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# Data-driven stochastic models for spatial uncertainties in micromechanical systems

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#### Abstract

Accurate uncertainty quantification in engineering systems requires the use of proper data-driven stochastic models that bear a good fidelity with respect to experimentally observed variations. This paper looks at a variety of modeling techniques to represent spatially varying uncertainties in a form that can be incorporated into numerical simulations. In the context of microelectromechanical systems, we consider spatial uncertainties at the device level in the form of surface roughness and at the wafer level in the form of non-uniformities that arise as a result of various microfabrication steps. We discuss methods to obtain roughness characterization data ranging from the use of a simple profilometer probe to imaging-based techniques for the extraction of digitized data from images. We model spatial uncertainties as second-order stochastic process and use Bayesian inference to estimate the model parameters from the input data. We apply the data-driven stochastic models generated from this process to micromechanical actuators and sensors in which these spatial uncertainties are likely to cause significant variation. These include an electrostatically-actuated torsion-spring micromirror, an electromechanical comb-drive actuator and a pressure sensor with a piezoresistive strain gauge. We show that the performance of these devices is sensitive to the presence of spatial uncertainties and a proper modeling of these uncertainties helps us make reliable predictions about the variation in device performance. Where data is available, we even show that the predicted variation can be validated against experimental observations, highlighting the significance of proper stochastic modeling in the analysis of such devices.

Keywords: Uncertainty quantification, microelectromechanical systems (MEMS), electrostatic

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actuation, spatially-varying uncertainties, stochastic modeling, profilometry, image segmentation, metrology.

## 1 Introduction

Spatially varying uncertainties are an important source of performance variation in microelectromechanical systems (MEMS). Most microfabrication methods that are used to generate mechanical or electronic structures on silicon wafers admit a large amount of non-unformity at wafer level, where the critical dimensions of devices in one part of the wafer may differ significantly from those in other regions. This variation may also extend down to the level of an individual device, where nominally uniform surfaces may exhibit significant amount of roughness or spatial variation. In order to ensure reliable performance, either by applying tighter tolerances on the fabrication equipment or by adjusting device design to reduce the sensitivity to these variations, it is important to first model the sources of uncertainty accurately and then quantify their effect on device performance. Accurate stochastic modeling is critical to achieving good predictions and this motivates the idea of using data-driven models that are directly estimated from experimental characterization data so that the input uncertainty is represented in a proper manner. This paper discusses several techniques for the generation of data-driven stochastic models for spatial uncertainties and applies these models to micromechanical devices in order to demonstrate that it is possible to make accurate predictions of variations in device performance.

There has been a lot of interest in modeling spatial variations in engineering systems, especially in the context of representing random, heterogeneous media [1, 2, 3]. In most cases, the variation is modeled as a stochastic process with a known local covariance structure [4, 5], whose parameters may either be assumed to be known or may be inferred from experimental measurements. Others have used self-affine roughness models that have a power law scaling [6, 7] to describe spatial roughness. In the context of MEMS, surface roughness has been studied in the context of mechanical contact [8] and stiction [9] as well as its effect on surface forces like the electrostatic force [10], Casimir force [11, 12, 7] and capillary forces [13, 14].

In this work, we use second-order stochastic processes to model spatial uncertainties. By using

 a generalized basis to represent the mean and covariance functions, we reduce the assumptions placed on the stochastic models and allow them to adapt themselves to fit the available data. This framework also allows for the inclusion of nonstationary covariance modeling, which is important in the context of electrostatic MEMS where variations in the device boundary affect the local electric field as well as the damping characteristics of the structure. The goal is to use characterization data obtained from actual examples of rough surfaces, to estimate the variation in device performance and wherever possible, to validate these predictions against experimental observations. The novel contribution of this work is to outline a proper data-driven framework that facilitates the incorporation of spatial uncertainties in MEMS modeling and to demonstrate its effectiveness in making reliable predictions.

The outline of this paper is as follows: Section 2 presents a generalized formulation for stochastic process modeling, which can easily be adapted to the situations encountered in the rest of the paper. Section 3 uses profilometric data corresponding to roughness along the floor of trenches etched using deep reactive ion etching (DRIE). This is then used to demonstrate the role of spatial uncertainties in a MEMS torsion mirror. Image segmentation-based methods are discussed in Section 4, where data extracted from scanning electron micrographs (SEM) is used to estimate the variation in side-wall profiles and then applied to a comb drive actuator example. Finally, Section 5 looks at wafer-level spatial uncertainties by estimating the thickness variation in a metal thin film process and its consequent effect on the uncertainty observed in batch-fabricated pressure sensor devices. Concluding remarks are mentioned in Section 6.

## 2 Mathematical framework for stochastic modeling

Spatial uncertainties like surface roughness can be represented within the numerical modeling framework as collections of random variables that are located at points distributed over the entire domain [15, 16, 17]. The spatial locations could correspond to points at which data is measured or could be randomly chosen in order to parametrize the uncertainty. This model assumes that there is some stochastic variation present at each spatial location used for parametrization and that this variation is correlated to the variation at neighboring points. Previous attempts at stochastic modeling in MEMS involving the measurement of electrical properties [6, 18] or for characterizing inhomogeneous material properties that affect thermoelastic damping in microresonators [5], use an assumed model for uncertainties based on prior knowledge that is available. In this work, we prefer a data-driven approach, where we try to keep the parametrization as generic as possible in order to obtain the best fit to experimentally measured data.

