

## SYSTEMATIC APPLICATIONS OF MULTIVARIATE ANALYSIS TO MONITORING OF EQUIPMENT HEALTH IN SEMICONDUCTOR MANUFACTURING

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### ABSTRACT

In this work, a systematic procedure of building a model for monitoring batch processes in semiconductor manufacturing and visualization of monitoring results will be presented. Semiconductor manufacturing batch-processing stages usually consist of many steps. Aging trends likely to be detected only in the steady state period of each step. Large fluctuations can be found in on-off period of each step. Hence "step-trend" variables, i.e. mean shifts from reference profiles of each steps, are defined to track aging trends. Residuals from this shifted profile are then used to provide a combined health index of each batch through Hotelling T2 analysis.

### 1. INTRODUCTION

Semiconductor manufacturing is one of the fastest development industries in the last two decades. To reduce cost and improve performance, wafer becomes larger and larger and gate width become smaller and smaller. Effective control of process operations to ensure final product quality has become one of the keys for maintaining competitiveness (Spanos and May, 2006). Semiconductor manufacturing is essentially a multistage process. For some of these stages (such as planarization and etching), inline metrology data are available as indicators of process performance, and the basis of run-to-run feedback control. For many other stages (such as implant and thermal annealing), tracking of process performance depends only on analysis of equipment sensor outputs. Multivariate statistical analysis (Smith, et al. 2004) is an ideal tool for such a purpose. However, in actual implementation, simple applications of multivariate analysis usually lead to frequent false alarms unless the model is frequently updated (Spitzlsperger, et al. 2005). This is due to the fact that processing equipments exhibit both short term fluctuations (such as "first-wafer effect") and

long term fluctuations (such as "aging"). Moreover, due to the multi-step nature of the stage, a sensor variable in different steps of the batch process may exhibit different trends. Such trends should be regarded as normal. Only substantial deviations from such trends should be detected as faulty operations. Failure to account for such variations so will lead to false alarm. In this work, a systematic procedure of building a model for monitoring batch processes in semiconductor manufacturing will be presented. Specific periods within the batch operation where aging trends is likely to be detected are identified. Explanations on why methods such as multiway PCA (Nomikos and MacGregor 1995) are no suitable.

### 2. PRETREATMENT OF BATCH PROFILE DATA

Each manufacturing stage in the semiconductor manufacturing workflow can be regarded as a multi-step batch (wafer or lot) process. Figure 1 shows a schematic illustration of a 2-dimensional (variable-time) data structure of sensor output from batch to batch.

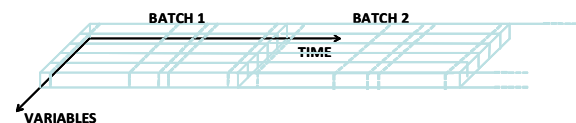


Figure 1: 2-dimensional (variable-time) data structure of sensor output from batch to batch

However, actual monitoring is performed from batch-to-batch. The changes of sensor variable within a batch should be regarded as a profile of variables. It is common that the processing times of each step vary from batch-to-batch and a synchronization procedure is required. The 3-dimensional (variable-profile-batch) data structure of sensor variable output and its synchronized

version is illustrated in Figure 2. In this work Akima spline (Akima 1970) is applied to each step for synchronization.

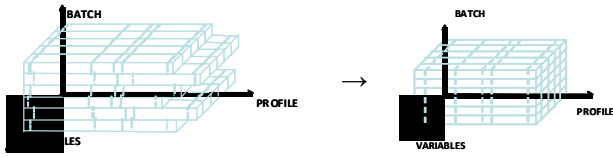


Figure 2: 3-dimensional (variable-profile-batch) data structure of sensor variable output and Synchronization

### 3. TREND IDENTIFICATIONS OF PROFILE DATA WITH SHARP CHANGES

Multi-way Principal Component Analysis (MPCA) (Nomikos and MacGregor 1995) is a commonly technique used to monitor a batch chemical or biochemical process (Kaistha et al. 2004). In this approach, the variables and profile are combined into a single dimension of numerous variables (Figure). It should be pointed out that it is often impossible to perform MPCA for the entire process due to the increase in number of variables and block PCA are used (Cherry and Qin 2006).

