Analysis of Interaction Structure Among Multiple Functional Process Variables for Process Control in Semiconductor Manufacturing

Xi Zhang and Qiang Huang

Abstract—Our previous work has shown that complex interaction patterns among functional process variables (FPVs) in semiconductor manufacturing processes can indicate process condition changes. We developed a nonlinear dynamics model to describe interactions among FPVs, which was further used to monitor process condition changes. However, the interaction structure among three or more FPVs has not been thoroughly investigated for the purpose of process control. In this work, we first extend our previously developed nonlinear dynamics model by considering the autocorrelation in each FPV. A generalized least square (GLS) method is applied to estimate the extended model. The interaction structure among FPVs is represented as a complex network in which the directionality and strength of interaction are discovered from the extended nonlinear dynamics model. To validate the proposed method, we first conduct simulation study using van del Pol oscillators. Then two sets of real experimental data from chemical mechanical planarization process are used to investigate the interaction structure change over a polishing cycle. The results show that the extracted patterns of interaction structure among FPVs aid to uncover the polishing mechanisms and provide more insights for condition monitoring and diagnosis.

Index Terms—Correlation pattern, interaction, multichannel signals, network, process monitoring.

I. INTRODUCTION

In semiconductor manufacturing many process factors are involved to affect product quality. As an example in chemical mechanical planarization (CMP), factors such as applied force, pad property, and slurry flow rate would jointly impact the quality of polished wafers. The interactions among process factors can be very complex. To understand the ways that process factors affect product quality, process variables such as coefficient of friction (COF) and polishing pad temperature are collected online to predict the realtime process conditions. If process variables are continuously observed and vary with time, these functional process variables (FPVs) may contain rich process information. For instance, COF between the wafer and the pad provides information regarding the tribological conditions at the interface. An abrupt and large variation in COF can be a realtime indication of pad failure, large particles on the pads, or underlying barrier layer exposure on the wafer. Highly correlated to COF, pad temperature is another important FPV that indicates heat variations generated through friction and chemical reaction. Previous studies have investigated FPVs both experimentally and analytically [1], [2]. Our experience suggested that certain process changes may not be easily detected without collectively studying these FPVs. Simultaneously analyzing these FPVs and their interaction patterns could bring additional insights into process condition changes and new opportunities for process improvement [3], [4].

In [3], [4] we have shown that the complex interaction patterns among FPVs in semiconductor manufacturing processes can indicate process condition changes. We developed a nonlinear dynamics model to describe interactions among FPVs, which was further used to monitor process condition changes. However, the interaction structure among three or more FPVs has not been thoroughly investigated for the purpose of process control. Below we briefly review related studies.

The common approaches of analyzing correlation or interaction over time are cross-correlogram and cross-spectrum methods [5]–[7]. They might be easily affected by artifacts and lead to improper detections, especially for the non-stationary signals collected in CMP process. Coherence and cross spectrum methods aim to analyze the correlation of paired signals in the frequency domain and are most commonly used with continuous signals [6], [8]. Phase synchronization was developed to detect timing-correlation in phase domain while discarding the effect of the amplitude of signals [8]–[10]. Similar to the correlation coefficient in the time domain, coherence, entropy, or mutual information indices in phase domain have been proposed to detect synchrony in paired signals [11]–[13]. A nonlinear dynamics model was further developed in [14] to study phase synchronization:

\[
\begin{align*}
\frac{d\phi_1}{dt} &= \omega_1 + q_1(\phi_1) + f_1(\phi_1, \phi_2) + \varepsilon_1(t) \\
\frac{d\phi_2}{dt} &= \omega_2 + q_2(\phi_2) + f_2(\phi_2, \phi_1) + \varepsilon_2(t)
\end{align*}
\]