Since this entire approach is centered around experimentally measured data, it is useful to examine the process of gathering data as a motivation for the development of the stochastic model. Figure 1 illustrates this process using a typical micromechanical device as an example. We consider an electrostatic microactuator that consists of a moveable cantilever beam suspended over a fixed substrate, where the substrate surface is assumed to be rough. In a typical microfabrication workflow, thousands of such devices may be batch-fabricated simultaneously on a single wafer. This means that the statistical variation in performance of a nominal device will be affected by variations that exist in the substrate material or that are generated during wafer processing. If the spatial uncertainty is due to surface roughness, we could run a profilometer probe over the substrate surface to measure spatial variation in the height of asperities as shown in Figure 1. Since spatial variations can change from one device to the next, we need to repeat the same process over a set of devices and gather multiple replicates of the data at corresponding spatial locations in the devices. This allows us to characterize the variation at each spatial location and thus lets us build a stochastic model for the uncertainty.

There have been several approaches that have been developed for the estimation of spatiallyvarying stochastic models [19, 20, 21]. Their underlying theme involves choosing a parametrization for the stochastic model in terms of some unknown hyperparameters and then estimating the values of these hyperparameters such that the overall model fits the given data well [15, 16, 22]. The actual task of estimating the model may be carried out by developing a maximum likelihood estimator [23] or using Bayesian inference [24]. A common assumption that is used is to approximate the stochastic process up to the second order in terms of its mean and covariance functions. Furthermore, if the joint distribution of the values at any set of locations within the domain follows a multivariate Gaussian distribution, we refer to this as a Gaussian random process [17].

Mathematically, a second order Gaussian process, f, is defined in terms of its mean, M(X),

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Figure 1: Process of sampling spatial uncertainties in microsystems.

and the covariance function, C(X, X'), where X and X' are two arbitrarily chosen points in the domain of the process [15]. In this work, we use a cubic B-spline representation for the mean function, which is a suitable form for a realistic scenario where the form of the function is not known *a priori*. B-splines are piecewise-polynomial functions that are expressed as the weighted sum of spline basis functions, which have a localized support [25]. They are a popular means of representing an unknown function in terms of basis functions that possess desirable smoothness properties and yet, are easy to evaluate due to their local support. Given a vector of knots,  $t = \{t_1, t_2, \ldots, t_{p+k}\}$ , a spline function of degree k may be expressed as,

$$S_k(X; \boldsymbol{t}) = \sum_{i=1}^p \gamma_i B_{i,k}(X; \boldsymbol{t}),$$

$$B_{i,1}(X; \boldsymbol{t}) = \begin{cases} 1 & \text{if } t_i \leq X < t_{i+1} \\ 0 & \text{otherwise} \end{cases},$$

$$(1)$$

$$B_{i,k}(X; t) = \frac{X - t_i}{t_{i+k-1} - t_i} B_{i,k-1}(X) + \frac{t_{i+k} - X}{t_{i+k} - t_{i+1}} B_{i+1,k-1}(X),$$
(2)

where  $\gamma_i$  is an unknown weighting coefficient associated with each individual basis. In order to equip the spline representation with a continuous derivative, we choose k = 3 corresponding to cubic B-splines.

Next we assume that covariance function belongs to the Matérn family, whose form is given by [17]:

$$Mat\acute{ern}\left(X, X', \nu, \phi, \theta\right) = \phi^2 \frac{1}{\Gamma(\nu) 2^{\nu-1}} \left(\sqrt{2\nu} \frac{\|X - X'\|}{\theta}\right)^{\nu} K_{\nu}\left(\sqrt{2\nu} \frac{\|X - X'\|}{\theta}\right), \qquad (3)$$

where  $\Gamma$  is the Gamma function, while  $K_{\nu}$  is the modified Bessel function of the second kind.  $\nu, \phi$  and  $\theta$  are unknown parameters that characterize the covariance function. Consider  $\mathbf{X} = \{X_j; j = 1, 2, ..., n\}$  to be the set of locations where measured data is available, as shown in the example in Figure 1. If  $\mathbf{d}$  is the set of random variables associated with each of these points, then it follows from the definition of a Gaussian process, that the joint distribution of these variables has a multivariate normal form given by,

$$\boldsymbol{d} \sim \frac{1}{\left(2\pi\right)^{n/2} \left|\boldsymbol{\Sigma}\right|^{1/2}} \exp\left[-\frac{1}{2} (\boldsymbol{X} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{X} - \boldsymbol{\mu})\right],\tag{4}$$

where  $\boldsymbol{\mu}$  is the vector of mean values such that  $\mu_j = M(X_j)$ , while  $\Sigma$  is the covariance matrix evaluated at the points in  $\boldsymbol{X}$  and is given by  $\Sigma_{ij} = C(X_i, X_j)$ , for i, j = 1, 2, ..., n [17]. We can assume each replicate of the data that is obtained from a single MEMS device as one instance of  $\boldsymbol{d}$ , which corresponds to a discrete sample of one instance of the random process. We thus pose

the task of estimating the stochastic model as an inverse problem, where we try to determine the unknown parameters that accurately fit a given set of measurements.

