Excursion Wafer Loss Prediction by Local Density Segmentation

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***Abstract*—The most obvious characteristics of an excursion wafer is an elevated defect density, either confined within a signature or distributed across its surface. Quantifying the impact of such abnormal levels of defectivity is the focus of this paper. Three methods are described which provide increasingly precise predictions of Defect Limited Yield. The methods are also intended to accurately handle excursion wafers that include highly divergent signatures, as well as non-optimized defect inspection recipes which may contain elevated levels of nuisance defects. This is achieved by combining the defect distribution with the kill ratio, via a geometric progression. The conditions under which each method is ideally suited are presented.**

***Index Terms*—Kill Ratio, defect limited yield, excursion wafers, geometric mean, segmentation.**

I. Introduction

DEFECT summary statistics have proved useful historically, when simplifying the estimation of the potential impact on yield. This is especially true where large numbers of wafers are aggregated together, but less so when dealing with individual wafers and are particularly poor when wafers deviate further from baseline behavior.

Thanks to this former success and familiarity, there is still a preference to use conventional summary parameters and models in spite of the advances in computing power which make the full, raw data utilization a practicality.

Over the previous decades, there has been much effort to improve the Defect Limited Yield (DYL) estimations. These have included the use of the ubiquitous defect size information [1], [8], [11], [13], [15], [16], clustering [1]–[4], [7], [10]–[12], [19]–[21] and defect classification [6], [11], [14], [22]–[24]. Regardless of these developments, many still prefer to use more conventional metrics for line-control [10], [23], [24]. This necessitates numerous independent limits that are far more laborious to maintain, while failing to capture excursions that are composed of previously unseen combinations of defect classes. All of these effectively subdivide the loss into separate categories, dividing some combinational effects, thus reducing control rather than increasing it.

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Furthermore, the rapid pace of development means that it is increasingly likely that technologies will go into production without all failure mechanism being fully characterized or even know. As a result, any system needs to be able to adapt to unforeseen interactions and their excursion mechanisms.

Root cause identification is certainly supported by the combination of various classes, but this should not distract us from the need to determine an accurate, total loss estimate for each wafer. There is a potential advantage to using DYL as an in-line control metric, if it can be demonstrated to be a robust means of assessing individual wafers.

Most of these aforementioned improvements have been directed towards more precise baseline loss estimates or root cause identification. However, performing these calculations on individual wafers, in particular excursion wafers, brings with it additional challenges.

II. Single Wafer Analysis

Turning our attention to previous work which has paid some attention to the characteristics of individual wafers rather than purely baseline yield estimation or prediction, we find that Warner and Hu examined the applicability of various models to individual wafer-sort results. Ott *et al.* [14] and Hessinger *et al.* [17] showed that accurate wafer-specific loss estimates require that kill ratios be determined specifically from each wafer. Tuohy [18] demonstrated how a dose-response analysis could be applied to individual wafers with extensive defectivity, in order to extract a kill ratio and loss estimate. Segal *et al.* [15] illustrated a real-time loss assessment utilizing a combination of kill ratios and Critical Areas, but restricted to random defectivity. Ott *et al.* [14] also identified the need to treat baseline and excursion wafers separately with independent class paretos. Riley [3] went further by separating each wafer according to random and clustered defects with the intention of improving yield loss predictions, while elaborating on the inadequacies of wafer-based assessments and the need to transition to die-based methods. Cummingham and MacKinnon [12] also pointed out the need for die-based or quadrat analysis to avoid the loss of information associated with the simplistic parameters such as defect counts or density, or the simple segregation into defective and non-defective die counts. Furthermore they elaborated on how clustering algorithms can vary considerably, this being due to their dependence upon fixed threshold values. However, Riley implemented his own dynamic algorithm based on the median number of defects-per-die. He also pointed out that

there may be better clustering algorithms but his intention was to separate die that are affected by significantly divergent levels of defects and he managed this without having to predefine threshold values. Ikota *et al.* [20] had proposed a least squares fit of the Poisson Model to the defect distribution in order to determine the threshold for clustering, which has an appealing universality. Mullenix *et al.* [25] did consider utilizing the numbers of defects-per-die when calculating the DLY, but applied independent kill ratios to each group of die affected by a specific number of defects. They described this approach as naive, presumably because defect capture-rates are imperfect. However, the observed number of defects can be considered to be proportional to the actual number and is illustrative of the resulting yield deltas. Additionally, they treated each defect class in isolation, requiring an assumption of independence in order to generate estimates for the total loss.

