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Statistical metrology: understanding spatial variation in semiconductor manufacturing

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ABSTRACT

Variation is playing an increasingly important role in microelectronics manufacturing; variation not only impacts yield but also limits performance and reliability. Statistical metrology is an emerging body of methods for the systematic characterization and study of variation in semiconductor manufacturing. This paper considers the key elements of statistical metrology and reviews current progress in these areas, including (1) measurement methods and data gathering, (2) variation modeling and data analysis, and (3) study of the impact of variation. Potential applications of the methodology are widespread, with significant existing work in equipment characterization, layout optimization, and circuit impact analysis. Statistical metrology is an exciting new area of research that will play a critical role in future design and manufacture practice.

Keywords: variation, statistical metrology, process characterization, intra-die variation, spatial modeling

1. INTRODUCTION - WHAT IS STATISTICAL METROLOGY?

The phrase “statistical metrology” carries with it more connotations than denotations: one has the sense that it has to do with measurements, but also deals with variation in some central way. The name itself, however, does not suffice to define what is meant. While there is still discussion about just what this newly emerging field of statistical metrology is [1, 2], a number of important elements can already by identified. It is the goal of this paper to consider the defining features of statistical metrology, to examine some of the tools and methods that have been developed to date, and to review current and potential application areas where statistical metrology will play an important role in the future. While many of the concepts may be applicable in other domains, we consider statistical metrology within the confines of microfabrication technologies.

We first propose the following definition: **statistical metrology is the body of methods for understanding variation in microfabricated structures, devices, and circuits**.

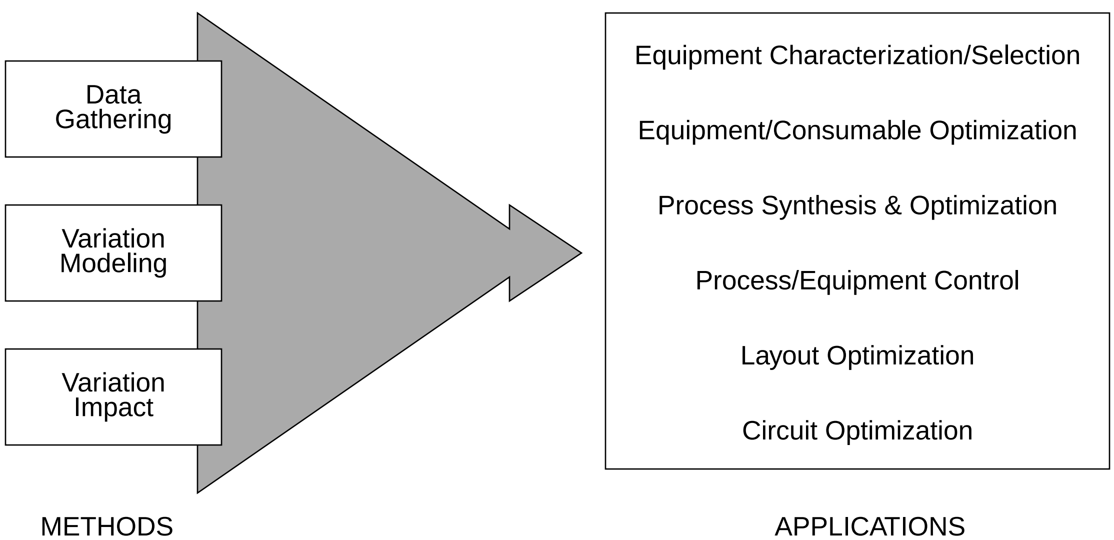

Figure 1. Statistical metrology methods and applications.

As summarized in Figure 1, statistical metrology methods fall broadly into three areas: (1) methods for gathering appropriate data to identify and assess variation, (2) methods for analysis and modeling of variation, and (3) methods to understand the impact of variation. These methods form the basis for application in a variety of areas, as summarized in Figure 1. In Section 2 we consider measurement types and variation concerns that progressively move from accurate estimation of single values, to representative values, random variation measurements, and finally identification of systematic variation and factors. In Section 3 the approaches and issues in modeling variation are discussed, particularly those dealing with spatial models. In Section 4 we examine the importance of connecting variation models to the experimental and theoretical consideration of the impact of that variation. Finally, in Section 5 we examine existing applications and future opportunities for the development and use of statistical metrology. Throughout this paper, examples will be drawn from current research into statistical metrology and its application to interlevel dielectric (ILD) thickness variation arising in chemical mechanical polishing (CMP) processes.