The formulation described above is suitable for modeling stationary covariance functions, where the covariance function between any two points depends solely on the distance between them such that the nature of roughness is similar at every point in the domain. However, this assumption may not be valid in a realistic scenario where the unknown underlying random process from which the data has been generated may not be stationary. This has been shown to be especially true when dealing with roughness and random topography [26]. The covariance function parametrization can be generalized by including a virtual displacement field, u(X), as an extra parameter. This displacement field transforms the position of a point, X, to a new position, x, given by x = X + u(X). We choose this mapping in such a way that C(x, x') is a stationary covariance function, which can be parametrized using the formulation given in Equation (3). This method of introducing nonstationarity in the model by transforming the co-ordinate system was proposed by Sampson and Guttorp [27] and subsequent research work has examined issues related to the uniqueness and identifiability of the nonstationary covariance function [28, 29]. Using this representation, we develop a nonstationary covariance formulation for stochastic processes as follows,

$$f|M, C \sim GP(M, C),$$

$$M : X, \boldsymbol{\alpha}, \boldsymbol{t}_{\boldsymbol{M}} \mapsto \sum_{i} \alpha_{i} B_{i,3}(X; \boldsymbol{t}_{\boldsymbol{M}}),$$

$$C : x, x', \nu, \phi, \theta \mapsto Mat\acute{ern}(x, x', \nu, \phi, \theta),$$

$$x : X, u \mapsto X + u(X)$$

$$u : X, \boldsymbol{\beta}, \boldsymbol{t}_{\boldsymbol{u}} \mapsto \sum_{i} \beta_{i} B_{i,3}(X; \boldsymbol{t}_{\boldsymbol{u}}),$$

$$\boldsymbol{d}|M, C \sim \mathcal{N}\left(M(\boldsymbol{X}), C(x(\boldsymbol{X}), x(\boldsymbol{X}))\right),$$
(5)

where  $t_M$  and  $t_u$  are the knot vectors for the mean function and displacement function respectively, that are chosen to lie in the domain of the stochastic process, while  $\alpha$  and  $\beta$  are the corresponding weight vectors that are unknown and are estimated from the data along with the other hyperparameters. It should be noted that although the B-spline representation developed in Equation (2) is for 1-D functions, it can easily be generalized to the multiple dimensions by taking tensor products of the basis functions along each individual dimensions. We shall use these multivariate B-splines when estimating 2-D stochastic processes to represent random surfaces.

## 3 Characterization of spatial variations using profilometric data

In order to estimate stochastic models to describe spatial uncertainties, we need to have multiple replicates of data, where each replicate is obtained by measuring the height of one instance of the random surface at several pre-determined points. This procedure is described in Figure 1, where a profilometer is used to scan the surface in order to measure the variation in height. In the case of MEMS, this kind of measurement is limited to those surfaces that are accessible to the profilometer probe; typically, those that lie in the plane of the substrate wafer. It must be noted that since this measurement of asperity height variation is independent of the nature of uncertainty, it can be applied to a variety of surfaces that are generated as a result of different etching/deposition techniques.

To illustrate this procedure, we model the random surfaces generated during deep reactive ion etching (DRIE), specifically along the floor of etched trenches. DRIE consists of short alternating steps, where an ion-assisted isotropic etch step by a chemical species is followed by a passivation step in which a polymer is deposited conformally in order to protect the side walls of the trench during subsequent etching steps [30]. The combination of passivation followed by etching allows for the creation of channels with high aspect ratios. A popular choice of the gas used for etching silicon is SF<sub>6</sub>, while the polymer-forming gas used for passivation is typically  $C_4F_8$ . DRIE has been widely accepted as the method of choice for etching, since it is capable of achieving higher etch rates and bigger aspect ratios, while maintaining a relatively uniform etch profile.

One of the side effects of using DRIE is the generation of spatial asperities on the floor of the etched trench which, in extreme cases, manifests as vertical filaments of silicon that are popularly referred to as "grass". Dixit and Miao [31] showed that the generation of grass is related to the flow rate of  $SF_6$  as well as the ratio of etching to passivation cycle times. They argue that the grass

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formation is caused by localized concentration of flouride ions at the bottom of the trench, which causes the resulting surface after etching to become uneven. For devices manufactured using DRIE, this roughness becomes a source of device-level spatially-varying uncertainty, affecting critical device parameters either directly or as a result of subsequent manufacturing steps.

The first step in estimating the stochastic model is to gather data characterizing the uncertainty. As explained in Section 2, in order to estimate the mean and covariance function for second order random processes, we measure the surface height at fixed locations across multiple replicates of the rough surface. For shallow trenches etched using DRIE, we can use a profilometer to measure the variation in surface height along the floor of the trench and use this data to estimate an appropriate stochastic model. We use experimental data obtained from 600  $\mu m$  wide trenches etched into silicon wafers, by scanning the trench width with a profilometer probe. Figure 2 shows the variation in surface profile over a 100  $\mu m$  section for 10 such datasets. The plots have been staggered by 5  $\mu$ m vertically for visual clarity. We see that except for a few outliers, the magnitude of roughness is fairly uniform over the entire section, indicating that a stationary stochastic model may be sufficient to capture the variation.



Figure 2: Profilometric data showing variation of trench floor after DRIE.

