905
upper 95% Mean	48.42024
lower 95% Mean	48.18834
N	665.00000

NU = σ/μ = 0.031525

- **"True" NU about 3.15%**
- **NOTE: R^2 still only 0.77. Cannot "model" away the random σ^2 = 0.49 noise!**

Summary of Fit

RSquare	0.768175
RSquare Adj	0.766416
Root Mean Square Error	0.735979
Mean of Response	48.30429
Observations (or Sum Wgts)	665

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	5	1182.8127	236.563	436.7318
Error	659	356.9575	0.542	Prob > F
C. Total	664	1539.7702		<.0001

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	49.883177	0.057113	873.41	0.0000
x	0.016497	0.000569	28.99	<.0001
y	0.0061666	0.000569	10.84	<.0001
y*x	-0.000007	0.000014	-0.50	0.6158
x*x	-0.000414	0.000012	-34.35	<.0001
y*y	-0.000214	0.000012	-17.72	<.0001

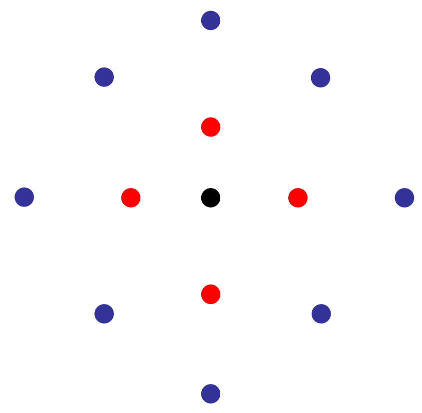
Robust Within-Wafer Uniformity Measures

- Davis et al.
  - Signal-to-noise (SNR) ratio for *systematic trends* is sensitive to location and number of measurements
  - Proposes an "Integration Statistic"
    - Base SNR on the total nonuniformity across an entire (spline) interpolated surface
- Simple approximation
  - Get much of the benefit by
    - Uniform sampling, or
    - Weighting importance of each measurement point by the amount of area that point represents

Typical: Linear Interpolation of Surface

Image removed due to copyright restrictions. Please see Fig. 1 in Davis, Joseph C., et al. “A Robust Metric for Measuring Within-Wafer Uniformity.” *IEEE Transactions on Components, Packaging, and Manufacturing Technology C* 19 (October 1996): 283-289.

E.g. 8 + 4 + 1



- Clearly only a coarse approximation of surface
  - Non-uniformity metrics based on this are subject to bias and variance errors

Proposed Interpolator: Thin Plate Splines

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- TPS: essentially localized polynomials with minimum curvature between "knots" or data points

Alternative to SNR (σ/μ): "Integration Statistic" *I*

$$I = \frac{I_n}{\text{Vol}_{target}} = \frac{\iint_{r,\,\theta} [T - g(r,\theta)] r \, dr \, d\theta}{\text{Vol}_{Target}} \quad (1)$$

where Vol_{Target} is the target volume, T is the target value of the response, and $g(r,\theta)$ is the function representing the response surface.

- Key ideas
  - Use interpolated surface *g(r, θ)*
  - Integrate deviations across the *entire* surface

Integration Statistic & Quality Loss

- Concern: cancellation in simple integration statistic
- Alternative: modify with a loss transformation

$$I = \frac{\iint_{r,\theta} h(T - g(r,\theta)) r \, dr \, d\theta}{\mathrm{Vol}_{Target}} \tag{2}$$

where $h(\,)$ is a general loss transformation such as $|x|$ or x^2 .

Approximation to Integral

$$I \approx \frac{\sum_{j=1}^{M} AC_j h(T - x_j)}{\text{Vol}_{target}}. \quad (6)$$

- Where C_j weight accounts for interpolation
  - Davis et al.: weights from coefficients of spline interpolation function
  - Alternative: the area that the point x_j represents

Improvement – Radial Nonuniformity Example

- Typical radial spatial pattern
  - SNR = μ/σ with radial measurements
    - **See bias for small # data**
  - Integration statistic based on TPS
    - **Removes bias**
    - **Reduces variance**

300 runs

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15% deterministic
+ 2% random

5, 13, 25, 73 points

Improvement – Asymmetrical Pattern

- Asymmetrical nonuniformity
  - 13 measurement sites
  - SNR with angular rotation
    - **Highly sensitive to angle**
  - Integration statistic based on TPS
    - **Reduced (but not eliminated) bias (20% smaller variation)**

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Agenda

- Spatial Sampling
  - Example: impact of sampling plan on response regression

- **Spatial Non-Uniformity Models**
  - **DOE/RSM with both process and spatial dependencies**
  - "Multiple Response Surface" (MRS) vs. "Single Response Surface" (SRS) approaches

IEEE TRANSACTIONS ON COMPONENTS, HYBRIDS, AND MANUFACTURING TECHNOLOGY, VOL. 15, NO. 3, JUNE 1992 311

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

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

- Silicon nitride etch
- Want response surface models for:
  - Nitride and oxide etch rates: R(Si_3N_4) and R(SiO_2)
  - **Nonuniformity of etch rates: U(Si_3N_4) and U(SiO_2)**
  - **Selectivity of nitride to oxide: S(Si_3N_4:SiO_2)**

Typical Etch Nonuniformity – Oxide Etch Rate

- Typical spatial map:
  - 19 measurements
  - 2 concentric hexagons [octagons?] plus center point

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- Relevant Process Parameters:

Challenge: Spatial Parameters

- Rates have a **spatial** dependence
  - How model this, as a function of both spatial position and the process conditions?

