

## RUN-TO-RUN SENSOR VARIATION MONITORING FOR PROCESS FAULT DIAGNOSIS IN SEMICONDUCTOR MANUFACTURING

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### ABSTRACT

Tool behavior modeling and diagnosis is a big challenge in modern semiconductor fabrication, in particular, with high product-mix and complicated technology nodes. Tool condition monitoring has been long conducted by implementing the Fault Detection and Classification (FDC) system and analyzing the large amount of real-time sensor data collected during the process. The tool condition hierarchy developed in the previous work proposed that the excursions can be firstly detected by an overall condition indicator and then intuitively traced down to the level of sensor groups. In this paper, a Run-to-Run (R2R) variation monitoring technique is developed in order to correlate the tool excursions with individual sensors, instead of sensor groups, and thus to close the diagnostic gap in the hierarchy. Therefore, the tool condition can be efficiently monitored by one overall indicator and the detected tool faults can be systematically diagnosed at the sensor level.

### 1 INTRODUCTION

In addition to the R&D advancement, IC makers also have invested huge capital in the equipment procurement and implemented up-to-date IT systems to meet the continuously growing market demands. It is therefore very critical to optimize the tool utilization and production control plans. In particular, the “big data” collected continuously during production are not effectively analyzed to timely response and adapt to the dynamic changes. Nowadays the common practice for tool condition monitoring is to implement the Fault Detection and Identification (FDC) system. Current FDC analytics requires data pre-treatments, including predefining temporal windows and calculating representative statistics, such as the average and variance, for every SVID (Status VAriable IDentification) in each of the temporal windows. This easily generates hundreds of control charts to detect the shifts/drifts in the process profiles. Apparently, it is not an efficient way for tool condition monitoring.

Wang (2002) makes a comprehensive survey of machine maintenance models which are categorized in terms of the maintenance policies, such as the age replacement policy and failure limit policy. As can be seen in the survey, maintenance models majorly aim at estimating the expected life of tools and spare parts for preventive maintenance as well as predicting the unanticipated failure events for corrective maintenance. Most of these methods are model-dependent in terms of process physics or tool characteristics. Therefore, the maintenance policies are usually limited in certain area with specific data source. For example, the Preventive Maintenance (PM) system for epitaxial layer growth is based on the

relation of temperature to the deposited thickness (Susto, Beghi, and De Luca 2011). The proportional hazard model for the lithography steppers (Pampuri et al. 2011) and the multilevel linear model for chamber matching (Schirru, Pampuri, and De Nicolao 2010) are both process dependent. However, there are more than hundreds of process operations in current semiconductor manufacturing environments. The components inside process tools are of different physical characteristics. Deploying maintenance models and policies, and keeping them up-to-date would be very challenging.

Thieullen et al. (2012) make another comprehensive survey on the tool health indicator and prognosis specifically applied to semiconductor manufacturing process. The topic can be generally referred to Prognostics and Health Management (PHM) of the functioning tools. As can be seen in the survey, data driven techniques are usually employed based on the daily operational data. Empirical behavioral models are built to monitor the tool conditions and/or to predict the potential tool faults in the near future. These data driven techniques share one key feature in common by analyzing historical data from the processing tools and the product information in specific operations. Development of generic methods/algorithms for the whole fab seems to be impractical, considering the varying operating characteristics, processing physics, and the known failure modes.

Following the concept of consolidating multiple FDC SVID's into one single indicator based on Generalized Moving Variance (GMV) to monitor the tool condition (Chen and Blue 2009), Blue et al. (2012 and 2013) propose a hierarchical monitoring scheme to efficiently detect and diagnose tool faults. Figure 1 summarizes the concept of constructing the tool condition hierarchy and the manner of diagnosing detected faults. The first step to build the hierarchy is to cluster the SVID's into meaningful grouping scheme, with the validation of domain knowledge. In each sensor group, the GMV is calculated out of the FDC data to represent the group condition. Principal Component Analysis (PCA) is employed to generate a representative virtual sensor for each group such that all the representatives can be consolidated into one indicator, i.e., the overall tool condition, via calculating the GMV on all the representative virtual sensors.