2. MEASUREMENT METHODS: DATA GATHERING

Statistical metrology is different than “metrology” in a fundamental way: it is about measuring, identifying, and modeling variation itself. Here we first consider some of the key characteristics of variation. We then examine measurement types, from “single” value representations of a parameter through more sophisticated and complete measures of variation.

2.1 Systematic vs. Random Variation

Variation in some physical or electrical parameter may manifest itself in several ways. One key characterization is systematic versus random constituents in the parameter distribution. An important goal is to isolate those systematic, repeatable, or deterministic contributions to the variation from a set of deeply confounded measurements. As illustrated in Figure 2, without detailed understanding of the individual contributions, the distribution is typically considered to be “random” and large. Typical approaches for managing such large distributions include “worst-case” design windows. Better understanding of the contributions, on the other hand, enables one to focus variation reduction efforts more appropriately, or to design the device or circuit to compensate for the expected variation.

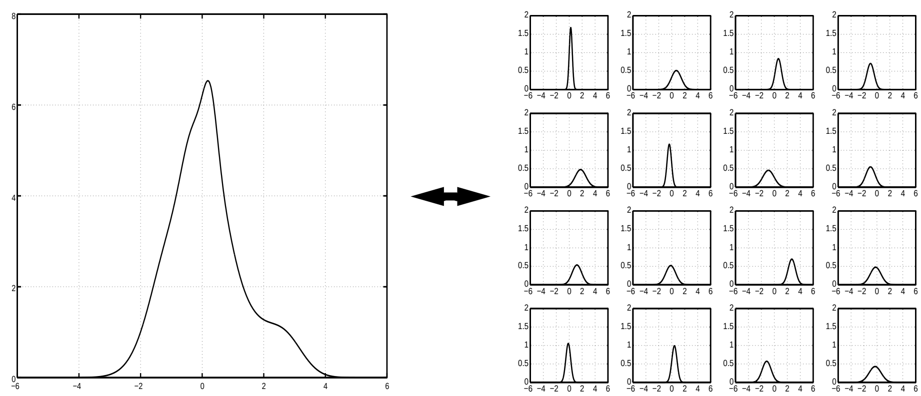

Figure 2. A large number of systematic or deterministic contributions (right) to a parameter will appear in aggregate as a single large “random” distribution (left). Statistical metrology seeks to deconvolve and identify both systematic and random elements.

2.2 Spatial vs. Temporal Variation

Variation manifests itself across time and across space. In each case, the variation appears at a number of different scales. Indeed, the separation of variation by unique signatures at different scales is a key lever used to pry apart and analyze such variation. In addition, an important requirement is the design of appropriate measurement strategies which can takes the scope of such variation into account.

Temporal and spatial variation at a number of different scales is shown in Figure 3. Process control has often been concerned with variation occurring from lot-to-lot. That is, some measure of a parameter for the lot may vary from one lot to the next as the equipment, incoming wafer batch, or consumable material drifts or undergoes disturbances. In a similar fashion, the temporal variation from one wafer to the next in single wafer processing equipment is also of concern. For example, in CMP the average oxide removal rate often suffers significant reduction or drift as the pad wears [3]. In typical practice, only simple measures for the parameter are used (e.g. a representative or mean value for some structure), but it may also be of interest in the future to track spatial variation patterns as they change in time from lot-to-lot or wafer-to-wafer.

In addition to temporal variation, different spatial variation occurs at different scales. In batch processes, for example, the spatial variation from one wafer to the next (e.g. along a polysilicon deposition tube) may be a concern. In equipment design and process optimization, spatial uniformity across the wafer is a typical goal and specification. For example, in most deposition or etch processes, uniformity on the order of 5% across the wafer can be achieved. That is to say, if one examines the value for some structural parameter taken at the same point on every die on the wafer, a fairly tight distribution can be achieved. At a smaller scale, on the other hand, additional variation issues may arise. In particular, the variation within individual die on the wafer is emerging as a major concern, in large part because of potential yield and circuit performance degradation. If nominally identical structures within the die are measured, one may indeed find variation with a much larger spread than across the wafer. An important observation is that knowing something about one scale of variation says little about the variation at the other scales. This is because different physical causes are at work at each scale; e.g. wafer level uniformity in plasma etch is driven by macroscopic tool design issues, while pattern-dependencies arise through details of the etch process conditions. At a still smaller scale, variation within individual structures or devices may also be a concern, particularly with respect to device reliability.