(1)

where \(\phi_{1,2}\) are the phases of two coupling variables, \(\omega_{1,2}\) are the base angular frequencies or natural frequencies, and \(\varepsilon_{1,2}\) are the noisy perturbations. \(f_{1,2}\) are defined as functions which involve interactions between coupling variables, and \(q_{1,2}\) are self-provoked functions. This model can be easily extended to the case with more than two coupling variables.
The major challenge, however, is to find interaction functions $f_{1,2}$ in (1) with adequate orders after Fourier transformation. To improve the model, we defined main effects and interaction effects of FPVs in [3] and further demonstrated it in process monitoring. However, the temporal patterns, especially the often strong autocorrelation in FPVs were not considered therein. This could lead to inadequate phase dynamics models and provide an incomplete picture of spatio-temporal patterns in FPVs. Furthermore, the complex interaction structure among three or more FPVs has not been thoroughly investigated. As shown in Fig. 1, the general correlation analysis can not reveal the directionality and strength of interaction, and the network structure among multiple FPVs. Our case study later will show that analyzing interaction structures can provide more insights into the polishing mechanisms.

Rosenblum et al. [15] first investigated interaction structure based on mutual prediction. In their study the canonical structure (three oscillators in a ring) was identified through pairwise analysis of coupled oscillators. More complex structures were investigated using partial directed coherence method [16]. All these methods examined the directionality of two-way interactions to identify interaction structures. Three-way or high order interactions have not been considered. Moreover, variables in the interacting network are assumed to be known, and hence hidden influential variables can be missed. Therefore, a new method that can distinguish different orders of interaction is preferable so as to identify more complex interacting mechanisms.

In Section II we first extend our previously developed nonlinear dynamics model by considering the autocorrelation in each FPV. A generalized least square (GLS) method is used to estimate the extended model. The interaction structure among FPVs is represented as a complex network in which the directionality and strength of interaction are discovered from the extended nonlinear dynamics model. We demonstrate the interaction analysis approach through a simulation of van der Pol oscillators. In Section III, two sets of real experimental data from chemical mechanical planarization process are used to investigate the interaction structure change over a polishing cycle. Conclusion is given in Section IV.
As can be seen, although the fitted model (dash line) could capture the main trend of the original instantaneous frequency (bold line), the residuals show a strong autocorrelation. Overlooking the potential autocorrelation can lead to $Q_{k}(\cdot)$ with many sine and cosine terms which is hard to find physical interpretation. Therefore, we extend the model (2) by imposing a structure on residuals,

$$\text{Cov}[\varepsilon_k(t), \varepsilon_k(t+1)] = \sigma^2 \rho_l, \text{ time lag } l = 0, 1, 2, \ldots \quad (4)$$

Compared with the previous model based on the assumption of noise independence, the noise term in the new model permits an autocorreled structure, i.e., error terms at time $t$ and $t + l$ have correlation coefficients $\rho_l$. For example, the error $\varepsilon_1$ of the COF may follow a first-order autoregressive model (AR(1) model), $\varepsilon_1(t) = \eta \varepsilon_1(t-1) + \nu_1(t)$, where $\nu_1(t)$ is the white noise, $\nu_1(t) \sim N(0, \sigma^2)$. Then the coefficient $\rho_l = \eta^l$ and Cov[$\varepsilon_1(t), \varepsilon_k(t+l)$] = $\sigma^2 \eta = \sigma^2 \eta/(1-\eta^2)$. The first order derivatives of phase variables will serve as response variables, while cosine and sine functions in the Fourier expansion of $Q_k(\cdot)$’s will be predictors. The model coefficients $\omega_j, a_{m_1m_2m_3m_4}, b_{m_1m_2m_3m_4}$, and $\rho_l$ can be estimated using the Generalized Least Squares (GLS) method [17].