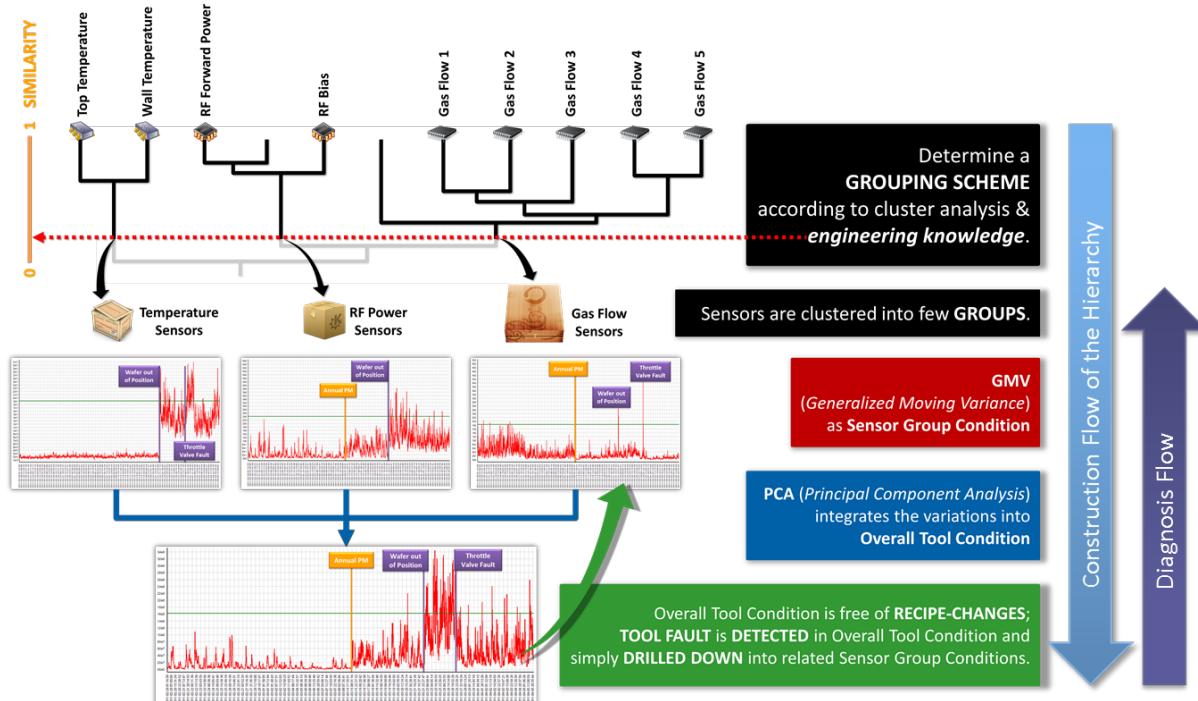


Figure 1: Illustration of the construction and diagnosis flows of tool condition hierarchy.

From the diagnostic viewpoint, the overall tool condition at the bottom in Figure 1 is going to provide an overview of the tool behavior. Given the mathematical property in applying PCA to consolidate the sensor groups into the overall indicator, the abnormal patterns displayed in the GMV of each sensor group will be kept in the overall layer and detected. It is therefore intuitive to drilldown the excursions detected in the overall indicator into the sensor groups by comparing the patterns between the overall and sensor group indicators. However, to make the hierarchy more practicable, the drilldown process should be extended to the sensor level, i.e., in the sense of SVID's (Moyné, Ward, and Hawkins 2012). Despite the fact that many univariate control charts already exist in the conventional practice, the diagnosis remains inefficient and nonsystematic, in particular, when one single SVID is summarized into several univariate indicators. In order to close diagnostic gap in the hierarchy, a temporal Run-to-Run (R2R) variation at sensor level is proposed in this paper to replace the conventional summarized indicators.

In the following section we are going to describe in details on the proposed methodology sensor level diagnosis followed by demonstrating a case study with real data from the local partner. Concluding remarking will be made at the end.

## 2 SENSOR LEVEL DIAGNOSIS

Tool condition can be evaluated based on very different data sources, such as Manufacturing Execution System (MES), FDC, or the wafer metrology measurements. Among these data sources, FDC data are collected continuously when the wafers are processed inside the equipment and thus shall provide comprehensive information about not only the process status but also the tool behavior. Therefore, most IC makers have implemented the FDC system in order to monitor process or tool faults. In this research, FDC data also serve as the study vehicle upon which we are going to develop the sensor level diagnosis.

Firstly we assume there are  $p$  sensors installed in one tool and thus these  $p$  SVID's:  $X_1, X_2, \dots, X_p$ , will be collected when one wafer is processed in the tool. The collected FDC temporal data for wafer  $k$  can be viewed as  $WT(k)$ :

$$WT(k) = \begin{bmatrix} x_{1,1}^k & x_{1,2}^k & \cdots & x_{1,p}^k \\ x_{2,1}^k & x_{2,2}^k & \cdots & x_{2,p}^k \\ \vdots & \vdots & \ddots & \vdots \\ x_{n_k,1}^k & x_{n_k,2}^k & \cdots & x_{n_k,p}^k \end{bmatrix}_{n_k \times p}, \quad (1)$$

where  $x_{i,j}^k$  denotes the collected FDC observation of  $j^{\text{th}}$  SVID at  $i^{\text{th}}$  time stamp for wafer  $k$ . The number of observations, i.e., the sample size, of each SVID for wafer  $k$  is  $n_k$  ( $i = 1, 2, \dots, n_k$ ) and is usually varying from wafer to wafer.

Under the original framework of the tool condition hierarchy, the tool fault diagnosis can be only drilled down to the sensor groups and thus the R2R variation of each sensor is proposed. Before going into the calculation of the R2R variation, there are two critical pretreating steps in order to have the meaningful R2R variation. Therefore, the two steps: recipe family grouping and FDC profile synchronization, will be introduced in the first two sub-sections followed by the concept of R2R variation.

