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Increasing detectability in semiconductor foundry by multivariate statistical process control

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Quality has become a key determinant of success in all aspects of modern industries. It is especially prominent in the semiconductor industry. This paper reviews the contributions of statistical analysis and methods to modern quality control and improvement. The two main areas are statistical process control (SPC) and experimentation. The statistical approach is placed in the context of recent developments in quality management, with particular reference to the total quality movement.

In SPC, Hotelling T^2 has been applied in laboratories with good result; however, it is rarely used in mass production, especially in the semiconductor industry. An advance process control (APC) of R&D study, involving Hotelling T^2 and principal component analysis (PCA), is performed on a high density plasma chemical vapour deposition (HDP CVD) equipment in the 12-inch wafer fab. The design of experiment (DOE) of gas flow and RF power effects is used to work the feasibility of PCA for SPC and examine the correlation among tool parameters. In this work, the Hotelling T^2 model is shown to be sensitive to variations as small as $(+/-)5\%$ in the tool parameters. Compared with classical PDCA and qualitative analysis, applying statistical in process control is more effective and indeed necessary. This model also is especially suitable to the semiconductor industry.

Keywords: statistical process control (SPC); advance process control (APC); fault detection and classification (FDC); Hotelling T^2 ; principal component analysis (PCA); semiconductor industry

Introduction

Statistical process control (SPC) is a tool of fault detection and classification (FDC) in advance process control (APC). SPC is an integral part of maintaining and improving quality. Failure to implement and operate SPC effectively can significantly impede a company's ability to meet product specifications, limit waste, reduce production costs and generally improve quality (Goetsch & Davis, 1994). In the semiconductor industry, process monitoring and continuing controls are used to reduce waste rate and product cost.

A lot of quality researchers have considered qualitative analysis, such as PDCA, variety of charts (Franceschini, 2002; Mukhopadhyay, 2001; Rahim & Ben-Daya, 2001; Tagaras & Nikolaidis, 2002);

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few used multivariate analyses. Qualitative analysis, however, cannot be elaborated to explain all the variations. It is especially true in the semiconductor chemical vapour deposition (CVD) process, where there are various chemical deposition reactions in the process. SPC is a statistical technique used to monitor and further control processes to reduce production variation. Variation reduction is a key aspect to improve quality. Although SPC was relatively complex and difficult for the majority of employees, clearly SPC is as important as it is difficult.

High-density plasma CVD (HDP CVD) is a high-density mixture of gases at low pressure, which is directed toward the surface of a wafer in the reaction chamber. Multivariate analyses have been extensively applied in process control in manufacturing (Kesavan & Lee, 2001; Dunia & Qin, 1998; Wang et al., 2002). In the operation and control of chemical processes, principal component analysis (PCA) has been applied for measured data, monitoring multivariate processes, understanding processes, reconstructing and identifying faults and so on (Kresta et al., 1991; Kongsanovich et al., 1996; Dunia & Qin, 1998). However, PCA is rarely used on real mass production lines, especially in the semiconductor industry, even though it has been employed in laboratories with good results. Thus, multivariate SPC was scarcely investigated by these relating studies. This paper discusses multivariate analysis of SPC applied in the HDP CVD process in an integrated circuit (IC) Foundry.

Statistical process control

The popularity of TQM and its related practices, such as statistical process control (SPC), quality circles, benchmarking and business process re-engineering, and ISO 9000 certification are always adopted in industries (Terziovski et al., 1999). SPC is the most potentially effective quality tool (Cheng & Dawson, 1998; Harris & Yit, 1994), through the development of diagnostic and problem-solving skills. In manufacturing processes and company management, SPC is an increasingly popular statistical technique used to control processes and to reduce variation.

