PECVD Chamber Cleaning End Point Detection (EPD) Using Optical Emission Spectroscopy Data

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In-situ optical emission spectroscopy (OES) is employed for PECVD chamber monitoring. OES is used as an add-on sensor to monitoring and cleaning end point detection (EPD). On monitoring plasma chemistry using OES, the process gas and by-product gas are simultaneously monitored. Principal component analysis (PCA) enhances the capability of end point detection using OES data. Through chamber cleaning monitoring using OES, cleaning time is reduced by 53%, in general. Therefore, the gas usage of fluorine is also reduced, so satisfying Green Fab challenge in semiconductor manufacturing.

Keywords: PECVD, Chamber cleaning, OES, Green fab

1. INTRODUCTION

The semiconductor industry has made an approximate 30% reduction in production cost during the last decade, through the shrinkage of device size, introduction of new material, and improved yield management [1]. 300 mm sized wafer manufacturing industries have already adopted advanced process control (APC) with real-time process monitoring technique, to reduce equipment wait time waste (WTW) and process cost waste (PCW), which is represented as a normalized difference between instantaneous throughput and averaged throughput over a period of time [2].

PECVD process is a workhorse for dielectric thin film deposition of various materials, but during the deposition process, the chambers become coated with process chemicals. To maintain deposition process performance, the chambers are periodically cleaned with NF₃ to remove build-up polymeric materials inside the chamber; however, running a cleaning process for a prolonged time can increase greenhouse chemical usage and WTW. Despite the numerous efforts in the reduction of perfluorocarbons (PFCs) in semiconductor manufacturing to satisfy the Green Fab challenge [3], no significant practice of efficient fabrication equipment operation has been reported from the semiconductor fabrication research area.

Generally speaking, the chamber cleaning time and amount of gas usage varies, depending on the type of material and the amount of deposited layer in previous processes. Real-time monitoring of chamber cleaning with added sensors has been investigated, to improve productivity, waste reduction and cost reduction. One can expect to prevent failure by cross-contamination from imperfect chamber cleaning. Fourier transform infrared (FTIR) was used to optimize the type and usage of cleaning gases in CVD for manufacturing cost reduction [4], and multi-sensor study on reducing PFC gas emission in CVD chamber cleaning has been performed employing quadrupole mass spectrometry (QMS) [5]. FTIR and QMS can provide benefits of monitoring chamber residual gases from exhaust, but they require additional set up for real-time data acquisition.

Optical emission spectroscopy (OES) is a reliable, in-situ and non-invasive monitoring method in plasma processing, and it
is widely accepted as an end point detection (EPD) and process diagnosis in plasma etch [6-9]. In this paper, we practiced EPD of the PECVD chamber cleaning process, using OES. The targeted PECVD chamber for the cleaning process monitoring is the SiON thin film deposition chamber, which is under development of low-cost and comparable-quality process, for the purpose of dielectric deposition. Silicon-oxynitride thin-film in the form of SiO\textsubscript{N}\textsubscript{2}:H is widely used in semiconductor devices and solar cells [10]. Although silicon-oxynitride (SiON) thin film with SiH\textsubscript{4}, N\textsubscript{2}O, and NH\textsubscript{3} gases is already an established process, the manufacturing cost can be reduced, by replacing expensive process gases. While the development of the SiON thin film deposition process with SiH\textsubscript{4}, O\textsubscript{2} and N\textsubscript{2} gases, we experienced severe silane polymer power build-up, depending on the process recipe. Adoption of a real-time process and equipment monitoring technique can provide the benefits of reduction in greenhouse gases, and increase in tool operation efficiency. Therefore, in-situ cleaning monitoring was desired, to improve the process chamber condition.

Acquired real-time in-situ OES data was separated into two groups of process gases and by-product gases. Principal component analysis (PCA) was applied, to create a combined end point, tracing signals for the respective groups. Overlapping the two end points traces from the feeding gas group and by-product group provided a straightforward intuition on the end point of PECVD chamber cleaning. Section II describes how the cleaning experiment was performed in the university research environment. EPD trace signal generation using PCA and its data analysis are presented in Section III. Finally, the conclusion is augmented with the Green Fab challenge in the research environment in Section IV.