The characterization data obtained using profilometry is then plugged into the estimation

framework outlined in Section 2. We first estimate the stochastic process using the full nonstationary covariance model and then set the displacement function to zero to mimic a stationary formulation. We compute the Bayes factor that compares the similarity between the two models. We obtain a value of 2.684, which indicates that there is no significant difference between the two [32]. This confirms our hypothesis that the data can be modeled well using a stationary covariance formulation. Figure 3 shows a few realizations sampled from the stochastic model estimated using a stationary covariance model, while Figure 4 approximates the posterior PDFs of the covariance function hyperparameters by computing histograms of the trace values generated by the MCMC sampler. The plots in Figure 3 have been staggered in the vertical direction by 5  $\mu$ m for visual clarity.



Figure 3: Realizations sampled from the estimated stochastic model.

In order to demonstrate the significance of this surface roughness, we apply the estimated stochastic model to a MEM device and examine the resulting variation in device performance. We choose a micromirror, whose schematic is shown in Figure 5. The micromirror is modeled as a flat plate with electrodes, that is suspended over a grounded plate by means of a torsional hinge. The device is actuated using electrostatic force, when a potential difference is applied between one of the electrodes and the ground plate (either  $V_1$  or  $V_2$ ). When a beam of light is incident on



Figure 4: Histograms of the covariance function hyperparameters.

the top surface of the micromirror, which is reflective, the rotation in the mirror can be used to steer the reflected beam in different directions. This kind of a device finds application in a variety of optical components including digital displays, where a displayed pixel can be turned on or off depending on the position of the mirror. It is important to tightly control the amount of rotation for a given voltage in order to reproduce the on and off states of the mirror with good fidelity. Moreover, since the dynamic characteristics of the movable electrode determine the transition time between the two states, it is important to understand the performance of the device with respect to these metrics in order to ensure long-term reliability.

We assume a simplified manufacturing workflow where a shallow trench is first etched into a silicon substrate wafer using DRIE to define the gap between the electrodes. We then planarize the top silicon layer of a silicon-on-insulator (SOI) wafer so that the silicon thickness is brought down to 3  $\mu m$  and define the conductor electrodes. This wafer is then flipped and anodically bonded with the substrate wafer so that the thin silicon layer on the SOI wafer fuses with the substrate wafer. The backing and insulating parts of the SOI wafer are then etched away revealing the 3  $\mu m$  silicon layer, which is then coated with a reflective layer, patterned and etched through to release the movable electrode. As in any electrostatically actuated system, the performance of the device is very sensitive to the gap between the electrodes. The dimensions of the gap, in turn, are controlled by the precision in the initial DRIE step. Consequently, we expect that any roughness on the trench floor that is generated during the DRIE step will result in a spatially-varying gap, which will change the performance characteristics of the device in terms of its static



Figure 5: Schematic of the micromirror with a torsional hinge showing the device with nominal dimensions at rest and in an actuated configuration.

as well as dynamic behavior.

In order to model the effect of spatial uncertainties on this device, we assume that the ground plate roughness can be represented as a stochastic process, which can be estimated using the procedure given above. The data for the stochastic model can be obtained by using a profilometer to map out the spatial variations immediately after the trench is etched into the substrate wafer. Using the trench floor profilometric data presented in Figure 2, we estimate a stochastic model for the spatial variation and use it to quantify the variation in device performance. The dimensions of the micromirror device are as shown in Figure 5 and the physical model for the device has been described in [33]. We use the electromechanical solver framework developed in [33] and model the hinge as a torsional spring with a stiffness of  $4.49 \times 10^{-7}$ N m rad<sup>-1</sup>. The ground plate profile is modulated by the spatial variation estimated from the stochastic model and we compute the variation in quantities of interest, like actuator displacement and damping ratio. Since the stochastic models obtained using the nonstationary and stationary covariance formulations are almost the same, we report results only from the latter method. By propagating the stochastic model, we obtain PDFs corresponding to the variation in various parameters of interest.

We first apply a static potential difference between one of the electrodes on the mirror and

the ground plate. This displacement causes the mirror to rotate until the displacement attains the steady-state equilibrium value. Due to spatial variation in the gap, we observe a spread in the steady-state displacement. This spread increases as the steady-state voltage in raised, due to the nonlinear nature of the actuator. Figure 6 shows the variation in the vertical position of the mirror edge as a function of the voltage applied. The red and green dotted lines correspond to the lower and upper bounds for the 95% confidence interval corresponding to the stochastic variation. The cyan dash-dotted line is the median displacement. For comparison, we also computed the mirror position in the deterministic case, where spatial variations are ignored. We see that there is a difference between the median value in the stochastic case and the deterministic value, especially at larger voltages. The realizations drawn from the estimated stochastic model, shown in Figure 3, show that the variation in the gap is roughly equal along both positive and negative directions, meaning that the mean trend is approximately zero. However, since the electrostatic force increases nonlinearly as the gap decreases, the variation in the displacement is amplified as the mirror edge gets closer to the ground plate. This causes the median edge position to be different from the nominal deterministic case, showing that a proper stochastic analysis is needed even in order to predict the average trend. In addition to the estimated stochastic process, we also randomly choose 6 replicates from the measured characterization data and propagate the raw variation through the numerical model. The corresponding results for 20, 25 and 30V are shown as black dots in Figure 6. We see that the spread in the dots corresponds well with the confidence interval predicted using stochastic analysis, which serves as an additional check for the whole exercise. We also plot the PDFs of the mirror edge position corresponding to actuation voltages of 20, 25 and 30V, as shown in Figure 7. Here we can clearly see the nonlinear behavior of the actuator that causes the spread in the displacement to increase, as the voltage is raised.