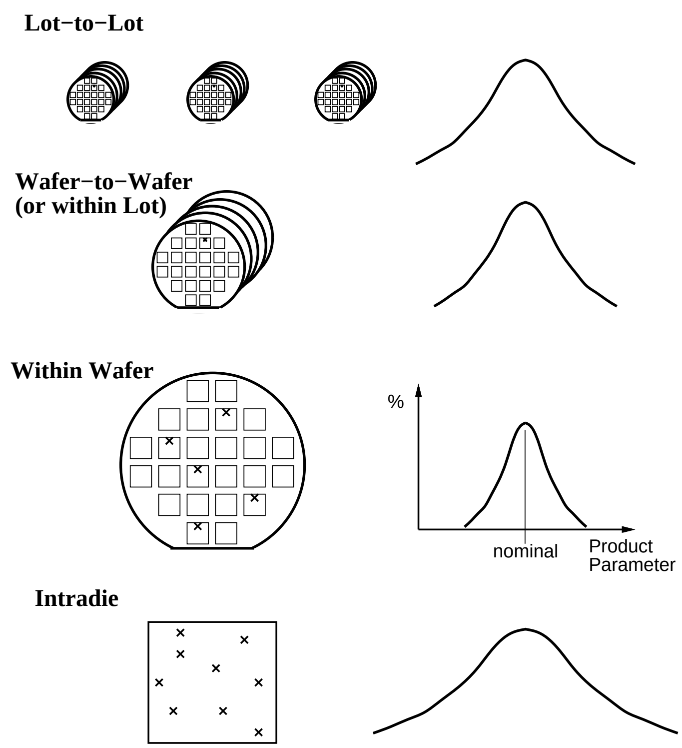

Figure 3. Spatial and temporal variation scales.

2.3 Measurement Types

Statistical metrology extends metrology or the measurement of parameters in an important way: we are concerned with understanding the variation in the structure, device or circuit, rather than studying the variation in the measurement itself. Reliable and repeatable measurements are increasingly difficult and statistical methods are crucial in the design of metrology tools and strategies, but for the most part such concerns are beyond the scope of statistical metrology. It is important, however, to consider the progression of measurement types and variation concerns that build up to statistical metrology.

2.3.1 Single value

Often a single value for some structural or device parameter is desired. An example is the accurate measurement of Leff for a specific transistor. Here measurement error or measurement variation is a key concern. Strategies include gage repeatability and reproducibility studies to understand limitations in the fundamental measurement. If a single value is of interest, then one can afford extensive characterization of the structure (e.g. TEM analysis).

2.3.2 Representative value

In many cases, an “average” or representative value for some parameter is desired. An example is the mean Leff over some ensemble of devices. Some of the important issues include what population to use and sample, and the number of measurements needed to obtain a good estimate. Approaches include robust estimators, e.g. the median, as well as application of basic statistical methods to bound or establish confidence on these estimates.

2.3.3 Variation measures

As one shifts from “nominal” design strategies toward manufacturability concerns, understanding something about the size of variation itself becomes important. In this case, not only is the mean (or median) a concern, but also other measures of the distribution of some parameter are needed (e.g. the standard deviation or moments for a known distribution type). At this level, variations are essentially treated as random, and the goal is simply to quantify these variations. Important tools at this level are primarily statistical: guidelines as to the number of samples required to reliably estimate the distribution can be applied.

2.3.4 Variation dependencies

At the next level, the power of statistical metrology approaches come into play. In this case, the goal is not only to quantify variation, but also to understand the fundamental dependencies in that variation. The goal is to identify the systematic components in the variation, and to develop functional relationships between other parameters and the variation. For example, one may be interested in understanding how oxide deposition varies over time, between wafers, as a function of position on the wafer, as a function of underlying pattern dependencies, etc.

In this case, a new set of methods and approaches are needed to guide data gathering and to feed the necessary analysis tools (discussed in Section 3). Specific tools include test structure design and experimental design and sampling strategies.

2.4 Measurement Approach and Test Structure Design

A key decision in gathering data for statistical metrology analysis is what physical measurement method to use. Several physical measurement approaches may be employed, providing different trade-offs with respect to ease, speed, and volume of data collection possible. For example, in advanced multilevel metallization schemes, the thickness of the dielectric layer between metal layers can be sensed or measured in several ways. The most detailed methods include SEM or cross-section TEM; such measurements provide information about variation within an individual structure, but are clearly limited in the number of samples that can be prepared. Optical thickness approaches can provide good throughput; depending on measurement tool and time available, hundreds to thousands of data points can be collected for a sample wafer, with good locational repeatability. Interferometric approaches do, however, impose a limit on the size of the lines or spaces that can be probed, requiring 10 - 20 μm dimensions for good repeatability. Surface profilometry also offers the opportunity for relatively efficient characterization of thicknesses at the die or wafer level, with various trade-offs in measurement sensitivity and measurement time. Finally, electrical measurements offer the opportunity for fast automatic probing to gather thousands of data points on the wafer, but require additional short-flow processing to build electrical test structures. Such test structures can also be designed to explore the submicron line widths and spacings present in advanced technologies.