2. MOTIVATION AND EXPERIMENT

Plasma enhanced chemical vapor deposition (PECVD) process requires a good amount of gas phase atoms or molecules to exist in the process chamber, and they are absorbed on the wafer surface to form a film. It is known that larger dissociation energy is required for O\textsubscript{2} than N\textsubscript{2}O in gaseous phase plasma, thus undissociated oxygen molecules easily react with gas phase silicon atom in the chamber. The large amount of required dissociation energy for oxygen molecules often leave unabsorbed silicon oxide compound in the chamber. For this reason, the semiconductor fabrication process employs N\textsubscript{2}O or NH\textsubscript{3} gas with SiH\textsubscript{4} for the formation of SiO\textsubscript{x} or SiN\textsubscript{x} thin film. The same thin film forming mechanism applies to SiON. However, it is also valuable to investigate the potential of O\textsubscript{2} and N\textsubscript{2} gas mixture for SiON film deposition, by optimizing the process condition, in order to reduce the cost of manufacturing.

During the effort to develop a new process, in fact, we experienced a good amount of unabsorbed silicon by-product inside the chamber, in the form of powder and film on the chamber. The required time and effects for chamber cleaning were significant under the university research environment, thus in-situ chamber cleaning monitoring was an urgent technical issue to solve, for the reduction of equipment wait time waste (WTW), and equipment output waste (BOW).

The PECVD system used in this research was the PECVD MINIPLASMA-Station, manufactured by Plasmart Co. Ltd., Korea. The process chemistry for SiON deposition is 2 sccm of 99.999% SiH\textsubscript{4}, diluted with 100 sccm of N\textsubscript{2}, while 3-5 sccm of O\textsubscript{2} is augmented for controlling the oxygen contents in SiON film. The cleaning process recipe is provided in Table 1. A total of eleven chamber cleaning runs were performed after every five SiON deposition runs. The amount of oxygen in our standard recipe for cleaning was set to be 40 sccm, but we noticed a lesser amount of oxygen was enough for the chamber cleaning recipe. The first five cleaning runs were performed with 40 sccm of oxygen, and the rest were run with 20 sccm. This change does not affect the purpose of our experiment, which is the model building for end time trace data generation.

To ensure the quality of OES data to include the cleaning end point, we intentionally double the five minutes of cleaning time, which was previously set up. Sulfur hexafluoride (SF\textsubscript{6}) is normally not used for chamber cleaning chemistry, but is used for silicon trench etching gas chemistry, with its isotropic etching characteristic. In this experiment, it is much desired to use nitrogen, fluorine (NF\textsubscript{3}) for the CVD chamber cleaning agent; however, the methodology for CVD chamber cleaning with monitoring of fluorinated gas chemistry still holds. The experimental apparatus in this research is illustrated in Fig. 1.

While five cleaning runs were performed, 200 e five cleaning runs were performed, in Fig. 1. with monitoring, and locally stored for further data analysis. The OES system employed is a CCD type spectrometer, SM440 with Toshiba TCD 1304 sensor array, manufactured by Korea Spectral Product, and the data acquisition software was sensor cluster manager (SCM) from Prime Solutions. Once the data collection was made, the selection of corresponding peaks to plasma gas chemistry, decomposition of process gas and by-product gas, and modeling for end point trace signal generation were performed as shown below.

Selecting corresponding emission peak lines of the OES signal may be arduous, when the possible combinations of by-product are many. To alleviate this concern, principal component analysis (PCA) has been applied, to reduce the data dimensionality. However, separating reactant and by-product gas species by engineering intuitive can also be beneficial in our case. The deposited material on the chamber was mainly SiON, and the reactant gases are SF\textsubscript{6} and O\textsubscript{2} for breaking silicon covalent bonding by fluorine, and forming volatile products of SiF\textsubscript{4}, O\textsubscript{2}, F\textsubscript{2}, and N\textsubscript{2}. The detected emission peaks during the cleaning process are presented in Fig. 2, and this is in accord with the engineering principle.

It is also straightforward that, as cleaning is performed, the optical emission intensity of feeding (or reactant) gases gradually increases, and that of by-products decreases, near the cleaning end point. Figure 3(a) shows the reactant gases of fluorine and oxygen.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
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<tbody>
<tr>
<td>SF\textsubscript{6}</td>
<td>20 sccm</td>
</tr>
<tr>
<td>O\textsubscript{2}</td>
<td>20 and 40 sccm</td>
</tr>
<tr>
<td>Pressure</td>
<td>700 mTorr</td>
</tr>
<tr>
<td>Power</td>
<td>400 W</td>
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<td>Run time</td>
<td>10 min</td>
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trace signals, and Fig. 3(b) shows two peaks of SiF and one of N2 in volatile by-product. In Fig. 3, the end point can be assumed with the one chemical time trace peak, but there is less confidence in defining which peak shows the correct EPD signal. To ensure the cleaning end point, we then employed PCA, to combine each group of optical emission intensities that corresponds to feeding gases and by-products, in forming EPD trace data.