### 2.1 Recipe Family Grouping

FDC temporal profiles can only be compared when they share regular patterns induced by similar recipe settings, which are sometimes referred to recipe bodies. A recipe body should clearly define the targets (or set-points) of the process states as well as regulate the behavior of the tool signals. Consequently recipes of different products and technologies display very different patterns, and are sometimes fine-tuned according to the run-to-run information in order to match the tool capability. In high-mix, low-volume production environment, recipe management is a challenging and critical issue because IC makers have to efficiently setup appropriate recipes for the operations and, at the same time, alleviate the impact

of changeover. Since recipes are directly related to the product designs, the recipe management becomes a confidential activity and is usually under central control in the companies.

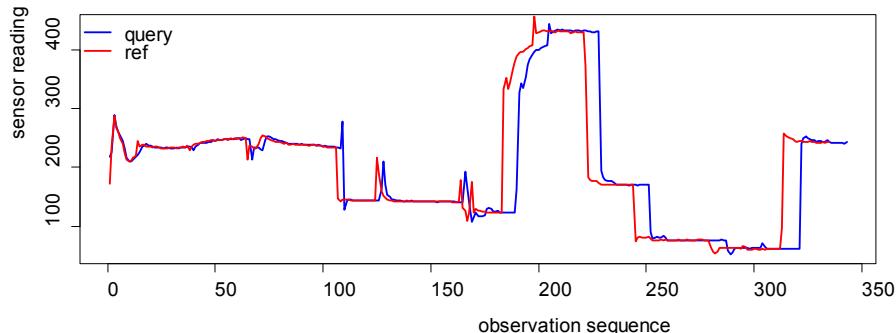
By comparing the FDC data among different recipes, not only the temporal profiles change significantly but also the numbers and types of SVID's vary notably. In order to have the fair comparison at the level of FDC temporal profiles, recipe grouping should be done beforehand to avoid detecting the excursion purely caused by the difference among recipes. In this paper, this step has been done by our industrial partner in the perspective of the physical design of recipes. Meanwhile, a mathematical/statistical grouping method is under investigation with the need of monitoring massive products and recipes at the same time.

## 2.2 FDC Temporal Profile Synchronization

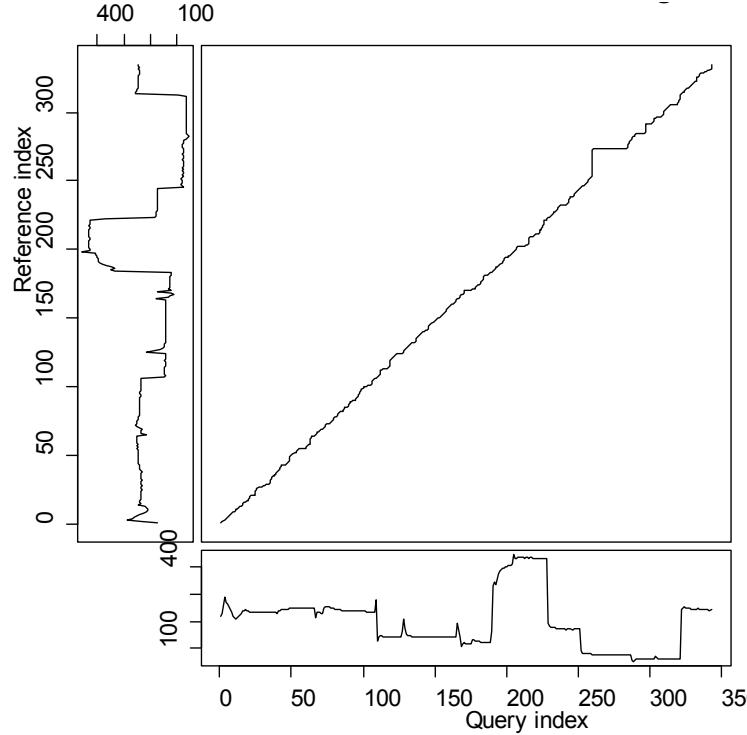
With the FDC data coming from similar recipe bodies, the comparison among wafer-to-wafer temporal profiles, ex: the comparison between  $WT(k)$  and  $WT(k+1)$  defined in (1), is still not easy. The main issue lies in the IT infrastructure. Current tools cannot perfectly handle the FDC data input/output interfacing and the production process at the same time. As one can imagine, the first priority is surely to keep the process running correctly and stably. Moreover, the timestamps between database servers and the tools are not well synchronized (SEMATECH 2013). This is causing missing values in FDC data and thus a Data Collection Quality Value (DCQV) is evaluated to monitor the data reliability and the process stability as soon as the FDC data of one wafer are collected. Another issue is related to the process characteristics because the process time would vary from one wafer to another based on the process physics. For example, the etching process will continue until the stop layer is reached. The process time might be different from wafer to wafer and, consequently, the length of FDC data collected is varying, i.e.,  $n_k \neq n_{k-1}$ .