For the measurement approach selected, designs for appropriate test structures that facilitate the collection of large volumes of data are an essential ingredient for statistical metrology. The critical issue here is to design the structure so as to block out or account for undesired variation factors, in order to accentuate or isolate the variation factors that are of interest. As an example, an electrical test structure for the measurement of interlevel dielectric (ILD) thickness is shown in Figure 4. Here a measured capacitance can be converted to infer the ILD thickness. For this structure, however, the capacitance is not only inversely proportional to ILD thickness (as desired), but is also strongly affected by any perturbations to the line widths of the underlying fingered capacitor plate. Thus, the test structure and measurement strategy must account for this variation source. In this example, local line width and sheet resistance measurements are also gathered for each probe structure, as shown in Figure 4. An integral element to the basic measurement approach, then, is the conversion of multiple direct measurements (capacitance, resistance) into the parameter of interest (ILD thickness). Additional device or interconnect simulation tools may need to be employed to accomplish this conversion, highlighting the strong coupling between statistical metrology and TCAD.

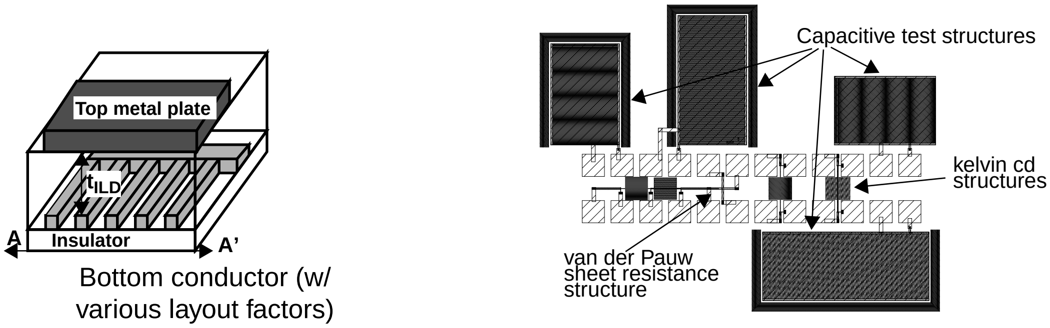

Figure 4. Electrical test structure for probing dielectric thickness (left). Corrections for variation in underlying line widths are computed from local Kelvin and van def Pauw structures.

2.5 Design of Experiments

In addition to new test structures, new design of experiments or DOE approaches are needed for statistical metrology. The traditional goal and purpose of DOE is to understand the influence of some number of factors on the parameter of concern. This is also a goal in statistical metrology, but in this case the goal is also to understand how *variation* depends on those same factors. In some sense, statistical metrology can be viewed as an extension of Taguchi experimental design and process optimization approaches [4]. In Taguchi methods, the goal is to find an operating point where the "signal" or desired output is strongest and the "noise" or variation is weakest. In statistical metrology, optimization is only one potential application; understanding and modeling of the variation is the underlying goal, and application may include robust design, variation reduction efforts, or compensation approaches.

Experimental designs in statistical metrology must therefore be customized to explore spatial or pattern-dependent factors that contribute to variation. The design must be carefully constructed to handle the multiple scales of variation. At the individual structure level, the design may systematically vary layout factors to explore their effect on the parameter of interest. In some cases, interaction between structures across larger spatial dimensions may occur (e.g. interaction across several mm in oxide planarization), so careful decoupling or accounting of such interaction must be undertaken. Finally, replication and organization of the structures within each die and repetition of the die across the wafer is important to identify die and wafer-level variation.

Methodologies to guide experimental design are just emerging in statistical metrology. Three phases or types of experimental designs can be identified (with some overlap between them). First, "screening experiments" are designed to explore a large space of possible layout or process factors that might affect the parameter of interest. Based on identification of important factors, the second type is an "environmental experiment" that more closely mimics the layout of particular product families (e.g. microprocessor, memory, ASIC) and which is designed to understand how the critical parameter depends on the factors in a realistic environment. Finally, more detailed "modeling experiments" may be employed. In this case, multiple levels of the important factors may be explored, with the goal being to build empirical or physical models that capture more fundamental dependencies in the parameter of interest. Examples of the first two experiment types, both of which use the electrical test structures from Figure 4, are shown in Figure 5. The first mask explores the influence of line width, line spacing, orientation, number of fingers, line length, and the presence or absence of a near-by structure on resulting local ILD thickness [5]. The second mask adds metal fill to the layout to more closely mimic the metal densities typical in ASIC circuits, and also systematically varies the separation distance between the test structure and this dummy fill to explore the effect of interaction between structures (or longer range density) on ILD thickness in CMP [6, 7, 8].