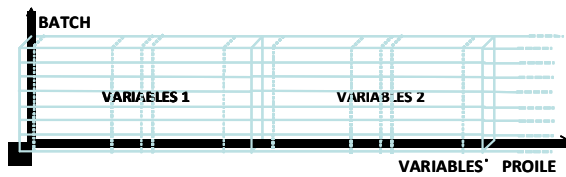


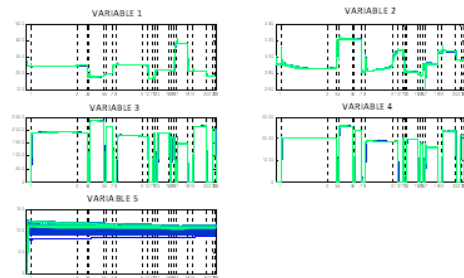
Figure 3: Combination of Variable and Profile Dimension in MPCA

However, unlike a chemical or biochemical process in which most variables vary in a relatively slow and continuous manner, semiconductor manufacturing processes often consist of on-off steps that involves variables with sharp and large changes. Figure 4a shows sensor output of 5 variables of 364 batches of a semiconductor manufacturing stage from a local company. Differences between steady states values of each step between batches are barely observable.

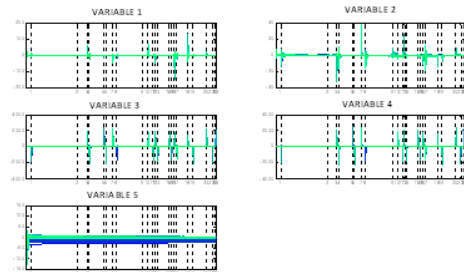
Let us denote batch (wafer or lot), variables, and profile points by indices  $i,j,k$  respectively. A deviation sensor output  $D_{ijk}$  can be estimated from the raw sensor using a reference profile. If such a reference is not known, the average of a set of batches can be used.

$$D_{ijk} = \begin{cases} X_{ijk} - X_{jk}^o & \text{with a known reference profile} \\ X_{ijk} - \bar{X}_{.jk} & \text{without known reference profile} \end{cases} \quad (1)$$

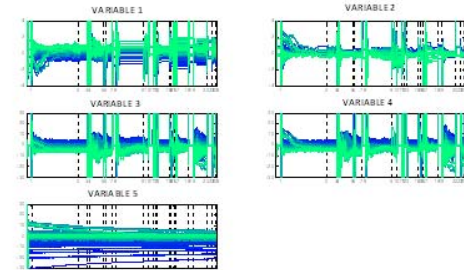
It can be seen that large variations can be found during the initial periods of each on-off steps (Figure 4b). Rescale of the variations show that a batch-to-batch drifting can be found during the stable periods of each step, but no such trend can be found at the initial turning-on periods (Figure 4c).



(a) Original



(b) Mean-centered



(c) Rescaled mean centered

Figure 4: Typical Profiles of Variables in a Semiconductor Manufacturing Stage

To separate this trend of batch-to-batch behavior, a set of step-trend variables are defined as the mean shifts of each sensor variables in each step from the reference profile:

$$\min_{b_{js}} \sum_{k \in \text{step } s} \left( \frac{D_{ijk} - b_{js}}{\hat{\sigma}_{jk}} \right)^2 \quad (2)$$

Figure 5 illustrates the 23 step-trend variables obtained from VARIABLE 3 in Figure 4. Obvious drifts can be found in many steps 2,4,3,5,7,9,10,12,14,16,18,20,22. Scores of 1st PC from weighted PCA analysis of the step-

trend variables (Figure 6) shows an unequivocal aging trend with first-wafer effect in many of these lots.

Figure 7 illustrates scores of 1st PC obtained from MPCA analysis of profiles of VARIABLE 3 in all 23 steps. Trends can be found in only step 3 and 5. It is due to the fact that the 1st PC captures the variables with largest fluctuations, which correspond to profile points at the initial periods of each steps.