Quality is therefore an important aspect for any company to maintain competitiveness. Wang & Eldon (2003) pointed out that SPC is a measurement procedure or instrument that is adequate for monitoring the performance of a process. The classical control chart method is widely used and calculated in process control (Lewis, 1993; MacCarthy & Wasusri, 2001; Wang & Eldon, 2003); however, this approach only provides the point estimates on the variance components of the measurement error study (Wang & Eldon, 2003). SPC is effective in process of control; Tagaras (1994) supported that SPC activities can contribute to modelling and cost minimisation. Many processes must be monitored by using observations that are correlated, and SPC is able to provide an attractive solution for the performance monitoring. Modarress et al. (2000) applied SPC as a means to predict uncertainties in production demand in the short run. Mandal (2004) also supported that large businesses today maintain large databases for controlling and improving their business process, and therefore for addressing the data quality problems that may be faced in implementation of SPC. SPC was applied to reduced the moisture content percentage (MC%) in tobacco (Mukhiopadhyay, 2001). As the relevant studies show above, multivariate analysis is a comprehensive fullness tool for data mining.

Dale et al. (1990) conducted a study involving the use of SPC by part/component suppliers in the automotive-related industry, but 77% of 158 respondents had experienced difficulties in introducing SPC. In addition, 82% of the respondents indicated that they had encountered difficulties with its applications and development. Multivariate analysis is hard to master, and rarely is it utilised in mass production. Our study, therefore, is to hold an experiment to perform multivariate analysis of SPC in the CVD process.

High-density plasma CVD and shallow trench process

A recent development in plasma-assisted CVD is high-density plasma CVD (HDP CVD). This method of deposition became extensively accepted in advanced wafer fabrications in the mid-1990s. As its name suggests, the plasma in HDP CVD is a high-density mixture of gases at low pressure, which is directed toward the surface of the wafer in the reaction chamber. The main advantage of HDP CVD is that it can deposit films to fill gaps with high aspect ratios over a range of deposition temperatures of 300 to 400°C. HDP CVD was initially developed for interlayer dielectric (ILD) applications, but is also being employed for deposition in ILD-1, shallow trench isolation, etch-stop layers, and the deposition of low- κ dielectrics.

The HDP CVD reaction involves a chemical reaction between two or more gas precursors. In the deposition of oxide ILD, oxygen (or ozone) is frequently used with a silicon-containing gas, such as silane (SiH₄) or Tetraethoxy silane (TEOS), along with argon. A source excites the gas mixture with radiation frequency (RF) or microwave power (2.45 GHz) and directs the plasma ions into a dense region above the wafer surface to generate the high-density plasma.

For a long time, local oxidation of Si (LOCOS) was the standard technology for providing electrically isolating active devices in integrated circuits (IC). As the demands for smaller geometry and higher circuit density increases, even more stringent requirements are being placed upon the isolation performance, and problems with LOCOS are beginning to surface. To overcome these limitations, IC manufacturers have actively pursued an alternative process called shallow trench isolation (STI) as a substitute to LOCOS for isolating devices (Fazan & Mathews, 1993). STI allows for higher chip density and so increases the efficiency of use of Si wafers. A typical STI process involves etching a trench pattern through a nitride layer, through a thin pad oxide layer and into the silicon. Subsequently, a chemical vapour deposited (CVD) oxide is laid over the entire wafer, filling the trench area and overlying the nitride-protective active region. Chemical mechanical polishing (CMP) is then used to planarise the topography obtained by the preceding deposition processes, stopping on the nitride layer. The remaining nitride is subsequently removed by wet chemistry or reactive ion etching (RIE).

The STI CVD process is more complex than the general production process. Hence, SPC of univariate analysis is inadequate within the various parameters.

Principal component analysis and Hotelling T²

Principal component analysis (PCA) is one of the most popular statistical methods for extracting information from measured data in the operation and control of chemical processes design of experiment (DoE).

If the tool parameters as a function of time are considered as a data matrix X , then this data matrix can be modelled using PCA as

$$X = 1 \times \bar{X} + T \times P' + E$$

where \bar{X} is the average matrix; T is the score matrix, P' is the loading matrix, and E is the residual matrix.

The principal component scores (t_1, t_2, t_3, \dots) are columns of the score matrix T . The residual matrix E can be used to calculate the distance to the model in X space (DMod X). The residual standard deviation (RSD) of an observation in X space is proportional to the observed distance to the hyperplane of the PC model in X space. The observed distances to the PC model in X space

(DModX) are presented as linear plots. A DModX that exceeds the critical DModX reveals that the observation may be an outlier in X space. Normally, such distances are determined after all components have been extracted.