With the issues mentioned above, comparison among FDC temporal profiles will suffer fundamental pattern shifting or miss matching such that the detected excursion might not be meaningful again. Therefore, a synchronization of FDC temporal data is needed. Dynamic Time Wrapping (DTW) (Müller 2007) is a technique for efficiently finding the alignment among shifted signals and has been used widely in many areas such as gesture recognition, robotics, speech processing and manufacturing.

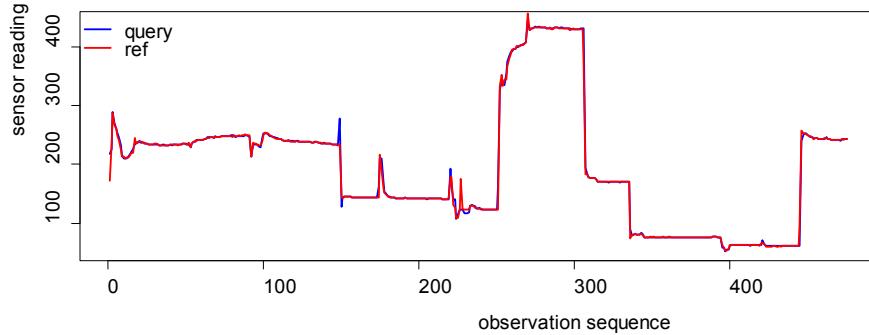
Considering two temporal series with  $n$  and  $m$  observations respectively, an  $n$  by  $m$  cost matrix, typically in terms of the Euclidean or Manhattan distance, can be constructed based on all the possible alignments. A feasible aligning path, also referred to a wrapping path, is subject to three constraints: boundary conditions, continuity and monotonicity (Keogh and Pazzani 2001). By minimizing the overall aligning cost via dynamic programming, the path can be found efficiently.



(a) The SVID profiles of two wafers from the same recipe show visible shifts, where the query series in blue has 343 observations and the reference series in red is of length 335;



(b) The optimal aligning path along the distance-based cost matrix;



(c) The SVID profiles of two wafers after DTW aligning are well synchronized. However, the final length of both series is augmented to 475.

Figure 2: A demonstration of DTW aligning (wrapping) path.

DTW works well only if the time shift (on the x-axis) exists between two temporal series with the completely similar pattern in terms of the value scale (y-axis). However, in FDC temporal profiles, local differences on the y-axis, i.e., the numerical magnitudes, of the series sometimes occur and cause the DTW algorithm ineffective. For example, two data points may share the same value but fall on different patterns such as one on the rising trend and the other on the down slope. DTW might have the chance to align the two points together due to the identical values. When two series do not share a similar pattern, they don't present in a simply time-shifted way in neither x nor y direction. It is very likely to happen in the semiconductor manufacturing environment when the severe process faults occur. DTW algorithm, in this situation, still takes granted that the two series shall be synchronized by matching head-to-head and tail-to-tail, instead of treating the abnormal one to be an outlier. Moreover, DTW tends to augment both

series in order to achieve the optimal warping condition such as shown in Figure 2(c). This is not a desired result if we would like to synchronize a group of FDC series, where an exemplar series with the fixed length will be assigned as the basis of synchronization. This basis is obtainable simply because the recipes with similar patterns are clustered or assigned to a recipe family wherein profile synchronization is demanded.

With the characteristics of FDC temporal data from the same recipe (or recipe family), not only time shifts but also measurement changes can be observed. Ideally, Derivative DTW (DDTW) can be employed to synchronize the FDC data and the experimental study was already done in Blue, Roussy, and Pinaton (2014). However, the designated patterns of different recipes are either slightly or significantly diverse from each other. By means of using the first derivative as the shape information in DDTW, the FDC temporal profiles after synchronization can be distorted.

Latecki et al. (2007) propose the Minimal Variance Matching (MVM) algorithm to work on the elastic matching of two series with distinctly different pattern while it is still possible to keep a fixed synchronized length. As can be seen in Figure 3, the two series form Figure 2(a) are aligned to have the same length 343. Therefore the MVM algorithm will be adopted in this research to synchronize the FDC profiles and the related notations are defined in the following.

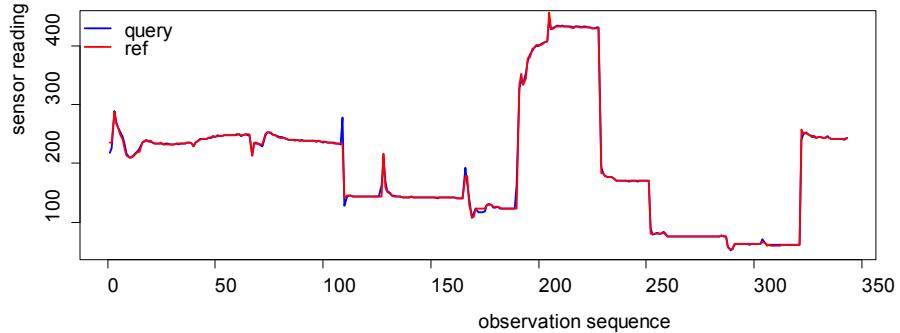


Figure 3: The SVID profiles of two wafers after aligning based on MVM are well synchronized. The final length of both series is fixed to be 343, same as the one in blue.