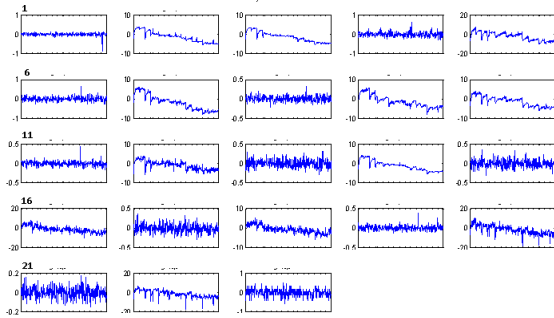


Figure 5: Trend Variables of Variable 3 in All 23 Steps

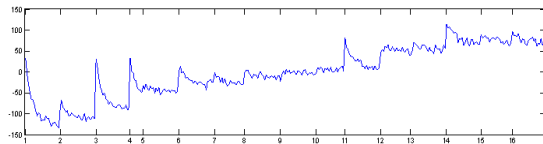


Figure 6: Weighted PCA Analysis of Step Trend Variables

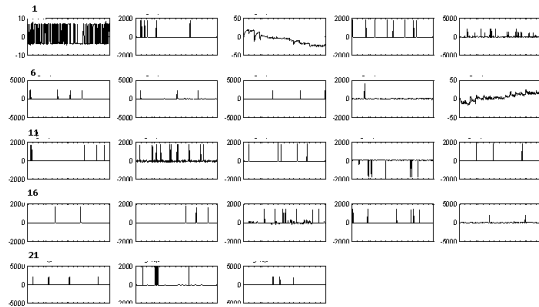


Figure 7: Scores of 1st PC obtained from MPCA Analysis of Each Step

The residual from these trend variables can be calculated as

$$e_{ijk} = D_{ijk} - \hat{b}_{ijs} \quad (3)$$

They show no aging or first wafer trends since they should have been already captured in the step-trend va-

riables; while the residual from MPCA analysis will not be rid of such trends (Figure 8).

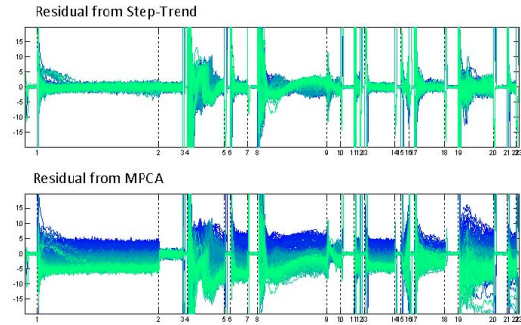


Figure 8: Trends of Residuals

#### 4. FAULT DETECTION

Given successful isolation of aging trends, the residual variables can be used for fault detection analysis. First, Hotelling  $T^2$   $H_{ik}$  can be estimated for each batch at each profile points .

$$H_{ik} = \text{diag} \left\{ \mathbf{E}_{i-k}^T \left[ \mathbf{E}_{i-k}^T \mathbf{E}_{i-k} \right]^{-1} \mathbf{E}_{i-k} \right\} \quad (4)$$

In the model construction, a chi-square distribution is assumed:

$$(N - I)H_{i-k} \sim \chi^2(p(k)) \quad (5)$$

while an F-distribution is used in the monitoring phase

$$\frac{N-p(k)}{p(k)} H_{ik} \sim F(p(k), N - p(k)) \quad (6)$$

Using equations 5 and 6,  $H_{ik}$  can be converted into a cumulative probability  $CP_{ik}$ , which can be summed into a single cumulative probability of each batch  $CP_i$ :

$$CP_i = \sqrt{12K} \left( \frac{1}{K} \sum_{k=1}^K (CP_{ik}) - \frac{1}{2} \right) \sim N(0, 1) \quad (7)$$

Graphical illustrations of the cumulative probability of each batch and at each profile point are shown in Figure 9. For example, it is found that  $CP_{ik}$  of stage 2 of batch 108 contributed substantially to the abnormality of this batch.