### 3. OES DATA ANALYSIS FOR CHAMBER CLEANING END POINT DETECTION

Principal component analysis (PCA) is an eigenvector-based multivariate analysis method that utilizes an orthogonal transformation, to reform the observation of interrelated variables towards the value of uncorrelated variables, called principal components (PCs) [11]. PCA has been widely used for multi-dimension data analysis, pattern recognition, and predictive regression models. PCA finds combinations of variables or factors that represent majority trends in a data set. PCs can be derived by an eigenvector decomposition of the covariance matrix of $X$.

$$X = t_i p_i^T + p_{i+1} p_{i+1}^T + \cdots + p_n p_n^T + E$$

where the data matrix $X$ is the sum of the outer product of vectors $t_i$ and $p_i$, plus a residual matrix $E$.

Here, $n$ is the number of principal components, which must be less than or equal to the smaller dimension of $X$, and the $t_i$ is known as scores that contain information about how the sample data is related to each other. The $p_i$ is a loading vector that represents how the original variables are related to each other. In the PCA decomposition, the $p_i$ vectors are the eigenvectors of the covariance matrix, i.e. for each $p_i$:

$$C(X) p_i = \lambda_i p_i$$

Here, $\lambda_i$ is the eigenvalue associated with $p_i$ and $C(X)$ means the covariance matrix of $X$. For a given data matrix $X$ with $m$ samples (rows) and $n$ variables (columns), the covariance matrix $X$ is defined as

$$C(X) = \frac{X^T X}{m - 1}$$

This assumes that the columns of $X$ have been mean-centered, i.e. adjusted to have a zero mean by subtracting off the mean of each column. The covariance matrix of $X$ can be calculated in Eq. (3). The projection of the observations of $X$ into the reduced dimensional space is contained in the $i$th score vector $t_i$, which defined as

$$t_i = X p_i$$

$p_i$ pairs are arranged in descending order, according to $\lambda_i$. The $\lambda_i$ present a measure of the amount of variance described by the $t_i$ and $p_i$ pairs.

Raw data is normalized with the Z-score, with $Z(0,1)$. The
quantity $Z$ represents the distance between the raw score and the population mean, in units of the standard deviation. A covariance matrix is calculated from the Z-score data, and eigenvectors and eigenvalues of the covariance matrix are represented in Table 2. Eigenvalues show their percentage of each $p_i$ score. In Table 2, 99% of the raw data is understood in $p_1$, because of the corresponding peak classification. Not only $p_1$, but also a new signal $t_1$ for EPD represent approximately 99% of raw data that contains combined information of each peak. One of the $t_i$ signals coming from process gas is defined as $t_p$, and the other one coming from by-product is defined as $t_b$, and those are used for EPD.

Figure 4 shows the newly generated $t_p$ and $t_b$ signal, and the detected end point of chamber cleaning. The end point of chamber cleaning is detected as a continuous 3 seconds saturation state of $t_p$ and $t_b$. However, the signals are not stabilized perfectly, because noise is included in each signal. Therefore, the steady state is defined if the signal is waved in the 4σ region guaranteeing 99.997% reliability. Figure 5 illustrates the reduced cleaning time by the PECVD chamber cleaning process monitoring with OES. That end of cleaning time is sufficiently considered as a reliable cleaning end point by the EPD algorithm. Although the cleaning time is reduced, the chamber condition is the reinstated innate condition of the chamber. As the result, the cleaning time is reduced by approximately 53%. That percentage means saved cleaning time, as well as gas usage reduction and power saving. Furthermore, product production time reduction and cost reduction is also expected by the chamber cleaning process monitoring.

4. CONCLUSION

In this paper, we presented the usefulness of in-situ chamber cleaning monitoring and its end point detection in the PECVD process. Although in-situ optical emission spectroscopy (OES) data includes some data preprocessing for mathematical model building, the established model can efficiently detect the chamber cleaning end point. The result shows a cleaning time reduction of about 53% was achieved by employing the suggested chamber cleaning EPD, and this methodology can contribute to the semiconductor industry, by reducing wait time waste (WTW), and process cost waste (PCW).

The PECVD chamber cleaning process employs fluorinated gas, and over use of the cleaning agent should be minimized, to satisfy the Green Fab challenge. Although this fundamental research was performed at a laboratory level, it is desired to continuously expand it to semiconductor manufacturing facilities, by utilizing the currently available in-situ process monitoring technique.

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