III. Excursion Wafer Analysis Options

Returning to the main topic of excursion wafers, they are most often found to include elevated defect densities either across the whole wafer surface or localized within a signature and these are the types of excursions that will be focused upon here. These density changes will invariably also change the observed pareto of defect classifications. Less common are excursions driven exclusively by a shift in defect sizing and are unlikely to be captured by traditional summary statistics. Depending upon the defect classification system, changes in the size distribution may be visible in the classification pareto. However, these types of excursions will not be considered here, although they can be expected to occur infrequently.

As a possible solution, we could imagine implementing some signature analysis and aggregate the classification data within each signature [6]. Alternatively, some two-dimensional methods [7], [12] could provide a workable alternative.

The simplest and perhaps the most obvious two-dimensional alternative would be to consider segmenting the data according to some zone-pattern that results in the greatest differentiation in kill ratios between zones. This approach can initially seem straightforward, however as ever more exceptions are discovered and zone-patterns are added, such systems would become intractable and difficult to anticipate its behavior in all cases, while still delivering poor segregation.

There are also the more conventional one-dimensional wafer-level summary statistics. A firm favorite among these metrics are those where the clusters are counted as single events. This is a satisfactory simplification when modeling baseline effects and when the number of cluster-per-wafer and numbers of defects-per-cluster, remain stable. Over extended periods of time these assumption will not hold and certainly do not in the case of excursion wafers.

Nevertheless, there may be a convenient middle ground between these multi-dimension spatial solutions and the one-dimensional wafer-level parameter summaries which could be explored.

Recognizing that all models are wrong on some level and cannot be corrected by excessive elaboration, we should seek out the simplest solutions that also reflect the natural phenomena we are attempting to model. As previously stated, a significant proportion of excursion wafers include defect signatures that are spatially distinct. Perhaps less obvious is that these independent signatures are almost as distinct in terms of density, on individual wafers. It is this trait that we seek to utilize in this paper.

Density variations integrate more directly with the cumulative defect distribution but require that any changes in the kill ratio with defect counts per die, be examined and potentially used to segment the cumulative defect distribution. So rather than separating the data into numerous classification categories and smaller samples of local density to be analyzed independently and later combined, we identify potential points where the complete cumulative defect distribution should be segmented, in order to separate dissimilar signatures with divergent kill ratios.

It is our intention to extend the Single Wafer Analysis work to utilize the defect-level data via the cumulative distribution, rather than using spatial methods or handling various aggregate summary statistics, and to improve the precision of the resulting loss estimates, while paying particular attention to the analysis of excursion wafers.

We can always identify a more complex and potentially superior solution, but that should not deter us from pursuing a simpler and more robust solution with greater bandwidth.

IV. Pre-Classification Data

In order to avoid any misconceptions that the loss estimates are some estimate of the final yield, the term Pass Rate was chosen to more succinctly describe the conventional Defect Limited Yield (DYL), but without reference to the term "yield". Unfortunately, in some cases the Pass Rate has been assumed to be merely the complement of the kill ratio. This can occur, but only if each die on a wafer has exactly one defect.

It should be stated that while it is often the intention to extract the kill ratio in the belief that there is a single representative value, in reality each die can experience a different kill ratio and there is in fact a distribution of values. We can of course, later distill the impact on yield, down to a average kill ratio which explains the visible loss seen on a typical die, or per defect, at Wafer-Sort.