Using the stochastic model, we also predict the variation in the pull-in voltage of the micromirror device. The pull-in voltage defines the limit of operation for the actuator and in some situations, the pull-in instability is directly used to switch the mirror between two different states. Hence, it is an important metric that governs actuator performance. Figure 8 shows the PDF of pull-in voltage for the micromirror along with the results corresponding to six randomly chosen replicates from the measured data. We see that the pull-in voltage varies by over 10V, showing



Figure 6: Variation of vertical position of mirror edge with voltage. The black dots correspond to results obtained using 6 randomly chosen replicates from the measured data.



Figure 7: PDFs of vertical position of mirror edge for actuation voltages of 20, 25 and 30V.

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that the effect of spatial uncertainties cannot be ignored in such a device. We also examine the effect of spatial uncertainties on the dynamic behavior of the actuator by computing the damping ratio. The PDF of the damping ratio is shown in Figure 9 and we see a 20% variation on either side of its median value. Again, we see the importance of incorporating spatial uncertainties during uncertainty quantification in order to make accurate predictions of the variation in parameters.



Figure 8: Variation in pull-in voltage of the micromirror due to spatial uncertainties. The black dots correspond to results obtained using 6 randomly chosen replicates from the measured data.

## 4 Extraction of data using image segmentation

Generation of data using profilometry is a particularly fast and easy way of obtaining characterization data to estimate spatial uncertainties. However, profilometry is limited to measuring surface roughness along the surface of the wafer and cannot be used to measure variations in orthogonal planes that go into the wafer substrate e.g. spatial variation in the side-wall profiles produced during the etching of channels. Another disadvantage of profilometry is that it is primarily suited to measuring the physical height of surface asperities and cannot be directly used to measure variation in other physical properties like electrical conductivity. In this context, image-based



Figure 9: Variation in damping ratio of the micromirror due to spatial uncertainties. The black dots correspond to results obtained using 6 randomly chosen replicates from the measured data.

techniques provide alternate tools to extract spatially varying data that can be used in stochastic model estimation framework in a manner similar to that for profilometric data. The idea is to gather multiples images corresponding to the spatial variation in different replicates of a device and to then digitize these images using a combination of various image processing techniques in order to obtain a coherent dataset that quantifies the spatial variation at certain fixed spatial locations. Since we are dealing with images, this method can be applied to other situations as well that do not involve surface roughness e.g. in quantifying the spatial variation in the boundaries of infected regions in biological tissue samples that have been stained using a suitable method.

In this work, we consider the variation in side-wall profiles of channels etched using DRIE. As explained in Section 3, the Bosch process used for DRIE consists of a series of alternating etching and passivation steps to achieve large aspect ratios. However, a curious side-effect of this process is that the side walls developed a characteristic wavy pattern known as "scalloping". This scalloping is a result of the anisotropic nature of the  $SF_6$  etch step being periodically interrupted by the passivation polymer [34]. The magnitude and extent of scalloping depends on the width and aspect ratio of the etched channel. In general, it is observed to be most prominent near

the top of the channel and gradually disappears as the channel depth increases [34, 35]. The surface roughness produced by scalloping has been extensively studied in the context of optical MEMS, where the smoothness and optical quality of the sidewalls governs the performance of the device [35, 36, 37].

In order to generate a stochastic model to describe the variation in sidewall profiles of DRIE channels, we use cross-sectional images of the channels obtained using scanning electron microscopy (SEM). Figure 10a shows one such example of the sidewall profile variation in a cross-sectional image of a channel in a silicon wafer. We clearly see the presence of scalloping in the top portion of the channel. In order to quantify the variation of the sidewall profile, we first perform image segmentation to identify the boundary between the channel interior and the silicon substrate. There are several sophisticated techniques to perform image segmentation and they mostly involve using local changes in contrast to identifying the boundary between adjacent segments. We employ a simpler method which involves applying a Sobel filter [38] to the image. The Sobel filter is a discrete differentiation operator which can be used to extract gradients along either the row or column direction for a 2D image array. Since the channel walls are fairly vertical, we use the filter along the direction perpendicular to the channel walls in order to identify the points where the gradient is maximum. Mathematically, this can be seen as the convolution of a  $3 \times 3$  matrix with the image array is as follows,

$$\boldsymbol{G}_{x} = \begin{bmatrix} -1 & 0 & +1 \\ -2 & 0 & +2 \\ -1 & 0 & +1 \end{bmatrix} * \boldsymbol{A}$$
(6)

where A is a 2-D array corresponding to the original image and  $G_x$  is the result of applying the Sobel operator. The 2-D convolution operation is denoted using the \* symbol. The array,  $G_x$ , can be thought of as the discrete directional derivative along the x-direction. By scanning each row in  $G_x$ , we can identify the points where the gradient is maximum or minimum. These correspond to location of the right and left walls, respectively. We can thus obtain the pixel locations of the points that form the sidewall boundary. The segmented image that we obtain after applying the above edge extraction algorithm is shown in Figure 10b. We thus obtain the pixel locations for two sidewall profiles for every available image replicate.



(a) SEM image of channel etched using DRIE

Figure 10: Image processing of SEM micrograph showing (a) the cross-sectional view of a channel etched using DRIE and (b) the binary image obtained after segmentation.