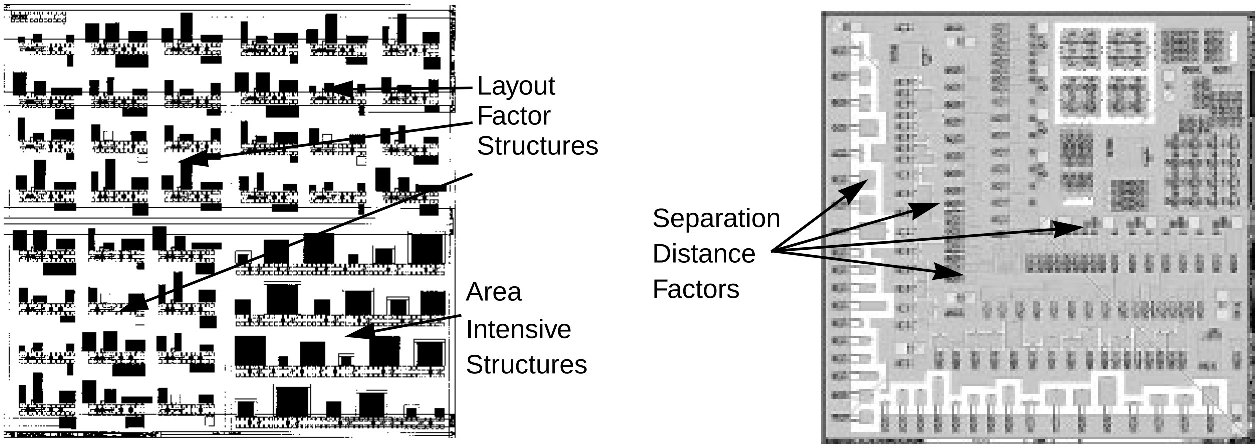

Figure 5. Example test chip experimental designs. A screening experiment (left) explores the influence of local layout factors on the ILD thickness of individual structures. An environmental experiment (right) more closely mimics an ASIC layout, and also explores the effect of separation distance between structures and nearby dummy fill.

3. MODELING VARIATION: DATA ANALYSIS

Time and space are generally “stand-ins” for more fundamental sources of variation. This is an important underlying principal used to gain understanding of variation through decomposition approaches. In lot-to-lot or wafer-to-wafer variation, for example, fundamental causes for equipment drift may be film buildup on chamber walls in plasma processes; both buildup and the resulting variation signatures are related through a similar dependence on time. Similarly, a key contribution to intra-die variation is pattern dependency; understanding positional dependencies and correlations between both die-level variation patterns and layout patterns gives a clue as to the key causal forces at work.

Statistical metrology analysis methods fall broadly in two categories. First are variation decomposition methods which seek to separate out the different variation scales in the data. Again, the key principle is that different physical causes are at work at these different scales (e.g. wafer-level versus die-level). Decomposition thus enables one to focus on the variation of most interest and filter out other issues. The second category of analytic methods are those which seek to develop more detailed dependency models, particularly in terms of more fundamental parameters rather than the “stand-in” spatial or temporal factors. For example, models relating specific layout practices to the resulting parameter variations are desired. Progress toward development of methods in each of these areas are next briefly reviewed.

3.1 Variation Decomposition

Figure 6 shows a flow diagram for a general spatial variation decomposition algorithm [9]. A hierarchical model is assumed in which the residuals (the output of the previous estimator minus its input) from one estimator becomes the input to the next estimator. There are three main estimators depicted in Figure 6: the wafer-level estimator, the die-level estimator, and the wafer-die interaction term estimator. The final box in Figure 6 represents the residual terms, or that portion of the variation that is left over and assumed to be purely random in nature.

This variation decomposition algorithm can be expressed in the framework of an additive model [10, 11] in which the total variation is represented as the sum of individual variation terms:

$$\begin{aligned} f_{RAW} &= f_{WLV}(x, y) + f_{DLV}(x, y) + f_{WLV \otimes DLV}(x, y) + \varepsilon \\ &\quad where \qquad \varepsilon \sim N(0, \sigma^2) \end{aligned} \quad . \tag{1}$$

In (1), x and y are spatial coordinates on the wafer while f_{WLV} is the wafer-level variation, f_{DLV} is the die-level variation, $f_{WLV \otimes DLV}$ represents the wafer-die interaction terms, and ε corresponds to the residual terms. Thus, the variation decomposition is able to (1) identify systematic spatial components in the variation, and (2) quantify these variation components.