The distance to the model (DModX) of an observation in a worksheet which is part of the model is

$$s_i = \sqrt{\frac{\sum e_{ik}^2}{(K - A)}} \times v$$

where v is a correction factor (which is a function of the number of observations and the number of components), and slightly exceeds unity. This correction factor takes into account the fact that the DModX is expected to be slightly smaller than the actual value for an observation in part of the training set because it has affected the model.

The normalized distance to the model is the observed absolute DModX divided by the pooled RSD of the model s_0

$$s_0 = \sqrt{\frac{\sum \sum e_{ij}^2}{(N - A - A_0) \times (K - A)}}$$

where $A_0 = 1$ if the model is centred at zero; otherwise $(s_i/s_0)^2$ has an approximate F distribution from which the probability of membership to the model can be determined.

The distance to the model in X space (row RSD), after A components (the selected dimension), for the observations is used to fit the model. If you select component 0, which is the standard deviation of the observations with scaling and centering as specified in the worksheet (without row means subtracted), it is the distance to the origin of the scaled coordinate system.

In complex tool state monitoring, the Hotelling T^2 control chart is employed as a tool for detecting and classifying faults. It summarises all the process variables and all the model dimensions, indicating how far from the centre (target) the process are along the principal component model hyperplane.

The Hotelling T^2 for observation i , based on A components is,

$$T_i^2 = \sum_{a=1}^A \frac{t_a^2}{s_{t_a}^2}$$

where $s_{t_a}^2$ is the variance of t_a according to the class model

$$T_i^2 \times N(N - A)/A(N^2 - 1) \sim F_\alpha(A, N - A)$$

where N is the number of observations in the model training set, and A is the number of components in the model or the selected number of components.

Therefore, if

$$T_i^2 > A(N^2 - 1)/N(N - A) \times F_\alpha(p = 0.05)$$

then observation i lies outside the 95% confidence region of the model.

The confidence region of a two-dimensional score plot of dimension a and b is an ellipse with axis

$$\left[s_{t_a \text{ or } t_b}^2 \times F_\alpha(2, N - 2) \times 2(N^2 - 1)/N(N - 2) \right]^{1/2}$$

At zero significance level, the confidence region becomes infinite and is not shown on the plot.

Traditionally, FDC is regarded as a two-step process in manufacturing. Recently, Goodlin et al. (2002) proposed a simultaneous fault detection and classification technique that utilises the fault vector approach to minimise the time to find, classify and correct the faults. The method reveals that different faults occur with different vector units in the space, and so provides a means of concurrently detecting and classifying faults.

This work examines an approach to simultaneous FDC that involves the PCA method, Hotelling T^2 and the DModX control chart to detect the designed faults of gas flow and RF parameters and classify the faults using PCA vector space on HDP CVD equipment.

Experiment

This study is dedicated to the shallow trench isolation (STI) CVD process, performed on the commercially available Applied Material 300 mm HDP CVD tool. The purpose of this process is to deposit a USG stack using high-density SiH₄/Ar plasma. The STI CVD process is composed of a series of 17 steps. The first three steps stabilise the wafer load and pressure stabilisation. Step 4 is a brief plasma ignition step. Steps 5 to 8 cause the gas to flow and heat the chamber. Steps 9 to 11 are the main steps for depositing the STI layer. Steps 12 to 17 shut off the gases, cool the chamber, shut off RF and unload the wafer. The process chemistry is identical from Step 9 to Step 11. However, this experiment only focuses on the main deposition steps, which are key to the entire process; all the analysed data are based on these steps (Steps 9 to 11).

A data collection module was installed in an HDP CVD tool to collect real-time tool state variable parameters (SVIDs) during the processing of the wafer. Forty-five parameters were used in the collection plan and the sampling rate of the collection was set to 1 Hz. Ninety-six golden wafers data were identified to build up the distinguished model. Twenty-five wafers (No. 51 ~ 75) were designed to study the effects of gas flow and RF power variation during the main deposition step, and we set the variance range within $\pm 5\%$. Table 1 lists the information on the controlled wafers.