The determination of the defect kill ratio requires the use of a model which explains the cumulative effect of multiple defects-per-die. Our expectation is that the number of defects-per-die affects its yield geometrically, in accordance with Equation (1), which requires no special measures to avoid exceeding a Pass Rate of 1. Examining this equation we see that for it to be valid there needs to a stable defect-level kill ratio, for all values of n.

$$PR = \sum_{n=0} P(DD_n)(1 - K_1)^n \tag{1}$$

$n =$ number of defects per die

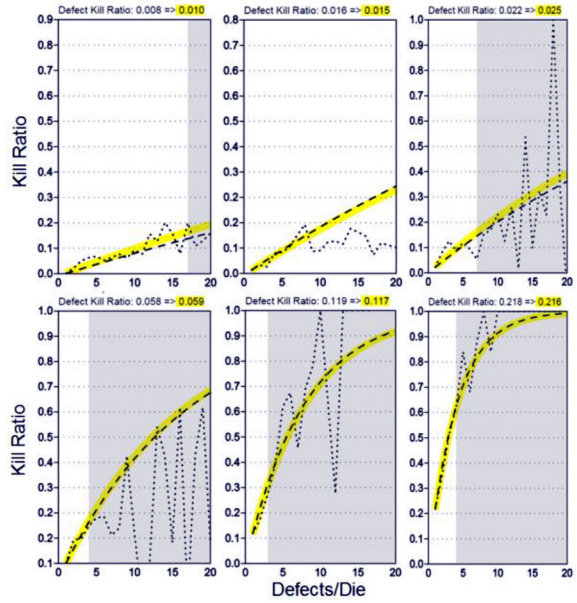

Fig. 1. Pre-Classification defect-level kill ratios versus point density. The dotted curves show the measured data; the dashed curve extends the kill ratio obtained from die with one defect; the yellow curve is a weighted fit for all point densities.

DD_n = Defective die with n defects

$P(DD_n)$ = Proportion of die with n defects

K_1 = Defect kill ratio

This can be determined by plotting the relationship between the kill ratio experienced by die versus the mean number of defects-per-die. Figure 1 displays this relationship for data aggregated from multiple lots and grouped according to different combinations of Product and Inspection Step. The first and last die in each row of the wafer-maps (taking the inspection orientation into consideration) are excluded because of typically having lower sensitivity. Including these data can distort the curves. Any regions of systematic loss will also adversely affect this process and should preferably be excluded. This can generally be considered as a reason to exclude all edge die.

The yellow curves in Figure 1 show the weighted fit of the geometric sequence to the observed data (black dotted curve) and the resulting defect-level kill ratios are also displayed (the black dashed curve extrapolates the defect-level kill ratio seen for die with a single defect).

The quality of the fits suggest that our assumptions regarding Equation 1 are sufficiently valid to pursue further.

V. Classified Defect Data

Next we must ask if these assumptions also hold true when the classification data is added to the system. Once again we need the defect-level kill ratios to be invariant with the number of defects-per-die.

Figure 2 displays two cumulative defective die distributions (blue curves). Figure 2a represents an excursion consisting of random defects, while Figure 2b shows a clustered excursion. In both cases, the random component is illustrated by the grey

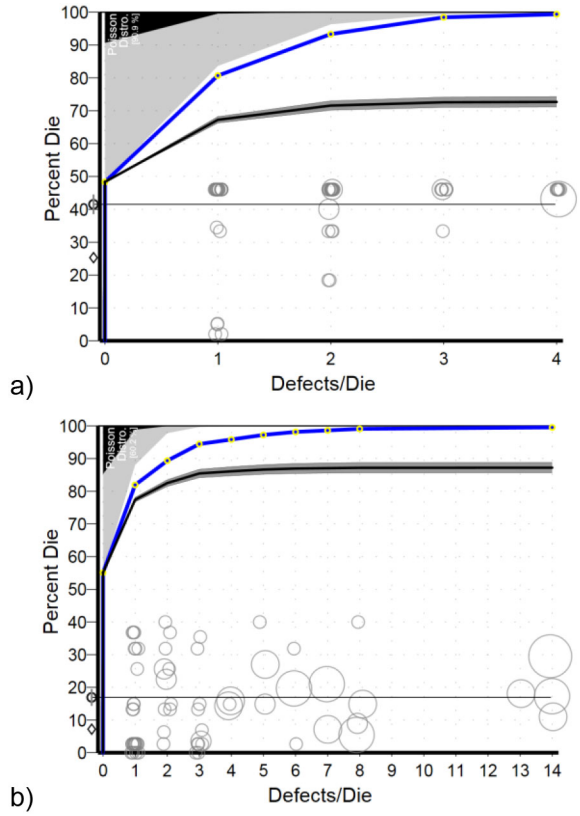

Fig. 2. Cumulative defects-per-die charts including mean kill ratios for classified die, indicated by grey circles. The size of the circles indicates the number of classified defects within each die. The horizontal black line shows the geometric mean kill ratio for all review defects. The 95% confidence Interval on this value is illustrated by the grey vertical bar through the circle to the left of the y-axis.