After image segmentation, we compute the pixel-length of the calibration scale included at the bottom of Figure 10a. This allows us to convert the pixel locations of the sidewalls into real-world coordinates. Since the left and right wall variations are approximately mirror images of each other, we flip the data from the right sidewalls so that it aligns with the data from the left side. The coordinates are then rotated by  $90^{\circ}$  so that the edge data from the vertical sidewalls is aligned horizontally. This is followed by a normalization step, where we fit a linear regression to each sidewall dataset and subtract this value from the entire dataset. This centers all the datasets and removes any rotations introduced during image capture. This entire sequence is repeated for each

<sup>(</sup>b) Image after segmentation

available image. In this work, we use SEM images of channels etched at 5 locations on a silicon wafer namely, along the four cardinal directions and at the center of the wafer. The resulting set of ten replicates is shown in Figure 11a, where the individual datasets have been staggered by 2  $\mu m$  in the vertical direction for visual clarity. We notice that in addition to the scalloping, there are large artifacts at certain locations. If we compare these artifacts with the original images, we see that they correspond to foreign material occluding the sidewall in the SEM image. This is seen near the top of the channel on both sides in Figure 10a. This foreign material could either be stray substrate material that is thrown up during the dicing step that is performed prior to imaging or it could be a result of the substrate material being cut in a haphazard matter during dicing. In either case, the presence of these artifacts confounds the image extraction process, resulting in abnormal variations being seen in the final digitized data.

Since these variations are not characteristic of DRIE, it is best to ignore them when generating the stochastic model. This is done by marking the data at these locations as invalid before passing the data to the stochastic model estimator. Unfortunately this has to be done manually, since the image extraction algorithm has no way of automatically knowing whether an artifact is naturally present or generated during dicing. The data after clean-up of imaging artifacts is shown in Figure 11b. As long as we have a sufficient number of datasets, we can handle missing data by estimating the stochastic variation using data from other datasets at the same location. This is formally handled during the stochastic model estimation step, where we extend the Bayesian formulation to include additional hyperparameters corresponding to the missing data values. We assign uninformative priors to these parameters and use Monte Carlo sampling to estimate their posterior PDFs. This is automatically taken care of by the PyMC [39] software package, which is used to set up the Bayesian network and to perform MCMC sampling.

We employ the formulation developed in Section 2 to estimate the stochastic model corresponding to the sidewall profile data. From Figure 11b, we see that the effect of scalloping is mostly present for about the first 60  $\mu m$  into the channel and is significantly diminished after that. This suggests that the corresponding stochastic model is likely to have a nonstationary covariance function in order to handle the variation in the roughness profile. We plot the estimated mean function and the virtual displacement function in Figure 12a and Figure 12b respectively.



(a) Raw data obtained after image processing



(b) Data after removal of imaging artifacts

Figure 11: Digitized data extracted from SEM images of DRIE channels (a) before and (b) after clean-up of imaging artifacts. The datasets have been staggered vertically for visual clarity.

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We see that the estimated mean function is more or less zero, indicating that there is no average trend in the data. This is expected because the normalization step during data extraction removes any linear trend in the data. We also see fluctuations in the mean profile that have roughly the same period as that seen in the input characterization data, which might be related to the natural scalloping pattern seen in DRIE. However, the magnitude of the fluctuations is lower than that seen in the input data. This is because the scalloping pattern in different datasets is not necessarily aligned and the phase differences that exist between them causes the mean function to average out to a very small value. It may be possible to capture this variation more accurately by aligning the peaks in the datasets, but we have not attempted to do this because of the complication of missing data and because of the scalloping periods not being exactly equal across all datasets. The virtual displacement function shown in Figure 12b clearly captures the extent of nonstationarity in the covariance function. From Section 2, we know that the displacement function transforms the coordinate system by applying a compressive or a tensile strain field at different points in the domain. In regions where the gradient is close to zero, there is no relative movement between adjacent points and the resulting covariance function is locally stationary. From the Figure, we expect the estimated covariance function to have a high degree of nonstationarity until about 60  $\mu m$ , after which it becomes more or less stationary. This corroborates well with the data shown in Figure 11, where we see that most of the nonstationary variation due to scalloping is contained within the first 60  $\mu m$  or so, after which the variation is uniform.

Setting the displacement function to zero results in a stationary covariance formulation. However, unlike the example presented in Section 3, here we expect to see a significant difference between the stochastic models estimated using stationary and nonstationary covariance functions. Comparing the likelihoods of the two models, we get a Bayes factor of 9.73, which indicates a significant difference between the two. This shows that the results predicted by the nonstationary and stationary covariance formulations will also show a fair amount of discrepancy. Hence, we perform uncertainty propagation with the two models separately and compare the results obtained from the two.