Results and discussion

Figure 1 plots the PCA scores of the first two principal components (t_1 , t_2) of the sample wafers. The figure shows that O₂(side), SiH₄(side) and He(top) DoE wafers are the strong outliers, at a 95% confidence level, indicating that the three gas flow parameters may have stronger

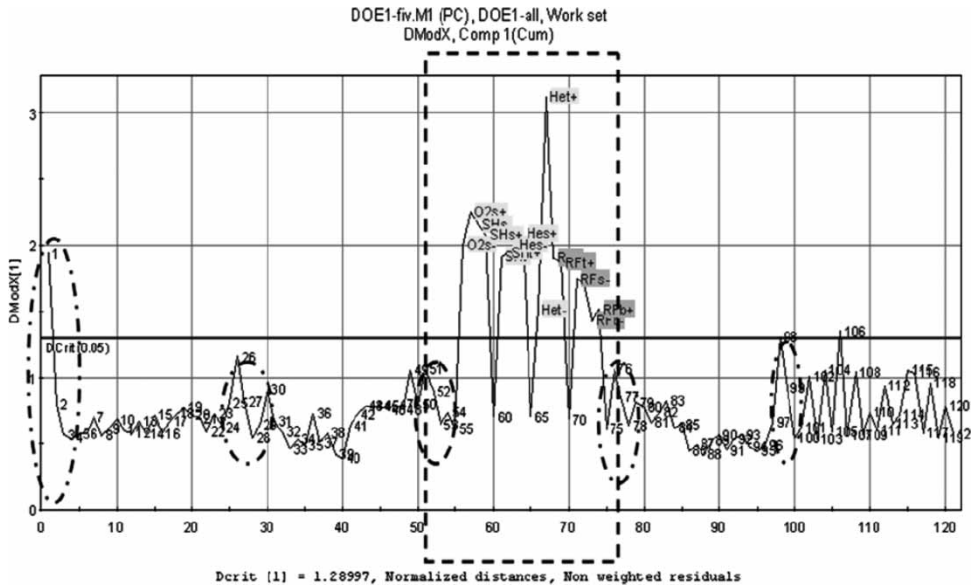


Figure 2. The plot of PCA distance to model versus sample wafer number.

reveals that the He(top) and SiH₄(side) DoE wafers are also found in the DModX vacuum subgroup system, indicating that He(top) and SiH₄(side) might affect the integrity of the vacuum. The reason requires further investigation. The first wafer effect is significant in the thermal subgroup system, as depicted in Figure 3d, indicating that the first wafer effect follows primarily from the thermal variation, as clearly indicated by the chamber dome heater temperature as a function of the sample wafer (Figure 4). The dome heater shows a period of fluctuation during every first wafer processing.

The fault classification method is based on the fault space vector technique. In the multivariate tool-variable parameter space, the basis for the use of the fault-specific space vectors is the notion that different classes of faults are typically associated with unique directions (paths) away from the normal condition. The deviation from the normal process is thus expected to fall on a straight line as the number of faults as a particular class is increasing. Such faults can then be linear combinations of tool-variable parameters.

The DoE faults are projected onto the three-component PCA space. Each fault is represented by a unique space vector (Figure 5).

In this study, using multivariate analyses, some phenomena became more apparent. First, the SiH₄(side) and He(top) gas flow seem to affect the stability of the vacuum. The reason must be investigated further. Second, the variations of O₂(side) and SiH₄(side) gas flow disturb the RF power and affect the chamber impedance condition. The RF system subgroup DModX results indicate that O₂(side) and SiH₄(side) gas flow are highly significant compared with other parameters. This is because the variations of O₂(side) and SiH₄(side) dominate the plasma quality in the oxide deposition process. Third, the fault space vector method approach can be used for classifying faults. Eigenvectors can be used to classify each fault according to a specific space vector, which can be treated as an index of fault classification, enabling the root causes of process fluctuation to be traced.