### B. Interaction Structure Analysis

The proposed interaction structure analysis approach is outlined in Fig. 3. Since the complexity of interaction analysis increases exponentially with the number of FPVs, we use a network involving three nodes as an example to demonstrate the procedure. With the extended phase dynamics model we will first identify the strength of interactions. As defined in [3], the main effects include $\cos(\varphi_1(t))$, $\cos(\varphi_2(t))$, $\cos(\varphi_3(t))$, $\sin(\varphi_1(t))$, $\sin(\varphi_2(t))$, and $\sin(\varphi_3(t))$. The two-way interaction effects or the first order interactions include $\cos(\varphi_1(t) + \varphi_2(t))$, $\cos(\varphi_1(t) + \varphi_3(t))$, etc. The three-way interaction effects or the second order interactions contain $\cos(\varphi_1(t) + \varphi_2(t) + \varphi_3(t))$, etc. The term $\sqrt{(a_{k,m_1m_2m_3}^2 + (b_{k,m_1m_2m_3}^2)}$ represents the amplitude in signal processing and $[(a_{k,m_1m_2m_3}^2 + (b_{k,m_1m_2m_3}^2)]^2$ is related to the power of that frequency component. The strength of each frequency component in a main effect or an interaction effect can be thus defined using the concept of the power, e.g., $[(a_{k,m_1m_2m_3}^2 + (b_{k,m_1m_2m_3}^2)]^2$. The strength of the main effects/interaction effects is defined as the summation of the power of every frequency component in all the main/interaction effects, e.g., $\sum_{m_1m_2m_3m_4}[(a_{k,m_1m_2m_3}^2 + (b_{k,m_1m_2m_3}^2)]^2$. Then we can construct a bar chart for each FPV which shows the strength of main effect and interaction effects (see an example in Fig. 9).

From the bar charts we will investigate interaction patterns. We analyze four important cases of interaction structures:

- **Self-oscillated FPV** As illustrated in Fig. 4, if main effect of a FPV is dominant and all of the two-way and high order interaction effects are insignificant, the FPV does not interact with others.

- **Clockwise interaction pattern** In this case, each FPV is affected by the other in clockwise manner (Fig. 5). From the bar chart, both interaction effects are significant, but one
is stronger than the other. Meanwhile, the main effect and three-way or high order interaction are relatively weak.

- **Symmetric interactions among FPVs** If strengths of all two-way interactions are similar and higher order interactions are insignificant, we may encounter symmetric interaction structure (Fig. 6).

- **Hidden FPVs in a network** If only one three-way interaction effect is significant, we may suspect that at least one hidden variable exists in the network. As shown in Fig. 7, the bar chart displays interaction strength for node 2. If three-way interaction effects are weak in all the other FPVs, a hidden FPV might interact the network through node 2. Similar idea for identifying hidden variables could be found in [18].

The last issue is to determine the directionality of an interaction. If the strength of two-way interaction in node \( j \) is stronger than that of the corresponding two-way interaction in node \( i \), then node \( j \) has stronger influence on node \( i \).

To validate the proposed approach for analyzing interaction structures, four-channel van der Pol oscillator system is simulated using Matlab [19] as (5), found at the bottom of the page, where \( x_{1,2,3,4} \)'s are four FPVs, \( u \) is the nonlinear self-weight parameter, \( \omega_{1,2,3,4} \)'s are linear self-weight parameter; \( \lambda_{i\rightarrow j} \)'s are weights from coupled variables, and \( \xi_{1,2,3,4} \) are white noises with normal distributions.

Three canonical types of interaction structures are generated by varying parameter values (Table I). The figures on the right column depict interaction structures under variant dynamical systems. Nodes 1, 2, 3, and 4 represent simulated FPVs, and arrows between nodes represent directed interactions determined by those parameters. Since some important process variables might be missed in a real dynamical system or process, we choose node 4 as hidden variable to be discovered by the proposed approach. The nonlinear parameter \( u \) is fixed to 3 for high nonlinear feature in dynamical systems. To avoid one FPV being modulated by another, small values were given to \( \lambda_{i\rightarrow j} \) and \( \omega_i \).