Assuming the temporal series of  $i^{\text{th}}$  SVID across all wafers from one recipe family,  $\mathbf{R}$ , are firstly collected from (1) and expressed as  $SVID_i(\mathbf{R})$ :

$$SVID_i(\mathbf{R}) = \begin{bmatrix} x_{1,i}^1 & x_{1,i}^2 & \cdots & x_{1,i}^r \\ x_{2,i}^1 & x_{2,i}^2 & \cdots & x_{2,i}^r \\ \vdots & \vdots & \ddots & \vdots \\ x_{n_1,i}^1 & \vdots & \ddots & \vdots \\ & \vdots & & x_{n_r,i}^r \\ & x_{n_2,i}^2 & & \end{bmatrix}, \quad (2)$$

where  $\mathbf{R}$  is the collection of  $r$  wafers,  $\{WT(1), WT(2), \dots, WT(r)\}$ , from the same recipe family. It is worth noting that the  $r$  series lengths of the same SVID from the  $r$  wafers are different, i.e.,  $n_1 \neq n_2 \neq \dots \neq n_r$ .

After applying MVM algorithm to (2), we get:

$$\overline{SVID}_i(\mathbf{R}) = \begin{bmatrix} x_{1,i}^1 & x_{1,i}^2 & \cdots & x_{1,i}^r \\ x_{2,i}^1 & x_{2,i}^2 & \cdots & x_{2,i}^r \\ \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ x_{n,i}^1 & x_{n,i}^2 & \cdots & x_{n,i}^r \end{bmatrix}, \quad (3)$$

where  $n = \max(n_1, n_2, \dots, n_r)$  is the unique wafer process length after synchronization. In the following sub-section, the R2R variation of one SVID will be calculated based on the aligned profiles in (3).

### 2.3 SVID Run-to-Run Variation

The concept of R2R variation starts by expanding a group of FDC temporal profiles of one SVID from a two-dimensional trend chart to a three-dimensional topography. It is done by simply adding the third axis “wafer ID in processing sequence” as shown in Figure 4. The topography can be viewed as a two-dimensional contour in Figure 5 with respect to the data arrangement in (3).

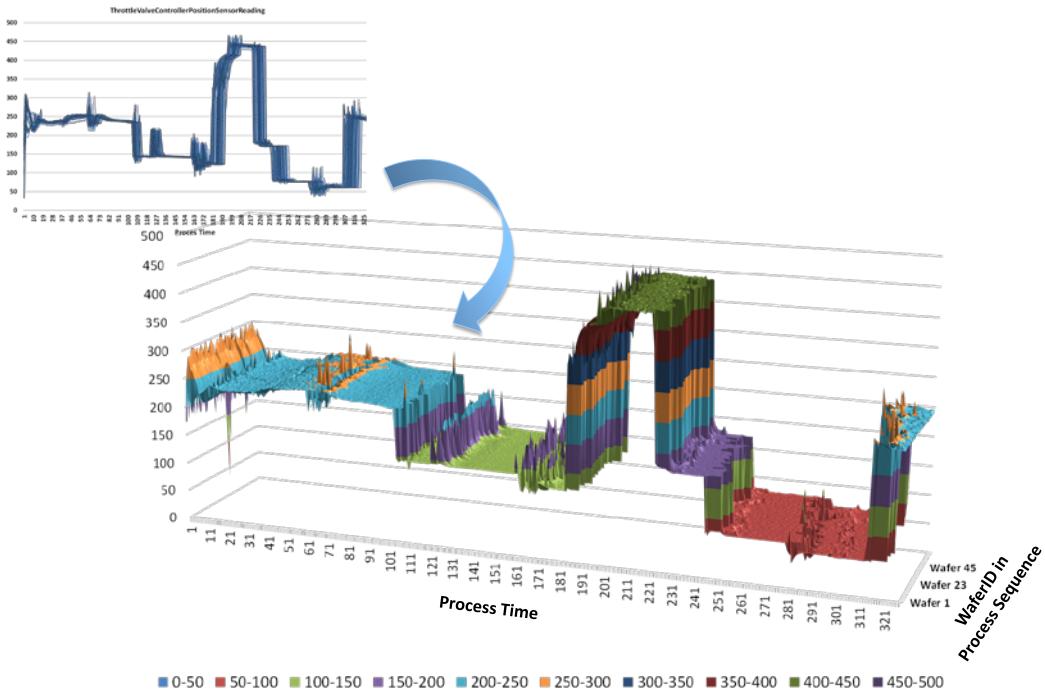


Figure 4: A 2-D wafer-to-wafer FDC temporal profiles of the SVID “ThrottleValve” is transformed into a 3-D topography.