shaded region above the cumulative curves. This represents the maximal Poisson Distribution that can fit inside the cumulative distribution. The black inset regions represent the baseline random defect component that is expected for these Inspection Steps. The pre-classification kill ratios are illustrated by the diamonds positioned to the left of the y-axis. These can also be combined using Equation (1) to estimate the expected baseline Pass Rate for the wafer-step. Dividing this value into the actual Pass Rate will return the additional loss, relative to the expected final SORT Yield.

The grey circles illustrate the average post-classification kill ratios, for each reviewed die. The size of the circle indicates the number of reviewed defects within each die. In the absence of these review data we would apply the single defect, pre-classification kill ratio via Equation (1) to determine the Pass Rate. The question this raises is if we can effectively apply the same method to the post-classification data and how can we obtain a single kill ratio value from these data, or do we need to return to more traditional normalization loss estimation methods. Mullenix *et al.* [25] warned that the recombination of the components of such methods requires that they be independent. Although, they found no evidence for any gross dependence in their analysis, we can expect dependence between classes is far more likely to occur on excursion wafers. As a result, it is preferable to avoid

any method where independence between components is a requirement.

Fundamentally, we must examine how the post-classification kill ratios respond to the increase in defects-per-die, if at all. As previously stated, the Pass Rate as given by Equation (1) assumes that there is a single defect kill ratio that can be applied to a wafer. This fits the pre-classification case as illustrated by Figure 1, where there is no additional information regarding the defect classes to disturb the model.

It is important to recognize that Review Sampling faces competing requirements: a) to identify any excursion with sufficient accuracy in order to maximize the likelihood of root cause identification and b) generate an unbiased sample of the defects types present on a wafer. The former criteria will dominate and so measures have to be taken to unbias the review sample before loss estimation is attempted. Fortunately, segmentation provides a natural solution to this problem, in the form of marginalization (see Section VIII).

This has implications for traditional methods of Defect Normalization which assumes typical defect densities and sizes and cannot assess the impact on excursion wafers. Additionally, small signatures with critical defect mechanisms often have the majority of their die classified and normalization will scale the impact beyond the affected area and perhaps significantly, invariably exaggerating the loss.

The usual die-level kill ratios could be scaled by observed density increase if typical values are known or preferably, modeled from defect kill ratios. Of course, as the number of classes increase (as they can even within a single signature), accurately determining a representative density for a specific class is increasingly difficult, much less the density distribution for an individual defect class. This can be a reasonable approach if we restrict ourselves to a minimum numbers of groups (random and clustered defects [3]).

VI. Aggregate Statistic

Any move to defect-per-die based assessment of excursion wafer raises an additional issue as to what aggregate statistic to use for the kill ratios.

A possible option is the median. This gives satisfactory results for humongous signatures affected by uniformly distributed kill ratios. However, the typical excursion wafer often contains a mixture of defects with divergent kill ratios. Using a median in such situations can have unexpected results for similar wafers where the proportions of the constituent defects changes only slightly. Moreover, the fact that the median could correspond with a nuisance class (i.e., kill ratio = 0) indicates that median values cannot provide a general solution.

The arithmetic mean may seem to be a more obvious choice. However the geometric nature of Equation (1) means that applying an arithmetic mean will always result in an underestimate of the loss. Of the two remain Pythagoreans means it is the geometric mean that provides a natural fit for Equation (1). Furthermore, since it is the complement of the kill ratio that is geometrically manipulated in the Pass Rate equation, it is the complement for which we must obtain the geometric mean. Otherwise the geometric mean of the kill ratios would