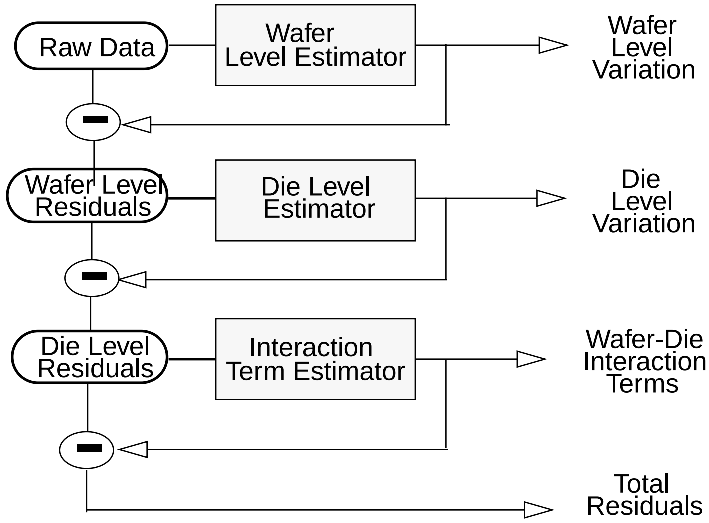

Figure 6. Variation Decomposition Flow Diagram

Wafer level estimators: A number of methods are under development for each of the estimators in Figure 6 [9]. Wafer level estimation approaches include moving average filters, spline-based approaches, and regression to assumed parametric forms. These approaches take advantage of assumptions on the shape of such variation: gradual trends are typical, or known functional forms are used (e.g. radial dependencies, sloped planes, or combinations of these).

Die-level estimators: When die-level spatial dependencies are examined, the key assumption is that the intended pattern imposes repetition among the many die on any one wafer. The decomposition methods exploit this repetition. Spatial repetition imposed by the stepping of the die across the wafer suggests the use of frequency-based analysis methods. A 2D spatial Fourier transform approach [12], for example, results in isolation of those components corresponding to the fundamental die frequency and its harmonics, as pictured in Figure 7. Alternatives based on modified multivariate ANOVA approaches for decomposition and modeling of die-level variation components are also under development [13]. These methods are helpful in overcoming limitations of the frequency-based approach, including die-sampling requirements and lack of model confidence information.

Wafer-Die Interaction: An important interaction may occur between the “pure” die level variation pattern and wafer-level dependencies. For example, the die-level pattern may be attenuated or accentuated depending on the location of the die on the wafer. At the wafer scale, the center of the wafer is often better controlled and more uniform, while the edges of the wafer experience significant “bull’s eye” or other nonuniformities. As a result, the die-level pattern dependencies may be significantly worse near the edge of the wafer. If one is concerned about the total range of variation, then, a multiplicative or other interactive factor between the die-pattern and wafer location may be a very large concern. More work is needed to understand the relationships between the interaction and the constituent die and wafer components. Spatial modeling approaches include methods which examine the residuals in Figure 6 for remaining quasi-periodic energy [9], or that use modified ANOVA models that mix factor and spatial location effects [13]. In the case of poly critical dimension, a multiplicative model has been proposed by Yu et al. [14] to account for wafer-die interaction.

Decomposition Summary: Decomposition approaches as outlined above can be very effective in separating systematic from random components of variation. Figure 8 illustrates the wafer, die, and wafer-die variation components for ILD thickness variation within a sample die; we see that die-level variation is much more significant than wafer-scale variation at the scale of any one particular die. Figure 8 also shows the distribution in (normalized) ILD thicknesses before and after decomposition. It is important to note that the wafer, die, and wafer-die distributions are not random; the complicated shape of these distributions are a function of the variation itself as well as the test structure and experimental design factors used to study them. On the other hand, the residual component contains both truly random variation or other variation factors not comprehended in the analysis.