- Nonuniformity is a **derived** parameter:
  - Ratio of standard deviation to mean

Two-layered Spatial Model of Etch Rates

Process Terms

$$R(n) = [1 \quad x \quad x^2 \quad xy \quad y \quad y^2] M \begin{bmatrix} 1 \\ T \\ \vdots \\ H^3 \\ TP \\ \vdots \end{bmatrix} \qquad (3)$$

Spatial Terms

where

$$M = \begin{bmatrix} a_0^1 & a_{1,1}^1 & \cdots & a_{5,3}^1 & b_{1,2}^1 & \cdots & b_{4,5}^1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ a_0^6 & a_{1,1}^6 & \cdots & a_{5,3}^6 & b_{1,2}^6 & \cdots & b_{4,5}^6 \end{bmatrix}. \qquad (4)$$

Spatial Models: Regression Surfaces

$$R(Si_3N_4) = c_0^N + c_{1x}^N x + c_{1y}^N y + c_{2x}^N x^2 + c_{xy}^N xy + c_{2y}^N y^2. \qquad (5)$$

- Rate as function of position
- Spatial coefficients become functions of process conditions

Process Models: Polynomial Regression

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

- 2nd order + cubic term (in process conditions)
- Process DOE
  - Uses Latin Hypercube Sampling (LHS)

Uniformity & Selectivity Functions

- Build out of more **fundamental** rate functions

$$U(n) = \frac{R(n,\sigma)}{R(n,\mu)} \quad \text{where } n = SiO_2, Si_3N_4$$

$$S(Si_3N_4 : SiO_2) = \frac{R(Si_3N_4)}{R(SiO_2)}$$

- For models of given spatial form:

$$R(n) = c_0 + \frac{(c_{2x} + c_{2y})r^2}{4} \qquad (6)$$

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

Multiobjective Optimization

1. maximum $S(Si_3N_4 : SiO_2)$;
2. minimum $U(Si_3N_4)$ across individual wafers;
3. maximum $R(Si_3N_4, \mu)$.

$$\min_{T,P,p,N,H} w_{RO} R(SiO_2, \mu)$$

$$\min_{T,P,p,N,H} w_{UN} U(Si_3N_4)$$

$$\max_{T,P,p,N,H} w_{RN} R(Si_3N_4, \mu)$$

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IEEE TRANSACTIONS ON SEMICONDUCTOR MANUFACTURING, VOL. 6, NO. 1, FEBRUARY 1993

Modeling, Optimization and Control of Spatial Uniformity in Manufacturing Processes

Ruey-Shan Guo, *Member, IEEE*, and Emanuel Sachs

- "Site Models"
  - Build models for **each** spatial location as a function of the process conditions
  - Then **combine** these sites as necessary for any derived or spatial parameters

(Measurement Sites)

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SRS vs MRS

- Single Response Surface (SRS)
  - Directly model σ/μ:

$$\frac{\sigma}{\mu} = C_1 + C_2X_1 + C_3X_2 + C_4X_1^2 + C_5X_2^2 + C_6X_1X_2 \quad (2)$$

- Multiple Response Surfaces (MRS)
  - Lower order models of each site

$$Y_1 = C_{11} + C_{12}X_1 + C_{13}X_2 \quad (3)$$

$$Y_2 = C_{21} + C_{22}X_1 + C_{23}X_2 \quad (4)$$

$$Y_3 = C_{31} + C_{32}X_1 + C_{33}X_2 \quad (5)$$

  - Combine functionally to derive uniformity

$$\mu = \tfrac{1}{3}(Y_1 + Y_2 + Y_3) \quad (6)$$

$$\frac{\sigma}{\mu} = \frac{\sqrt{\tfrac{1}{2}[(Y_1 - \mu)^2 + (Y_2 - \mu)^2 + (Y_3 - \mu)^2]}}{\mu} \quad (7)$$

Claimed MRS Advantages

- Effective models from small number of data
- Rapid adaptation of models after a process disturbance
  - Important for cycle to cycle control
- Immunity of models to the presence of noise
- Model forms are compatible with process knowledge

Argument: Complexity of Uniformity

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Implications for Control

Example: LPCVD of Polysilicon

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- Goal is to optimize SNR defined as $(\mu/\sigma)^2$

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Model Fits with Injected Noise

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SRS

MRS

MRS vs SRS Modeling – Impact on Optimization

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Conclusions

- Spatial Sampling
  - Sampling plan impacts spatial modeling
  - Uniform sampling, or appropriate weighting
- Combined Process/Spatial Modeling
  - Generally better to model fundamental parameters as function of process
  - Create derived measures using combinations of the lower level models
    - E.g. spatial nonuniformity, selectivity