To calculate the R2R variation, two consecutive wafers in the same recipe family are selected, for example, the  $WT(1)$  and  $WT(2)$  in  $\mathbf{R}$ . Consequently the first two columns in (3) are picked up. The variances of all pairs of observations between the two wafers, i.e.,  $\text{var}(x_{1,i}^1, x_{1,i}^2)$ ,  $\text{var}(x_{2,i}^1, x_{2,i}^2)$ , ..., and  $\text{var}(x_{n,i}^1, x_{n,i}^2)$  are calculated. By taking the average of these  $n$  local variances, we get the first R2R variation of SVID  $i$ , denoted as:

$$s_{r2r,1}^2(i) = \frac{1}{n} \sum_{j=1}^n \text{var}(x_{j,i}^1, x_{j,i}^2). \quad (4)$$

The idea of R2R variation is to capture the local changes between two consecutive wafers from time to time. From the illustration in Figure 5, the first local variance is calculated from the pair of

observations of two consecutive wafers at the first second of the process, assuming the FDC data sampling rate is one observation per second. If the process lasts for 327 seconds, there will be 327 local variances from these two wafers. The R2R variation is calculated by taking the average of these local variances.

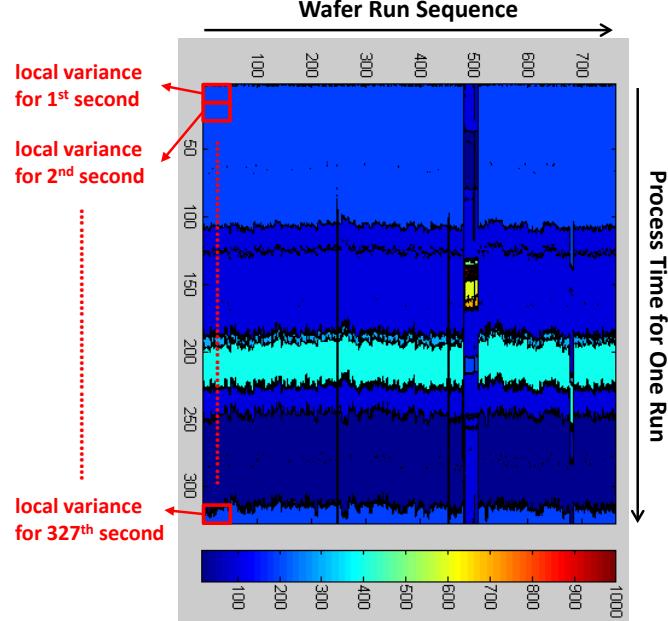


Figure 5: The FDC data in (3) is arranged in a 2-D contour. The local variances are calculated from two consecutive wafers and averaged to be the R2R variation.

## 2.4 SPC on R2R Variation

In order to detect the excursion of R2R variations, Exponentially Weighted Moving Average (EWMA) is employed. EWMA control scheme (Borror, Montgomery, and Runger 1999; Lucas and Saccucci 1990) is well-known for process dispersion monitoring (Castagliola, Celano , and Fichera 2006). Let  $Z_{i,k}$  denote the EWMA statistic of the R2R variation of SVID  $i$  of wafer  $k$ .  $Z_{i,k}$  can be calculated as:

$$Z_{i,k} = \lambda s_{r2r,k}^2(i) + (1 - \lambda)Z_{i,k-1}, \quad (5)$$

where  $\lambda$  ( $0 < \lambda \leq 1$ ) is the smoothing constant.

The steady-state EWMA Lower/Upper Control Limits (LCL/UCL) are defined as:

$$\text{LCL} = \mu_{s,i} - L\sigma_{s,i}\sqrt{\frac{\lambda}{2-\lambda}} \text{ and } \text{UCL} = \mu_{s,i} + L\sigma_{s,i}\sqrt{\frac{\lambda}{2-\lambda}}, \quad (6)$$

where  $\mu_{s,i}$  and  $\sigma_{s,i}$  are the mean and standard deviation of in-control  $s_{r2r,k}^2(i)$ 's, and  $L$  determines the width of the control window. For a standard Shewhart control chart (Castagliola, Celano, and Fichera 2006) on the normally distributed data, the Average Run Length (ARL) with  $3\sigma$  is known to be 370.4. Since  $s_{r2r,k}^2(i)$  is not likely to follow the normal distribution, we may follow suggestions by Borror, Montgomery, and Runger (1999) to use  $L=2.492$ ,  $2.703$ , and  $2.86$  with corresponding  $\lambda=0.05$ ,  $0.1$ , and  $0.2$ , respectively, for the EWMA control scheme to obtain approximately the same ARL=370.4. In this paper, after some experiments from the actual production data, we set  $\lambda=0.05$  and  $L=4$  for a lower false alarm rate acceptable to the semiconductor manufacturing practice. The setting of the EWMA control scheme should not be fixed across all tool types and should be adjusted according to the natures of the tool processes, which surely affect the false alarm rate.