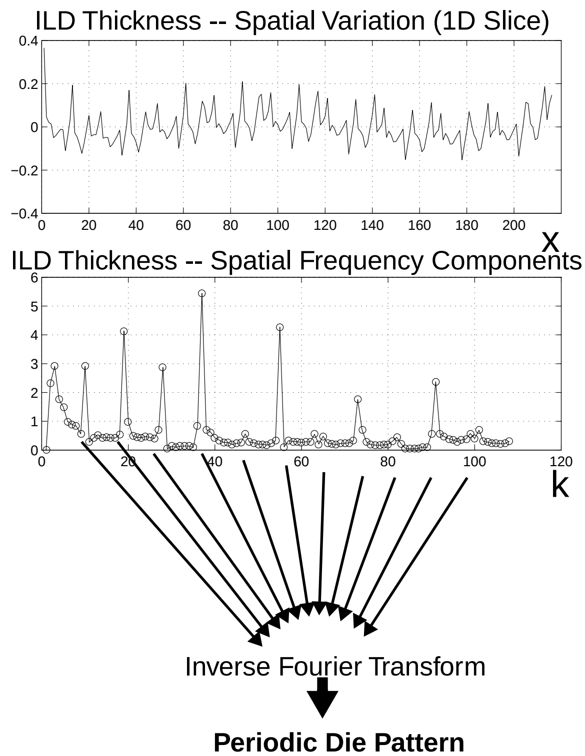

Figure 7. Spatial frequency-based estimator for extraction of perfectly periodic die pattern.

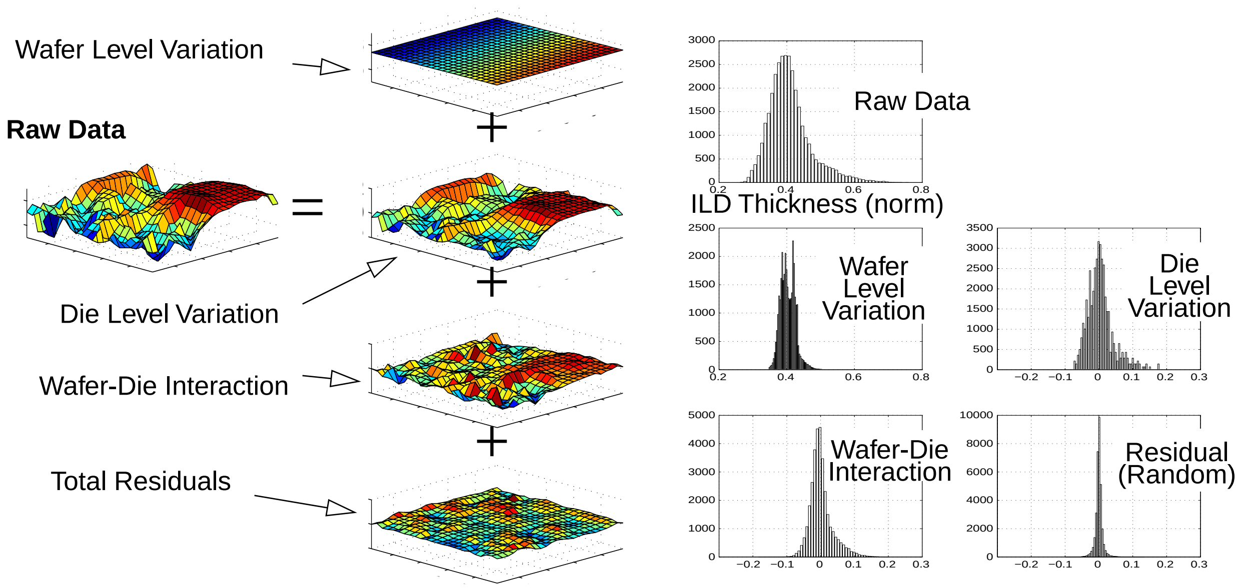

Figure 8. Components of ILD thickness variation for a single raw die (left) for the left test chip of Figure 5.. Resulting distributions after variation decomposition (right). The wafer, die, and wafer-die histograms correspond to systematic components in the raw data, while the remaining narrow residual component is random.

3.2 Variation Modeling

The methods described above emphasize the decomposition of variation into different components. While such decomposition alone is very useful in directing reduction efforts, comparing equipment, and gaining insight, it is also desirable to build explicit models that capture the functional dependency between the parameter of interest and the contributing factors. Methods for such modeling are just beginning to emerge in statistical metrology. One approach is to examine the extracted die-level variation for factor dependencies. A simple analysis of variance (ANOVA) approach can be used to compare the influence of individual factors, explore interactions between those factors, and construct models [5]. Manipulation of the underlying factors may be appropriate to construct good models. For example, the line width and line spacing factors in ILD thickness variation studies may be more efficiently modeled in terms of local or global layout density parameters, as pictured in Figure 9. Empirical models such as these can feed both flexible design rule generation, or can be integrated into quasi-empirical simulation tools (e.g.[15]).