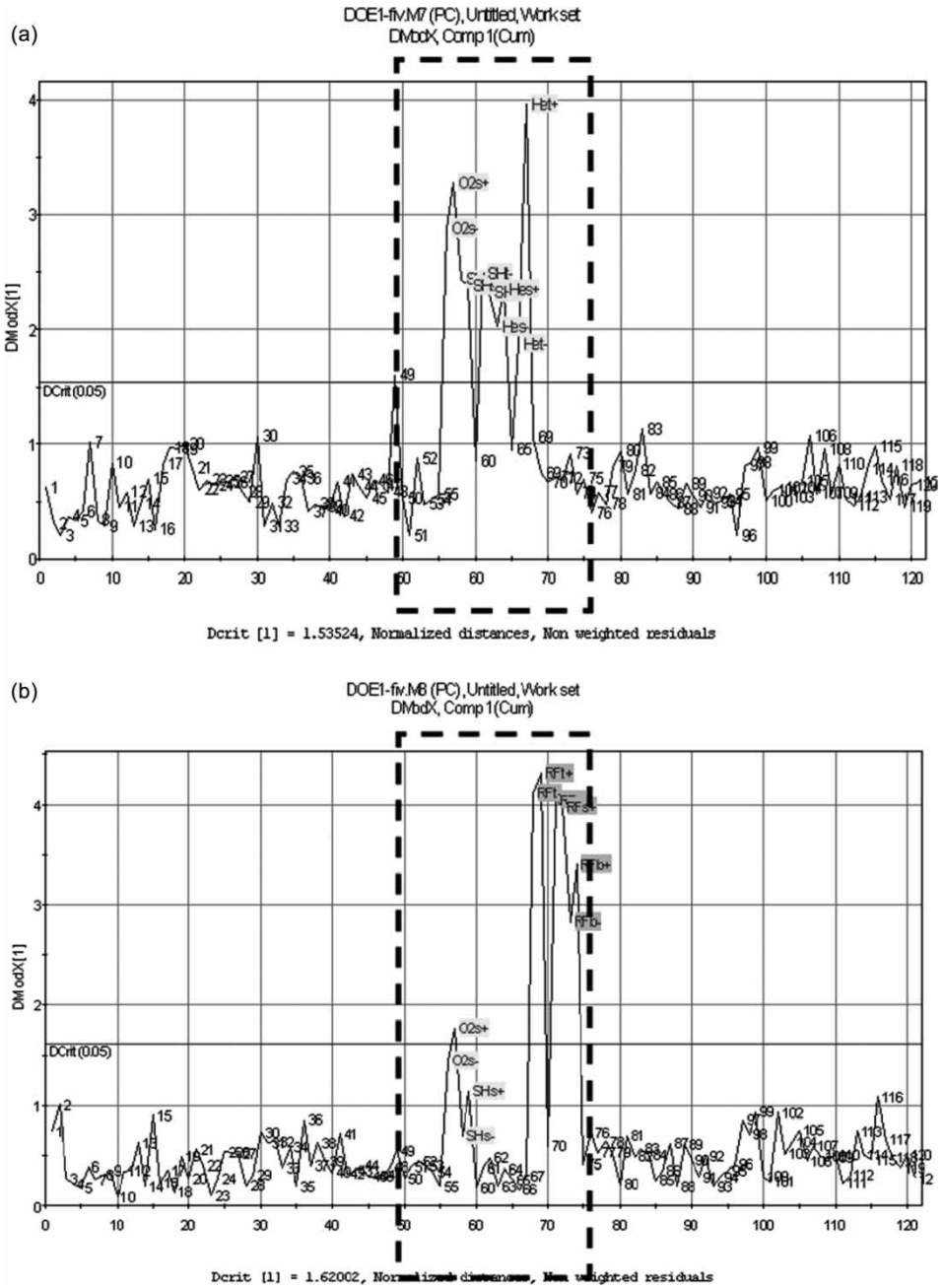


Figure 3. PCA distance to model analysis by delivery (3a), RF (3b), vacuum (3c) and thermal (3d) subgroup system.