### 3 EVALUATION OF CASE STUDY

The FDC data to be evaluated are collected from an etch tool, which are the same as the second case in Blue et al. (2012). Around 800 wafers with 31 SVID's from one family of eight GATE recipes are analyzed. The FDC profiles are also synchronized by DDTW firstly. Following the hierarchical analysis in Blue et al. (2012), it is known that there is a significant anomaly in the overall tool condition as shown in Figure 6. By looking into the conditions of four sensor groups: 11 SVID's in RF (Radio Frequency), 3 SVID's in temperature, 13 SVID's in gas, and 4 SVID's in pressure, the abnormal pattern in the overall condition can be directly identified as a fault from the *gas* group. To save the page in presenting the results of tool condition hierarchy, we simply put the overall tool condition and the gas group condition from here. For more analytical details of the tool condition hierarchy, please refer to Blue et al. (2012).

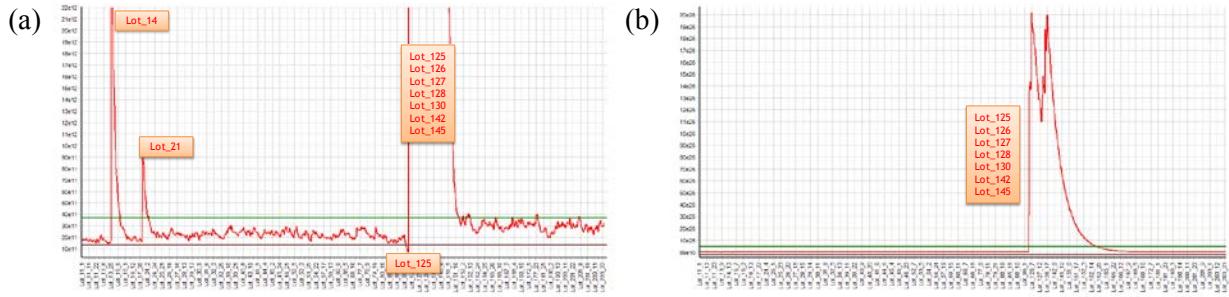


Figure 6: The simplified result from the tool condition hierarchy analysis: (a) the overall etch condition; (b) gas group condition, with EWMA UCL in green and LCL in dark red if non-negative.

Since the FDC data are already classified into one recipe family, the next step is to synchronize the FDC profiles for the calculation of the R2R variation. MVM algorithm is employed and the R package “dtw” is directly used to process the alignment for the whole dataset (Giorgino 2009). To further classify the root causes at the sensor level in gas group, the proposed R2R variation is calculated for the 13 SVID's. To make a clearer illustration, Figure 7 visualizes the contours of MFC1 (Mass Flow Controller 1) and MFC2 to provide a sketch on the wafer-to-wafer profile transition. As can be seen, MFC2 has no significant pattern compared to MFC1. The other 11 MFC's in the gas group exhibit consistent abnormalities in accordance with the phenomenon in MFC1.

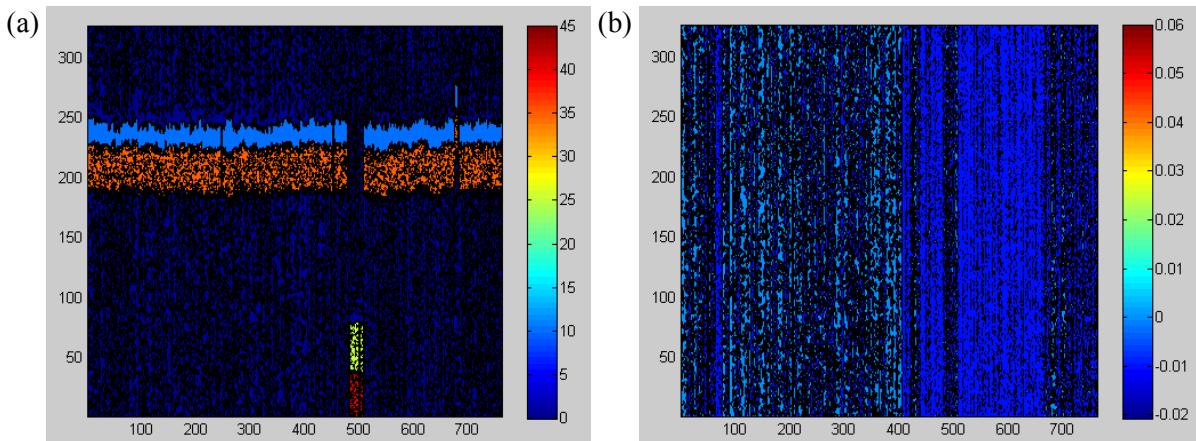


Figure 7: Contours of (a) MFC1 and (b) MFC2 out of the 13 SVID's in the gas group, where x-axis is the wafer ID and y-axis indicates the process time in one run.

R2R variations for these SVID's are also calculated and monitored according to the proposed control scheme. In Figure 8, only the R2R variation of MFC1 in contrast with MFC2 are shown and other gas flows are analyzed in the same fashion. After applying the EWMA control scheme, the R2R variation chart of MFC1 shows very similar pattern to the overall tool condition and gas group condition in Figure 6(a) while the one of MFC2 seems not to account for this main excursion. It is known from MES that this dataset covers a complete PM cycle followed by a Corrective Maintenance (CM) intervention for fixing the process drift. However, the process drift is not completely fixed until the end of the dataset. The big pattern here in Figure 6(a) is confirmed to be the period that covers the practiced PM followed by CM intervention when the tool started to collect unusual FDC profiles. It also shows that the tool condition after the CM intervention remains unstable around the upper control limit. Particularly, the mass flow controllers display totally different temporal profiles compared to the wafers processed before/after the abnormal period.