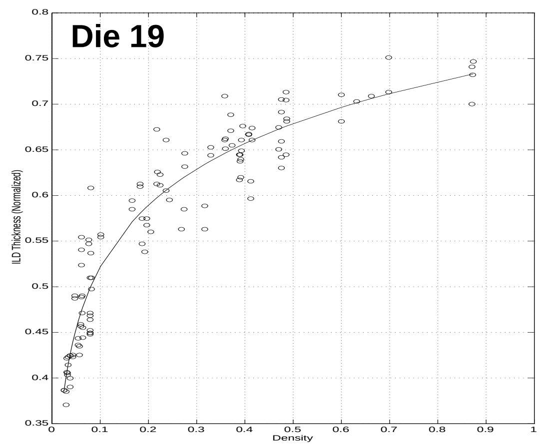

Figure 9. Model of ILD thickness as a function of layout density, constructed by analysis of data from the (right) test die in Figure 5.

The more general use of multivariate ANOVA approaches must be undertaken with care. One cannot assume that each die is a true replicate; rather, experiments with many die on the same wafer show some features of split-plot or repeated measure designs [16]. Recent work into a modified ANOVA approach which captures both the systematic (repeatable or shared) die-level variation and the die-wafer interaction terms shows great promise [13]. In this approach, ANOVA models are constructed for each die of interest, and then the ANOVA coefficients are compared and analyzed for their spatial dependencies. An important result of such work is that the range of validity of the models can also be more easily expressed, which is important for their application in variation impact studies.

More research is needed in mixed factor modeling methods for statistical metrology. Important issues are models that also capture spatial distribution or parameter dependencies on other factors, including time, process parameters, or other exogenous variables.

4. VARIATION IMPACT

A third key element of statistical metrology is the understanding of the impact that variation has on device and circuit performance, manufacturability, and reliability. Of the most immediate concern is yield impact: connection of variation models to technology CAD and physical modeling tools could be extremely useful to study the propagation of variation through multiple process steps, and understanding the yield cost of different levels of wafer, die, or other variation. In addition to yield, however, performance may be impacted as well. For example, ILD thickness variation over different topographies may induce capacitive skew differences between different signal paths and upset timing assumptions. Finally, interactions with device and circuit reliability may also be important. For example, understanding the factors which influence line width variation and line width distributions may be important for accurate modeling of chip-level electromigration reliability.

Variation impact on performance can also be examined using statistical metrology experimental design and analysis methods. In particular, spatial correlations between measured structure variation and full flow circuit test chip performance can pinpoint important factors and quantify their influence. Examples include evaluation of end-of-line electrical parameters such as Id(sat) as a function of polysilicon critical dimension variation [13], or ring oscillator frequency as a function of poly CD [17]. The analysis of variation impact on devices or circuits [18, 19] through both simulation and experimental means is an exciting current activity in statistical metrology research.

5. STATISTICAL METROLOGY APPLICATIONS

Statistical metrology is providing new tools and methods to guide the design of valid experimental designs and collection of data, to support the decomposition and modeling of the variation (spatial variation in particular), and to study the impact of that variation on manufacturability, performance, and reliability. We close the paper with a brief summary of some of the key application areas for statistical metrology.

One early application of statistical metrology is "fingerprinting" or characterization and comparison of different equipment sets. For example, the impact of different steppers on die-level line widths has been examined [14], and comparisons between typical wafer and die-level patterns in oxide polish using differenct CMP tools have been reported [20]. Such studies are immediately useful in equipment selection decisions, but can also be used to guide equipment or consumable optimization. Indeed, in CMP there is a strong demand for a "standard" means of characterizing spatial and pattern dependent performance of difference slurry or pad designs [21]; statistical metrology can supply experimental design and analysis methods for such standards. While this paper has focused on statistical metrology as applied to parametric variation, the spatial analysis of defect-related data to characterize or improve equipment and processes is also an important application [22].

In addition to characterization and optimization of the equipment, variation models are needed to guide process optimization and process synthesis. Short-flow methodologies are needed that can accurately characterize the performance of process modules, including their important variations and interactions, so that full flow processes can be more rapidly and easily assembled. An important element of this is the causal decomposition of variation - identifying the process steps or modules that contribute to overall variation. For example, the contributions of etch and lithography in line width variation have been studied by Yu et al. [23]. Once process design has been accomplished, there is a critical need for process and equipment control strategies that can monitor and minimize such variation. For example, any modification to process parameters in a production process, be they as simple as polish time or as sophisticated as full multivariate process control, will be undertaken only when the die-level variation implications of that change are well understood.

In addition to application in the manufacturing arena, statistical metrology will play an important role in product design as well. Statistical metrology can contribute to variation reduction through improved circuit design practice. In the case of CMP, for example, the experimental methods and models of ILD thickness variation dependencies on layout patterns are already contributing strongly to the development of metal fill patterning practices [8]. An important future opportunity is the use of variation models to design circuits which are robust to or compensate for known systematic variation sources.

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