\[
\begin{align*}
\frac{dx_1}{dt} &= u \left( 1 - \frac{x_1^2}{3} \right) \frac{dx_1}{dt} - \omega_1^2 x_1 + \lambda_1 \cdot \left( x_2 - x_1 \right) + \lambda_1 \cdot \left( x_3 - x_1 \right) + \lambda_1 \cdot \left( x_4 - x_1 \right) + \xi_1 \\
\frac{dx_2}{dt} &= u \left( 1 - \frac{x_2^2}{3} \right) \frac{dx_2}{dt} - \omega_2^2 x_2 + \lambda_2 \cdot \left( x_3 - x_2 \right) + \lambda_2 \cdot \left( x_4 - x_2 \right) + \lambda_2 \cdot \left( x_1 - x_2 \right) + \xi_2 \\
\frac{dx_3}{dt} &= u \left( 1 - \frac{x_3^2}{3} \right) \frac{dx_3}{dt} - \omega_3^2 x_3 + \lambda_3 \cdot \left( x_4 - x_3 \right) + \lambda_3 \cdot \left( x_1 - x_3 \right) + \lambda_3 \cdot \left( x_2 - x_3 \right) + \xi_3 \\
\frac{dx_4}{dt} &= u \left( 1 - \frac{x_4^2}{3} \right) \frac{dx_4}{dt} - \omega_4^2 x_4 + \lambda_4 \cdot \left( x_1 - x_4 \right) + \lambda_4 \cdot \left( x_2 - x_4 \right) + \lambda_4 \cdot \left( x_3 - x_4 \right) + \xi_4
\end{align*}
\]
TABLE I
INTERACTION STRUCTURE TYPES AND CORRESPONDING PARAMETERS

<table>
<thead>
<tr>
<th>Type A</th>
<th>$\lambda_{1-2} = 0.5$</th>
<th>$\lambda_{2-3} = 0.5$</th>
<th>$\lambda_{2-4} = 0$</th>
<th>$\lambda_{2-5} = 0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\omega_1 = 0.5$</td>
<td>$\lambda_{3-4} = 0.5$</td>
<td>$\lambda_{3-5} = 0$</td>
<td>$\lambda_{4-5} = 0$</td>
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<tr>
<td>$\omega_2 = 0.5$</td>
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<td>$\lambda_{4-5} = 0$</td>
<td>$\lambda_{5-5} = 0$</td>
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<tr>
<td>$\omega_3 = 0.5$</td>
<td>$\lambda_{1-4} = 0$</td>
<td>$\lambda_{1-4} = 0$</td>
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</tr>
<tr>
<td>$\omega_4 = 0.5$</td>
<td>$\lambda_{1-3} = 0.5$</td>
<td>$\lambda_{4-3} = 0$</td>
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<thead>
<tr>
<th>Type B</th>
<th>$\lambda_{1-2} = 0.5$</th>
<th>$\lambda_{2-3} = 0.5$</th>
<th>$\lambda_{2-4} = 0$</th>
<th>$\lambda_{2-5} = 0$</th>
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<tbody>
<tr>
<td>$\omega_1 = 0.5$</td>
<td>$\lambda_{3-4} = 0$</td>
<td>$\lambda_{3-5} = 0$</td>
<td>$\lambda_{4-5} = 0$</td>
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<tr>
<td>$\omega_2 = 0.5$</td>
<td>$\lambda_{4-5} = 0$</td>
<td>$\lambda_{4-5} = 0$</td>
<td>$\lambda_{5-5} = 0$</td>
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<tr>
<td>$\omega_3 = 0.5$</td>
<td>$\lambda_{1-4} = 0$</td>
<td>$\lambda_{1-4} = 0$</td>
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<tr>
<td>$\omega_4 = 0.5$</td>
<td>$\lambda_{1-3} = 0.5$</td>
<td>$\lambda_{4-3} = 0$</td>
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<tr>
<th>Type C</th>
<th>$\lambda_{1-2} = 0.5$</th>
<th>$\lambda_{2-3} = 0.5$</th>
<th>$\lambda_{2-4} = 0$</th>
<th>$\lambda_{2-5} = 0$</th>
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<tr>
<td>$\omega_1 = 0.5$</td>
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<td>$\lambda_{3-5} = 0$</td>
<td>$\lambda_{4-5} = 0$</td>
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<tr>
<td>$\omega_2 = 0.5$</td>
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<td>$\lambda_{4-5} = 0$</td>
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<tr>
<td>$\omega_3 = 0.5$</td>
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<tr>
<td>$\omega_4 = 0.5$</td>
<td>$\lambda_{1-3} = 0.5$</td>
<td>$\lambda_{4-3} = 0$</td>
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Five percent Gaussian white noise of original signal in decibel was added to each channel.