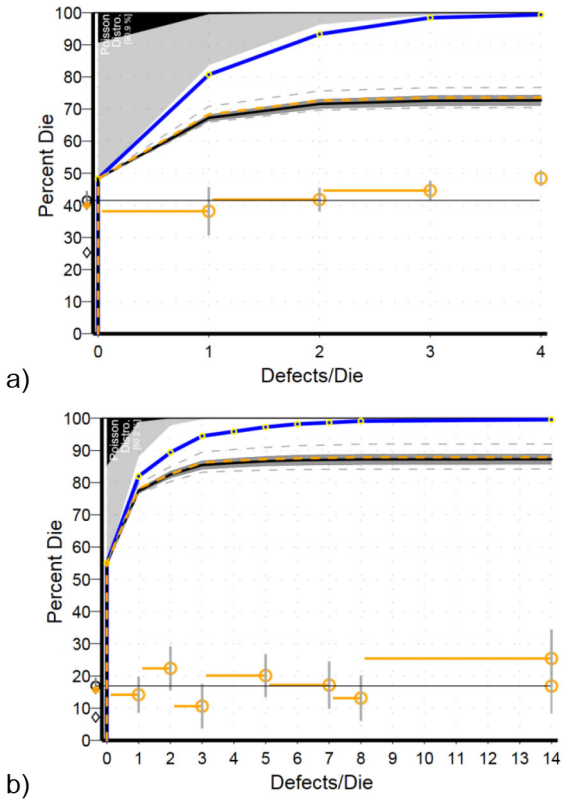

Fig. 3. Cumulative defects-per-die charts including aggregated geometric mean kill ratios for point-density ranges. The orange dashed curves show the Pass Rate that results from the application of the segmented kill ratios.

underestimate the loss more severely than the arithmetic mean and the presence of any nuisance defects will always result in a mean kill ratio of 0.

The black horizontal line across the chart with a circle to the left of the y-axis shows the geometric mean kill ratio for the post-classification data. The 95% confidence interval is illustrated by the grey vertical bar through the black circle.

Applying this geometric mean via Equation (1) generated the black curve whose final value is the Pass Rate for the wafer. The grey region around the curve is its 95% confidence interval.

As previously stated, the defect kill ratio should not vary with changes in the number of defects-per-die. It is not clear from the charts in Figure 2 what variation may be occurring in the average defect kill ratios versus the number of defects-per-die. Furthermore, we cannot expect a single model to explain all observed behavior. Therefore it is more straightforward to simply segment the values according to ranges of defects-per-die; creating a pseudo-Manhattan Diagram. The orange horizontal lines in Figure 3 show the geometric means for reviewed defects within those illustrated ranges. The vertical grey bars at the ends of these ranges indicate the 95% confidence intervals.

The resulting groups naturally lend themselves to an ANOVA and the Least Significant Difference could be used to identify clear separations in the kill ratio variation. Of course this is not a randomized control experiment for which ANOVA was intended. Additionally a monotonic change in

kill ratio may be visible (see Figure 3a), but with no point exceeding the Least Significant Difference.

VII. Segmented Pass Rate

Alternatively, we could simply apply the segmented kill ratios as they stand, in accordance with Equation (2), which contains a minor modification with respect to Equation (1). All terms are as before except for the inclusion of k_n which represents the segmented kill ratio that changes with the value of n.

$$PR = \sum_{n=0} P(DD_n)(1 - k_n)^n \tag{2}$$

$\mathrm{k_n}$ = Defect kill ratio for die with n defects

It should be noted that any excursion wafer is clearly a combination of baseline defectivity which could be expected to be largely randomly distributed and adhere to a Poisson Distribution, with an excursion mechanism that could also be randomly distributed (Figure 3a), but more often is clustered (Figure 3b).

Our initial example (Figure 3a) shows an almost ideal, random excursion defect mechanism where at least 90.9% of the defective die can be explained by a single Poisson distribution (see the grey shaded area above the blue cumulative curves). The inset black region shows the median baseline random defectivity. The defects on the die with higher defect counts can be expected to be from the same source due to autocorrelation and their kill ratio should asymptotically approach the value for the dominant excursion class.

As more high density die are reviewed the average kill ratio will skew more towards that of the excursion mechanism (i.e., 0.47). This is an issue where segmentation provides an ideal solution. Applying the segmented kill ratios to the data in Figure 3a increases the Pass Rate estimate from 72.7% to 73.6%, while Figure 3b displays a 0.6% increase; not a huge amount but nevertheless a systematic error that can and should be corrected for.