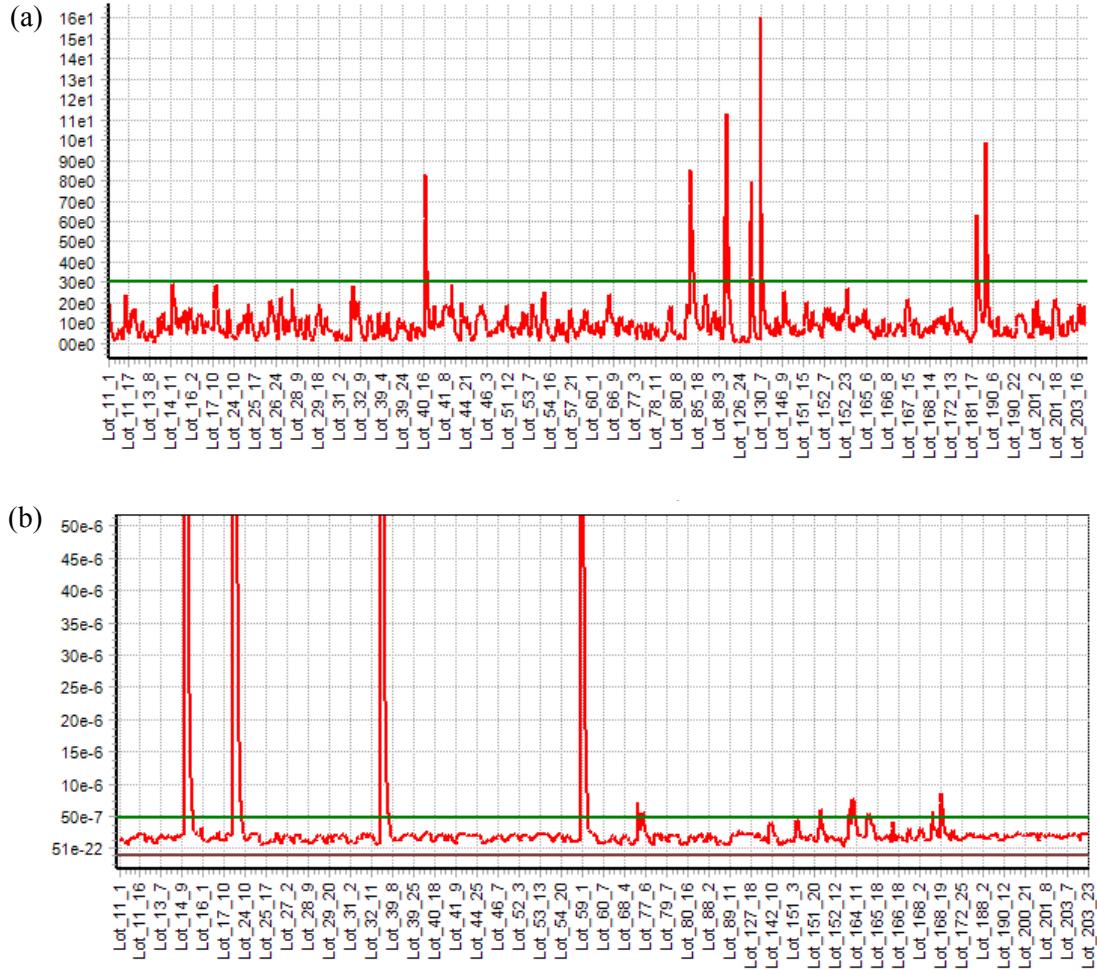


Figure 8: R2R variations of (a) MFC1 and (b) MFC2.

#### 4 CONCLUSION AND FUTURE WORK

The main contribution of this paper is to extend the diagnostic function in the tool condition hierarchy to the sensor level by calculating the R2R (Run-to-Run) variation of individual sensor. Given the fact that monitoring the enormous amount of summarized indicators conventionally implemented is inefficient and

ineffective, the proposed R2R variation is calculated directly out of the sensor temporal data and tries to detect the change of the variation from profile to profile. To ensure the robustness of monitor the R2R variation, two preliminary steps have to be done in advance: recipe grouping and temporal profile synchronization. The false detection of excursions due to simply recipe changes or inconsistent data structures can be then avoided. The use-case further validates the effectiveness of R2R variation.

Nevertheless, recipe grouping based on the physical definition will contradict against the advantage of recipe-independent hierarchical monitoring scheme. Furthermore, data transformation via Minimal Variance Matching (MVM) and Dynamic Time Wrapping (DTW) algorithms would surely cause information distortion. It is of our continuous goal to look for automatic recipe grouping mechanism with respect to the Fault Detection and Classification (FDC) profiles as well as to investigate the distortion after applying profile synchronization.

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