We apply the estimated stochastic models to electrostatic microactuators, specifically to the MEMS piggyback actuator example mentioned in [33]. This application is particularly interest-



(b) Virtual displacement function and its gradient

Figure 12: Plots of (a) the mean function and (b) the virtual displacement function as well as its gradient, corresponding to the stochastic model estimated from DRIE cross-sectional SEM data.

 ing because it employs a comb-drive mechanism for actuation. Comb-drive actuators consist of interleaving fingers shaped liked a comb. One set of fingers is movable while the other set is fixed. A potential difference applied between the two sets of fingers generates an electrostatic force that causes them to attract one another. The comb-drive structure is typically fabricated using DRIE in order to leverage the high aspect ratio etching technique to increase the surface area of interaction between the fingers and thereby increase the sensitivity. However, the disadvantage of using DRIE is that unless the process is well controlled, we expect to see asperities along the sidewalls, especially due to scalloping, which changes the inter-electrode gap and hence, the electrostatic force. This makes the comb-drive actuator an ideal application for testing the stochastic models estimated using DRIE sidewall profile data.

We take the comb-drive actuator example presented in [33], and consider a simplified version that comprises only one set of moving and fixed fingers. The behavior of the actuator as a whole can be calculated by simply multiplying the force generated by one set of fingers by the total number of fingers. We apply the spatial sidewall variation to the fixed ground plate and compute the variation in actuator displacement under a constant applied voltage, as well as the dynamic behavior in terms of the damping ratio. The results are presented in Figure 13 and Figure 14 respectively. We see that the range of variation predicted by the nonstationary covariance model is larger than that predicted using a stationary covariance.

## 5 Wafer-level stochastic processes

After developing methods for the estimation of stochastic models from spatial characterization data, we finally extend the framework to model wafer-level stochastic processes. Wafer-level uncertainties are very common in microfabrication process workflows, where controlling uniformity of a particular etching or deposition step across the entire wafer can be quite challenging. In terms of mathematical modeling, wafer-level uncertainties pose the additional challenge of handling 2-D stochastic processes whose domain covers the surface of a wafer. Finally, the biggest hurdle in the way of estimating 2-D stochastic processes is the lack of sufficient characterization data with the required spatial resolution in order to resolve the variations properly.

We first extend the stochastic process formulation to handle 2-D data. Since we express the



Figure 13: Variation in comb-drive actuator displacement due to spatial uncertainties estimated from DRIE sidewall scalloping data.



Figure 14: Variation in damping ratio of comb-drive actuator due to spatial uncertainties estimated from DRIE sidewall scalloping data.

covariance function in terms of the Matérn covariance function, which in turn is a function of the normed distance between two points, the extension of the covariance function to 2-D merely involves using the Euclidean norm in two dimensions. We need to modify the basis representation of the mean function and the virtual displacement function. Since we used cubic splines in the 1-D case, we can extend the framework to 2-D by using 2-D bicubic splines. This has exactly the same form as that used in Equation (5), except that the 2-D basis functions are obtained by taking the tensor product of corresponding 1-D basis functions.

We pick an example to demonstrate the application of stochastic analysis using 2-D wafer-level stochastic processes. We consider a MEMS pressure sensor that is manufactured using bulk micromachining techniques. The pressure sensor consists of a circular diaphragm that is suspended over an enclosed etched cavity. A glass wafer is bonded to the back-side of the pressure sensor wafer in order to enforce an air-tight seal around the cavity. The resulting device behaves as a pressure sensor, where variations in the external atmospheric pressure cause the diaphragm to flex. By measuring the strain in the diaphragm, we can estimate the corresponding fluctuation in atmospheric pressure using simple mechanical models for the diaphragm flexure. The most popular way of measuring strain is to use a piezoresistive contact strain gauge. A metal film deposited over the membrane and etched into an appropriate shape, has the property that perturbations in the membrane strain are translated into variations in the resistance of the metal element. This resistance change can be measured using a Wheatstone bridge network and calibrated to yield the corresponding change in pressure. Figure 15a shows the combined photolithography masks used to fabricate multiple pressure sensor devices on a single wafer, while Figure 15b shows the same thing for a single die.

We see the position of the metal piezoresistive element that is positioned directly over the circular membrane as well as the reference element with the same dimensions, that is outside the zone of deflection of the pressure sensor diaphragm. The primary source of variation in the piezoresistive element is the uncertainty in the thickness of the metal film. We note that although the metal film is deposited as a single layer over the entire wafer, the spatial uniformity in its thickness is rarely perfect. The variation in the thickness can be estimated by using a profilometer to calculate the step height of the conductor lines at different parts of the wafer,



(a) Top view of lithography mask for entire wafer

![](_page_27_Figure_4.jpeg)

(b) Top view of lithography mask for a single die

Figure 15: Combination of photolithographic masks used for fabrication of a pressure sensor, showing (a) the masks for the entire wafer and (b) the masks for a single die..

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after the conductor etch has been performed. Since the measurements are only taken at a small set of points (one per die), it is not possible to estimate any fine-scale roughness in the thin film. However, the resolution is adequate in order to generate a 2-D random surface corresponding to wafer-level variations in the thickness.

We choose the domain for the stochastic process by picking the smallest rectangle that covers the 21 points (corresponding to 21 dies) where the thickness measurements are available. The spatial coordinates are normalized with respect to the pitch distance from the center of a die to that of the adjacent one. This allows us to only deal with dimensionless data during estimation. The output from the estimation procedure is given in Figure 16, where contour plots of 9 randomly sampled realizations are shown in Figure 16a and a surface plot of a single representative realization is shown in Figure 16b. We also plot the estimated mean function in Figure 17. We see that the mean function is fairly uniform in the center, while there are fluctuations towards the periphery of the stochastic domain. This is likely due to the lack of information regarding the thickness near the periphery of the stochastic domain, since most of the sampled data is clustered in the center.