Some might expect the segmented kill ratio for die with one defect to be true value for an excursion wafer where the defects are distributed randomly and the increasing kill ratio with number of defects-per-die is merely an artifact of sampling a single defect from those die. Certainly, as the sample size falls the proportion of observed defects classes will skew towards any dominant class. However, the die with a single defects will contain the highest proportion of baseline defectivity classes.

It should be noted that the high density die usually attract a disproportionate level of classification and as a result can skew the unsegmented kill ratio average. A kill ratio for the excursion mechanism will be more representative of these die and we can expect a transition to occur between the baseline and excursion mechanisms. Small review samples of the defects within a die will increase the rate of any such transition. Where this is a concern, a **Dirichlet Distribution** can be used to provide a correction.

VIII. Marginal Kill Ratios

Segmenting the kill ratio range according to the local defect density slightly increases the complexity of the loss calculation. However, it allows for a more dynamic assessment as to the ground truth of loss, on excursion wafers. Figure 3b demonstrates the cumulative distribution for a more typical excursion wafer where there is a component of clustered defects. In this example only 60.2% of the defective die can be explained by a single, maximal Poisson Distribution and the remainder can be considered to be affected by clusters. The excursion is not confined to these clustered defects, but it is its most obvious component.

The resulting segmented Pass Rates (orange dashed curves) are usually greater than their respective unsegmented Pass Rate. The deviation rarely exceeds 0.5% and is always within the 95% confidence interval on the unsegmented Pass Rate. This would suggest that segmentation is generally unnecessary, where the review sample is unbiased and there are no nuisance signatures.

The potential dependence of the kill ratio upon the number of defects-per-die is suggestive of the conditional probabilities found within a Bayesian Framework. Another interesting term that is used with such a framework is the Marginal Probability. This can be derived by means of the **Law of Total Probability** as the sum of the sizes of mutually exclusive partitions of the sample space, times the conditional probability for each partition. This has the advantageous characteristic that it gives an unbiased estimate of the average probability.

Applying this to the task at hand, we can calculate a **Marginal Kill Ratio** by utilizing Equation (3), where k_n is the conditional kill ratio for die with n defects and the other parameters are as previously defined:

$$K_M = \sum_{n=1}^{Max} k_n P(DD_n) \tag{3}$$

Since we are concerned with calculating the kill ratio and the clean die have no influence, the sample space should be restricted to those die with defects. It is for this reason that the summation starts with a minimum value of 1.

There is not much value in pursuing these similarities with a Bayesian Framework any further as the Posterior Probability would merely give the probability of observing a specific number of defects on a die, given a particular kill ratio, which is of limited value.

The marginal kill ratio is effectively a rebalancing of the review sample to compensate for the local defect density from which it was collected. This minimizes any bias which almost certainly exists. For wafers without any nuisance signatures, simply applying the **Marginal Kill Ratio** instead of the geometric mean of the defect kill ratios, to the whole defect distribution will produce the same Pass Rate as the **Segmented Kill Ratios**. Substituting the constant, marginal kill ratio (K_M) for K_1 in Equation (1) is all that is required to calculate the **Marginal Pass Rate**.

Applying the **Marginal Kill Ratio** of 0.399 to the data in Figure 3a, instead of the geometric mean value of 0.415, also returns a Pass Rate of 73.6%, which is the value obtained from

the use of the segmented kill ratio. In the case of Figure 3b, the difference between the geometric mean and marginal kill ratio is slightly smaller (i.e., 0.169 and 0.157). Applying the marginal kill ratio does not entirely eliminate the difference between the segmented and unsegmented Pass Rates, but it does reduce it from 0.6% to 0.1%. This demonstrates that similar result can be achieved by using the simpler Pass Rate equation with the marginal kill ratio. However, the calculation of the marginal kill ratio still requires the segmentation of the sample space.

IX. Verlapping or Nuisance Signatures

Almost all signatures can be expected to overlap to some extent with other components on a defect map. Nevertheless, this should not be an issue as long as the Review Sampling strategy selects the divergent elements (e.g., nuisance and non-nuisance) with approximate equal likelihood. This is not an unreasonable assumption for a typical review sampling plan.