1500 data points were sampled for each FPV. The initial 200 points of data were cut off from original data series to avoid instability caused by initial values. Fig. 8 displays the simulated signals from each node in type A structure. Since the interaction relationship could not be distinguished via visual study, the proposed nonlinear dynamics models are applied to unveil the interaction mechanism.

According to the principles for modeling fitting discussed in Section II-A, low order of Fourier expansion is preferred. Stepwise regression was applied to screen out those insignificant terms in the phase dynamics model. Terms with very low strengths of main effects or interactions effect were also dropped off. The order of Fourier expansion was finally set to 2 with p-value being 0.05 in model selection. By computing the strength of main effects and interaction effects for each node, we obtain bar charts shown in Fig. 9.

Fig. 8. Four-channel simulated signals via van der Pol oscillators.
It can be seen clearly in the first row of Fig. 9 that both interaction effects are significant, but one is stronger than the other in each node. For instance, in node 2, the two-way interactions $2 \leftrightarrow 3$ and $2 \leftrightarrow 1$ are both significant, but $2 \leftrightarrow 3$ is more dominant. The pattern repeats at each node which suggests clockwise interaction structure (nodes in a ring pattern) in type A nonlinear system. Two-way interaction $2 \leftrightarrow 1$ in node 2 actually represents an indirect influence between nodes 1 and 2.

In the second row of the charts, the two-way interactions $1 \leftrightarrow 2$ (node 1), $2 \leftrightarrow 3$ and $2 \leftrightarrow 1$ (node 2), and $3 \leftrightarrow 1$, $3 \leftrightarrow 2$ (node 3) are significant. This indicates the structure of type B in Table I.

The third row is similar to the first row except that the three-way interaction $2 \leftrightarrow (1,3)$ in node 2 appears significant. Since all the two-way interactions suggest a ring pattern, the unexpected three-way interaction $2 \leftrightarrow (1,3)$ may be due to a hidden variable (node 4) which influences the network through node 2.

Remark: As clearly shown in the simulation study, our method determines the directionality of interaction via the definition of strength. Furthermore, we consider three-way or higher order interactions which assists to understand complex structure. The mutual prediction algorithm [15] constructs an index with value from $-1$ to 1 using two oscillators each time. Depending on the sign of the index, the directionality of each oscillator are able to be obtained for structures like Type A. Since high order interactions are not modeled, complex structures with hidden factors are hard to be determined by that method.

III. APPLICATION TO IDENTIFICATION OF INTERACTION STRUCTURE PATTERNS IN REAL CMP PROCESS

Understanding the interaction structures has important implication in semiconductor manufacturing process control. Specifically the discovered interaction patterns among process variables over time assist to understand the underlying physical mechanisms. In this section we will demonstrate this point in CMP process. Two CMP process conditions are investigated: diamond conditioners with abrasive size 8 $\mu$m and 100 $\mu$m were chosen to condition the polishing pads, respectively.

The whole polishing process was conducted on a bench-top CMP tester (model CP-4) manufactured by CETR Inc. The 6-inch diameter IC 1000-A4 perforated polishing pad (manufactured by Rodel, Inc.) was attached on the rotating bottom platen of the CMP tester. The 2-inch copper wafer coupon was attached to the upper polishing head. Cabot 5003 copper polishing slurry was mixed with 2.5% hydrogen peroxide. The slurry was fed into the center of the pad at the rate of 50 mL/min. The pressure were set to 2 psi both on conditioning and polishing process, and polishing head rotating speed was 150 rpm.

Three replicates under each pad condition were produced and each run lasted 3 min. During each polishing process, three FPVs were collected simultaneously at sampling frequency 20 Hz. The COF was obtained by gathering shear and normal forces with sensors installed on the polishing head, while the acoustic emission (AE) signal was collected through AE sensor on the back of wafer holder. A FLIR infrared thermal camera was used to collect thermal data. The focused thermal zone was selected on the polishing pad adjacent to the wafer-pad interface to record the average temperature. Since the temperature in this interface between wafer and polishing pad cannot be obtained directly, the selected zone is the best approximation of the average process temperature [20]. These three process variables are good indicators of chemical-mechanical polishing conditions [21], [22]. Fig. 10 shows one sample of the original signals collected under each process condition. Directly observing original signals provides limited information.