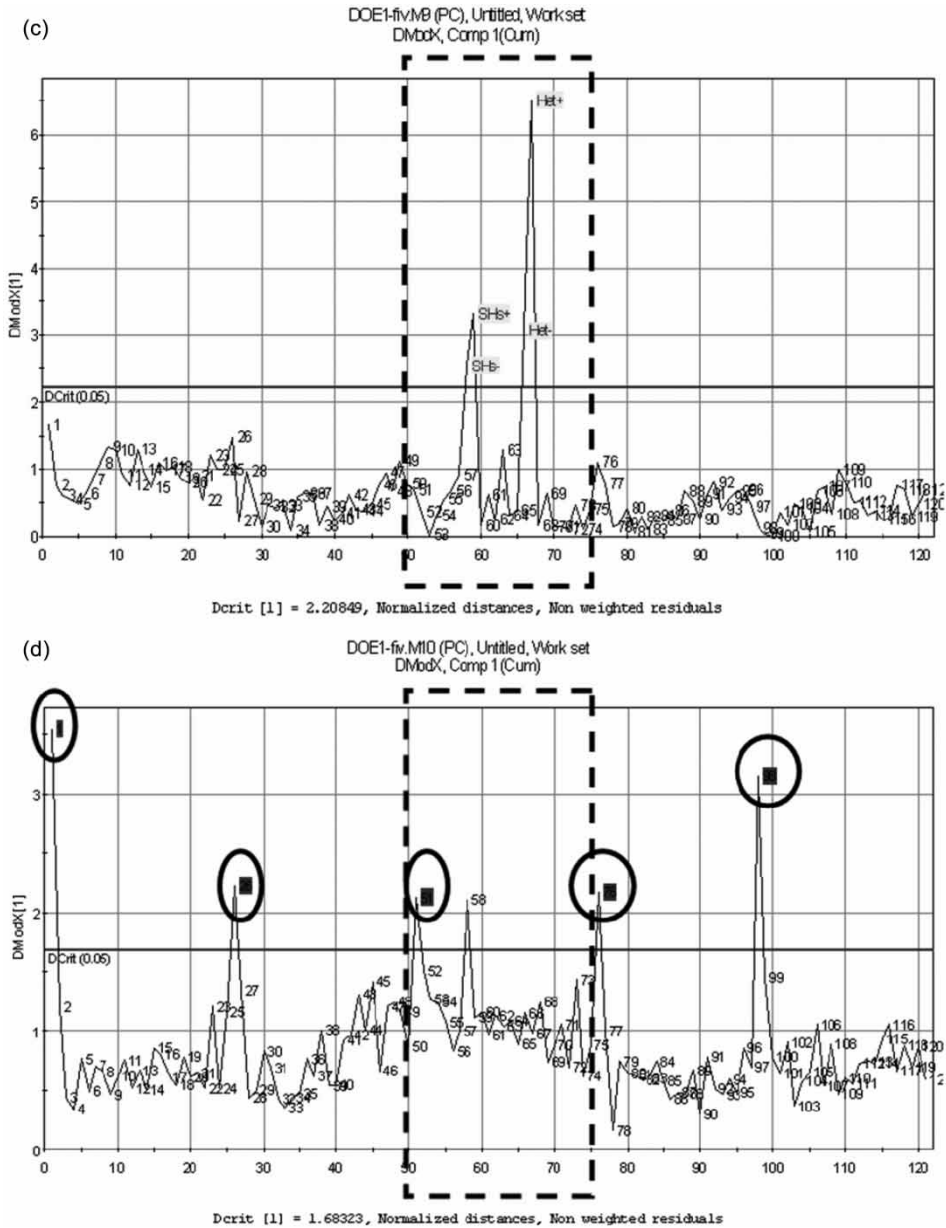


Figure 3. Continued.

This work presents a concept of simultaneous fault detection and classification by multivariate analysis of SPC, and addresses a few issues that affect manufacturing equipment. Multivariate control charts of the fault spaces are powerful tools for both detecting out-of-control situations and diagnosing causes. The only prerequisite for applying these methods is the availability of a good database on previous operations.

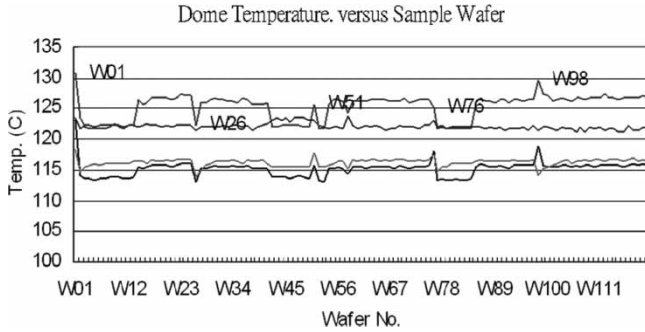


Figure 4. Four zones of dome heater temperature versus sample wafer number.