Furthermore, individual signatures can contain within themselves a portion of nuisance or low kill potential defects. As long as the sampling plan provides an unbiased estimate within these components, a geometric mean of the kill ratio can be used to estimate the loss. Extending this assumption, to separate signatures, but with partially overlapping densities, the geometric mean kill ratio can compensate for this eventuality. We do not have to expect that the sampling plan be unbiased across the whole wafer or even over a significant range of point densities in the cumulative defect distribution, but only that within the small density ranges where signatures may overlap, that any bias is negligible. Within this framework there should be no need to separate signatures with similar defect classes as they should either overlap in density of form part of a continuum. More specifically, if their kill ratios are similar, disparate signatures can be considered as a single entity.

There will undoubtedly be cases where such a simplification will fail to capture the true behavior. Nevertheless as long as such events remain sufficiently rare and the error is much less than 0.5% it can be considered an effective solution. Ideally, in order to resolve the dilemma of nuisance defects, we would exclude these defects from the defect map, if they could all be identified. Since this is not possible, alternative methods need to be used as we only know the location of a proportion of the nuisance defects. The most common approach is to nullify the nuisance defect contribution to the class-pareto by setting their kill ratio to zero. Unfortunately, this only generates satisfactory solutions when the nuisance defects are evenly mixed with the other defect classes but this is sufficiently rare and can be ignored.

Zhou *et al.* [16] correctly pointed out that defects at the minimum of the size distribution, because of limitations of Inspection Tool sensitivity, are often nuisance and eliminating these can often improve correlations and subsequently predictions. Unfortunately, nuisance or divergent signatures can occur anywhere in the size distribution and even at the maximum size value where poorly tuned recipes can incorrectly detect circuit patterns.

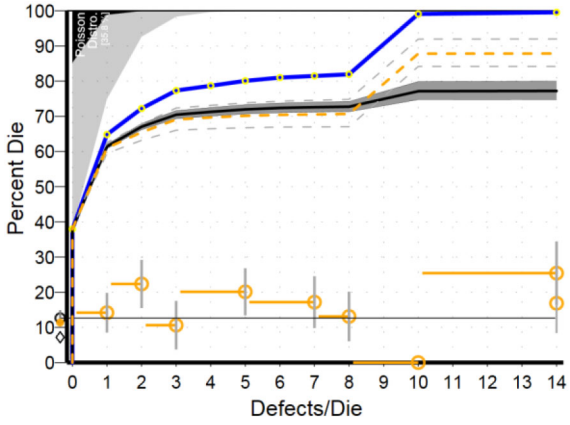

Fig. 4. Cumulative defects-per-die charts including nuisance signature at 10 defects/die and affecting ∼20% of die. The segmented Pass Rate was unaffected, while the unsegmented Pass Rate dropped by more than 10%.

Fortunately this is where our approach of transferring the kill ratios to the cumulative distribution can simplify matters. To illustrate this problem, Figure 4 contains the same data as in Figure 2b and 3b, but with a nuisance signature affecting ∼20% of die with 10 defects on every die. These defects have a kill ratio of zero (note the segmented kill ratio for die with 9 to 10 defects).Both the Unsegmented and Marginal kill ratios have been reduced by the introduction of this strong nuisance signature, dropping for 0.169 and 0.157 to 0.127 and 0.114 respectively. In spite of this reduction the unsegmented Pass Rate has decreased by 10%. However, the Segmented Pass Rate continues to provide the true Pass Rate value of 87.9%.

While there are various factors that can adversely affect loss estimations (e.g., inspection capture rate, classification accuracy), in their absence we can expect the segmented geometric Pass Rate to be well within 0.5% of the observed loss at wafer-sort.

X. Conclusion

A segmented, geometric progression has been presented for the accurate estimation of loss on excursion wafers. The basic method is sufficient for baseline wafers and pre-classification assessments. The method can be extended to include defect classification data. Review sampling skewing of these classification data can be compensated for by the use of a Marginal Kill Ratio. Segmentation of the kill ratios according to the corresponding number of defects-per-die, can adapt to the presence of nuisance or divergent signatures.

These methods can allow accurate loss assessments to be performed on baseline and excursion wafers alike, without the need to resort to multi-dimensional or signature analysis techniques. The segmented kill ratio method is robust enough to function with new or experimental defect inspection recipes that have not been completely optimized.

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