Since the main trend of each FPV would not be dramatically altered by interactions, we first remove the trend from collected data through cubic-spline smoothing method. Fig. 11 displays the one sample of temperature data before and after detrending.

To understand the dynamics of interaction mechanisms during the whole polishing process, we monitor the process via sliding windows. When determining window size and length of overlapping period, we intend to (1) maintain a smooth transition between adjacent windows based on the belief that there is no sharp change of polishing mechanism in a short period; and (2) avoid large window size for potential miss-detection of changes. We start first with large window size to test the polishing condition, and reduce the window size until difference is apparent between two windows. Finally, our sliding window size is determined to be 25 s (500 data points). We update the sliding window every 5 s (100 data points) for good computing efficiency without losing any information of condition change. The overlapping period is 400 points to have smooth transition between adjacent windows. In each window, the dynamics model was fitted by GLS, and the model adequacy was checked. Fig. 12 shows one sample of the instantaneous frequency extracted from original data versus fitted one in single window, and the residuals are also plotted to check the adequacy of autoregressive terms. It is found that model order $n = 2$ and autoregressive order $l = 5$ provide adequate prediction.
Strength of main effects, two-way and three-way interaction effects is computed in each window. The interaction structures and their changes are able to be deduced by analyzing the bar charts. Fig. 13 shows structure changes under polishing condition using 100 \( \mu \)m diamond particle size of conditioner.

As can be seen, the two-way interactions AE—temperature and COF—temperature are significant at the beginning, and they decreased gradually over time. Meanwhile, the strength of two-way interactions AE—COF and temperature—COF increased. Other interaction effects seemed not significant enough to affect interaction structures. The dynamics of interaction change were represented by network structure change in Fig. 13. The solid line with arrow represents significant affects, and dash line with arrow represents weak effects in term of strength. From the network, we could see temperature had greater impact on AE and COF initially, and COF influenced AE and temperature more afterwards. It is known that temperature on pad reflects the heat generated by friction and chemical reaction, AE is related to the material deformation, and COF is determined by the interface properties [21], [22]. We therefore interpret the network structure change as follows. The chemical reaction was dominant at the beginning and temperature on the polishing pad was mainly due to heat released from wafer surface softening and weakening caused by slurry. Afterwards, the mechanical friction played a bigger role because of the non-uniformity on the wafer surface in our polishing process.

Fig. 14 shows the analysis of polishing condition using 8 \( \mu \)m diamond particle size of conditioner. Compared with Fig. 13, strength of interaction effects is relatively mild. Initially only the two-way interaction COF—temperature was significant. This interaction also faded as the polishing process continued. The two-way interaction AE—COF appears relative strong compared to other interaction effects during the later period of
the polishing process. This pattern might be interpreted as that the smaller diamond particle size will generate smoother the polishing pad. This will lead to a weaker mechanical reaction relative to its chemical reaction.

IV. CONCLUSION

This paper developed a methodology to analyze the dynamic interaction structures among multiple functional process variables (FPVs). The analysis started with a phase dynamics model extended from our previous work by considering the temporal patterns in FPVs. By analyzing two-way and higher order interactions and their strength, directionality and interaction structures can be deduced from bar charts. The ability to model high order interaction among three or more variables is one unique feature of the proposed method, which enable us to analyze complex structures.

The method was validated using four-channel van del Pol oscillators. Four important cases of interaction structures were analyzed. The analysis can be extended to network with five more FPVs. To demonstrate the importance of understanding interaction structures in semiconductor manufacturing, we investigated two polishing conditions. The results show that uncovering the interaction patterns among process variables over time brings new insights into the underlying physical mechanisms. These
Fig. 14. Interaction structure analysis: 8 μm diamond particle size of conditioner.

results also provide a new perspective for process monitoring and diagnosis.

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REFERENCES


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