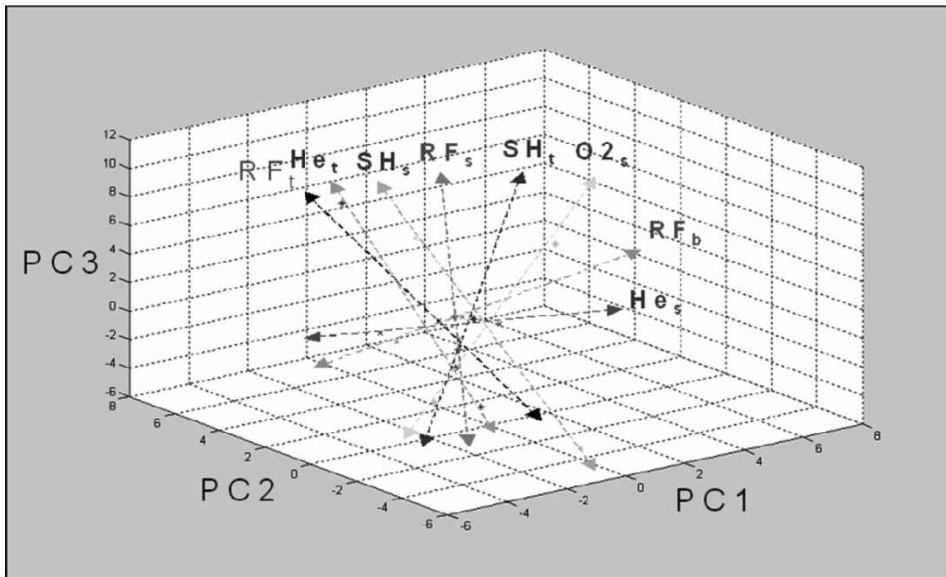


Figure 5. Fault space vectors are projected on the three-component PCA space.

Conclusion

Multivariate SPC of fault detection and classification is an important step in process control. From the experiment applying a HDP CVD above, we can advocate that SPC of multivariate analysis will be more elaborate than qualitative analysis will be for process management. This method represents a breakthrough in the monitoring of a semiconductor manufacturing production line; relevant inferences regarding the current state of the equipment can be drawn, preventing yield loss and eliminating further damage to machines.

In semiconductor manufacturing, thousands of parameters govern the production line and are hard to monitor simultaneously. The traditional SPC method can only provide a basic way to monitor several parameters, which are identified in advance as the key to the process or equipment. Accordingly, extending PCA of the Hotelling T² control chart is a powerful method of multivariate analysis that can reduce the current heavy data management problem to a single

process control chart. In addition, the Hotelling T^2 control chart can easily detect 5% variation in the single gas flow and RF power parameter. The model resolution is sufficiently high to detect faults with $\pm 5\%$ variation. The wafer selection associated with the model must be performed more strictly, and governed by more reasonable criteria, to increase the resolution.

The first wafer effect on the HDP CVD tool is primarily associated with the variation in the dome-heater/thermal system. The first few wafers always suffer some problems caused by the instability of chamber conditions or hardware transient states, which are responsible for the well-known 'first wafer effect'. There are also some limitations of the research to be considered. Sometimes, the root cause of the first wafer effect is not easy to extract from the thousands of data. The tiny variation in each parameter cannot be discriminated by the univariate analysis method but all variations in parameters will be summed to a single larger number in the multivariate analysis model, to discriminate a fault.

Future research should involve more external sensors (such as RGA, OES, V.I. Probe and others) on a tool to retrieve more detail chamber information, a golden model should be built, and sensor parameters should be matched to physical states and then an analysis undertaken. Predicting bottlenecks will help in extracting useful information from raw data and then identifying specific correlations between external sensors and actual components of a piece of equipment.

In sum, we expect to contribute to more elaborate analysis of process control. At a time when quality researchers are challenged to provide research with practical implications, it is also believed that this study may be used by managers to pursue processing control while taking multivariate analysis of SPC into consideration.

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