

Adaptive Multi-Way Principal Components Analysis Applied to Monitoring a Semiconductor Etch Process

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Introduction: Multi-way principal components analysis (MPCA) is finding utility in monitoring batch processes.[1] The steps included are data alignment (to account for differing batch lengths), data scaling, and construction of the MPCA model. In the present example, MPCA is applied to machine state measurements obtained during metal etch. (Wafer etch is analogous to batch processing in the chemical process industry.) In this case, the process mean drifts significantly between preventative maintenance cycles (PM) and slightly within a PM.[2] To account for this drift a moving window approach was used with the data mean reset at the beginning of each PM.

Experimental: The data set consists of 14 engineering variables from a LAM 9600 Metal Etcher processing 129 wafers over three PMs; 108 normal wafers and 21 wafers with intentionally induced faults (raw data available at www.eigenvector.com).[1,3,4] The PMs corresponded to three experiments, Numbered 29, 31 and 33, run several weeks apart. Data from different experiments have a different mean and slightly different covariance structure. Although faults were typically induced consecutively two to four at a time, in this simulation they were interspersed within the normal wafers with two or more normal wafers in between each fault. This arrangement was expected to simulate randomly occurring faults that might be expected in the process. The MPCA model was calibrated on a moving window of fourteen wafers and fault identification was based on the Q residual only. A warning was given at the 95% limit and a fault at 1.6 times the 95% limit. The model was not updated on fault wafers. For visualization, Q contributions were block scaled to the mean and standard deviation of residuals from the updated model.[5]

Results and Discussion: Data alignment is based on all fourteen variables (using the ALIGNMAT function) and the results are shown for the EndPt A variable (this is a broad band optical emission measurement) in Figs. 1 and 2. Alignment removes irrelevant variability that can reduce model sensitivity.

Figs. 3 and 4 show the difference between autoscaling and block scaling of the data. It is clear that block scaling (using the GSCALE function) retains relative variance within a single variable trajectory whereas autoscaling tends to inflate irrelevant variance that can desensitize the model.

Fig. 5 shows an RF fault identified in Experiment 33 and Fig. 6 shows the corresponding Q residual contributions (block scaled to the calibration model residuals – analogous to using standardized residuals). Patterns in contribution plots combined with process knowledge are useful for identifying the cause of a fault. For this simulation, the sensitivity (fraction of faults caught) was 0.76, and specificity (fraction of normal wafers not alarmed) was 0.99. This is consistent with results from previous studies.[1,3]



Figure 1: EndPt A for Experiment 29: not aligned.



Figure 2: EndPt A for Experiment 29: aligned.

Conclusions: MPCA and adaptive MPCA are useful process monitoring tools. Alignment of the process trajectory and block scaling were used to minimize



irrelevant variance in the process measurements. Block scaling of Q contributions also enhanced visualization of faults. Some faults are difficult to catch in any event, however the adaptive approach keeps the model local optimizing detection.[1]



Figure 3: EndPt A for Experiment 29: aligned and autoscaled.



Figure 4: EndPt A for Experiment 29: aligned and block scaled.

References:

[1] Wise, BM, Gallagher, NB, Butler, SW, White, D, and Barna, GG, "A Comparison of Principal Components Analysis, Multi-way Principal Components Analysis, Tri-linear Decomposition and Parallel Factor Analysis for Fault Detection in a Semiconductor Etch Process," *J. Chemometr.*, **13**, 379–396 (1999).

[2] Gallagher, NB, Wise, BM, Butler, SW, White, D, and Barna, GG, "Development and Benchmarking of Multivariate Statistical Process Control Tools for a Semiconductor Etch Process: Improving Robustness Through Model Updating", IFAC ADCHEM'97, Banff, Canada, 78–83, June (1997).





Figure 5: Q Residuals (top) and T^2 (bottom) normalized to their respective 95% limits for Wafers 81 to 106. Wafer 106 (RF Power-12 W) was indicated as a fault. Wafer 82 (TCP Power-20 W) and 101 (Cl-10sccm) were faults also.



Figure 6: Q Residual Contributions Wafer 106 (RF Power-12 W). Contributions are high on Endpt A and low on Pressure.'

[3] Wise, BM, Gallagher, NB, and Martin, EB, "Application of PARAFAC2 to Fault Detection and Diagnosis in Semiconductor Etch," *J. Chemometr.*, **15**(4), 285–298 (2001).

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[5] Warren, J, Gallagher, NB, "Heuristic and Statistical Methods for Fault Detection: Complementary or Competing Approaches?", SEMATECH AEC/APC Symposium XVIII, Westminster, CO, Sept. 30-Oct. 5 (2006).