Using the estimated stochastic model, we compute the variation in the output current obtained from the sensor as a function of the applied pressure. This gives an idea of the sensitivity of the pressure sensor. The use of output current as a performance metric is also motivated by the fact that we can experimentally measure the same quantity for the fabricated sensors so that the results can be compared with the predicted values. The results obtained by propagating the estimated stochastic model through a numerical model of the device are given in Table 1, where they are compared with experimentally determined values. In each case, we present the variation as a mean value with the corresponding standard deviation as an error. The observed drift in the predicted mean value from the experimental one is likely due to inaccuracies in the physical model used to simulate the device behavior. However, the predicted standard deviation of the output current is seen to be consistently lower than that observed in the experimental case. This is probably due to the fact that we have only considered uncertainty in the metal film thickness, whereas the actual device may have other sources of uncertainty as well. Nevertheless, it serves as a conservative estimate of the minimum amount of variation that we expect to see in the real

![](_page_29_Figure_2.jpeg)

(a) Contour plots of thickness (in  $\mu {\rm m})$  for 9 realizations

![](_page_29_Figure_4.jpeg)

(b) Surface plot of a single realization

Figure 16: Realizations sampled from the estimated stochastic model for metal film thickness, shown as (a) contour plots for 9 different realizations and (b) a surface plot of a single realization

 47.5

46.5

46.0

45.5

45.0

44.5

44.0

43.5

43.0

 $\begin{array}{c} 43.0 \\ 1.0.2 \\ 0.0.5 \\ 2.0 \\ -2.0 \\ 0.0 \\ -1.0 \\ 0.0 \\ -1.0 \\ 0.0$ 

Mean film thickness

![](_page_30_Figure_2.jpeg)

1.5

device. Overall, we see a reasonable match between the predicted results and the experimental ones, both in terms of the mean and the standard deviation.

Table 1: Comparison of experimental results with predicted values obtained from a 2D stochastic process and a univariate PDF, for the variation of output current with applied pressure.

Pressure (Pa)	Output current (nA)		
	Experimental	Estimated - 2D process	Estimated - Univariate PDF
1	$13.3 \pm 1.5$	$13.8 \pm 1.1$	$20.8 \pm 3.0$
2	$31.7 \pm 2.8$	$32.3 \pm 1.9$	$41.2 \pm 5.5$
3	$50.2 \pm 4.7$	$51.5 \pm 3.3$	$65.4 \pm 10.2$
4	$65.6\pm10.5$	$67.4 \pm 6.9$	$81.7 \pm 20.2$
5	$82.1 \pm 18.1$	$86.2 \pm 11.8$	$104.9 \pm 34.6$
6	$98.2\pm22.8$	$105.5 \pm 16.6$	$123.6 \pm 50.4$
7	$113\pm31.6$	$123.7\pm21.3$	$150.8 \pm 65.9$

In order to highlight the importance of stochastic process modeling, we perform an alternate simulation where we estimate a univariate PDF using kernel density estimation. We assume that the data for the estimation comes from the entire set of measured thickness values. This amounts to ignoring any spatial correlation in the data and treating each data point as independent from and identically distributed as every other data point. We propagate the estimated PDF through the numerical model of the device and compute the variation in output current as before. The results are presented in the last column in Table 1. We now see that this estimated model is neither able to predict the mean nor the standard deviation with any degree of accuracy. While the predicted means are consistently higher than experimental values, the predicted standard deviation values are almost twice that of their experimental counterparts. These results indicate that the univariate PDF model over-estimates the uncertainty in the device and is not as accurate as the full stochastic process model, where spatial correlations are included. This shows the benefit of proper stochastic modeling in being able to predict the output uncertainty with a greater degree of accuracy.

## 6 Conclusions

This work describes a comprehensive framework for performing uncertainty quantification in micromechanical devices. The overall goal is to advance the role of numerical simulations in the design process by augmenting their predictive capabilities when dealing with uncertainties in material properties or geometrical parameters. This includes developing techniques to employ experimental data to accurately estimate stochastic variations and then to use the estimated models to generate reliable predictions about variation in device performance with the least possible computational effort. Reliability is of key concern because it is important that the predictions ultimately corroborate well with experimental observations.

In order to expand the scope of uncertainty quantification, we introduce stochastic processes to model spatially varying uncertainties. We develop a nonstationary formulation to handle heterogeneous random processes. The transformation function used to introduce nonstationarity, is specified as an additive displacement that transforms the co-ordinate space to a deformed configuration in which the covariance between points can be represented by a stationary model. The stochastic modeling framework is modified to use a spline basis in order to make the approach more non-parametric. Bayesian estimation involving the Markov Chain Monte Carlo (MCMC) method is used to estimate the parameters of the stochastic model.

We finally employ these computational techniques to perform uncertainty quantification in a

variety of micromechanical devices that are affected by spatial uncertainties. We generate data for stochastic modeling either through profilometric measurements or from digitized data extracted from cross-sectional images of the roughness. We focus on spatial uncertainties encountered in the microfabrication workflow, specifically those resulting from variations in processes like etching and deposition. After estimating the stochastic models, we apply them to real-world MEM devices to demonstrate how UQ may be carried out for a real device. Where experimental results are available, we are able to validate the predictions generated through UQ, thus meeting the original goal of generating reliable predictions.

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