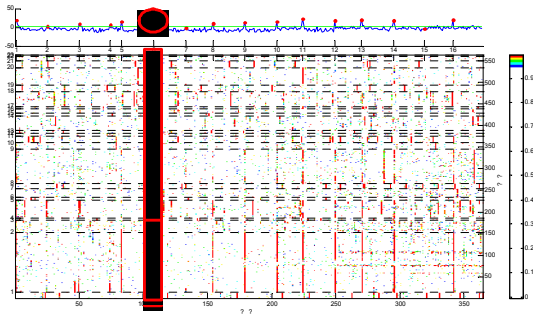


Figure 9: Cumulative Probability  $CP_1$  of Each Batch and at Each Profile Points  $CP_{1k}$

Contribution plot of Hotelling  $T^2$   $H_{108,k}$  (Figure 10) showed that variables except for variable 2 provide important variations. Actual variations are provided in Figure 11. Variables 3 and 4 at step 2 and 3 contributed substantially to this particular fault.

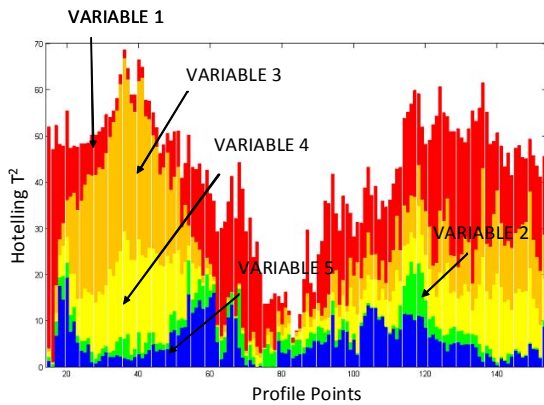


Figure 10: Contribution Plot of  $T^2 H_{108,k}$

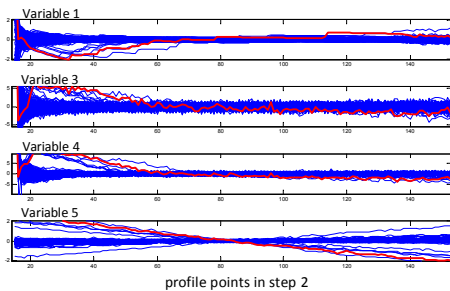


Figure 11: Deviations from Mean Profile in Step 2

## 5. CONCLUSION

In this work, a systematic procedure of building a model for monitoring batch processes in semiconductor manufacturing is provided. This procedure involves synchronization of batch profile data using Akima spline, use of mean-shift of reference profiles of each step to identify aging trends. Weighted PCA of step-trend variables can be used to monitor aging trends, and Hotelling  $T^2$  and cumulative probability of the residual variables to detect potential defective batch.

## 6. REFERENCES

Akima, H. 1970. A New Method of Interpolation and Smooth Curve Fitting Based on Local Procedures, *Journal of the Association for Computing Machinery* 17:589-602.

Cherry, G.A, and S.J. Qin 2006. Multiblock principal component analysis based on a combined index for semiconductor fault detection and diagnosis. *IEEE Transactions on Semiconductor Manufacturing* 19(2):159-171

Kaistha, N., C. F. Moore, and M.G. Leitaker. 2004. "A Statistical Process Control Framework for the Characterization of Variation in Batch Profiles," *Technometrics* 46:53-67

Nomikos, P., and J. F. MacGregor. 1995. Multivariate SPC Charts for Monitoring Batch Processes, *Technometrics* 37:41-59.

Spanos, C.J., and G.S. May. 2006. *Fundamentals of Semiconductor Manufacturing and Process Control* Wiley.

Smith, J.A., K.C. Lin, M. Richter, U. LevAmi. 2004. Practical, real-time multivariate FDC. *Semiconductor International* 27(13).

Spitzlsperger, G., C. Schmidt, G. Ernst, H. Strasser, and M. Speil. 2005. Fault detection for a via etch process using adaptive multivariate methods. *IEEE Transactions on Semiconductor Manufacturing* 18(4):528-33.

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