Virtual Metrology Modeling of Reactive Ion Etching Based on Statistics-Based and Dynamics-Inspired Spectral Features

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Virtual metrology (VM) refers to methods that employ available manufacturing process related data and relevant sensor readings to predict the properties of the resulting product. In micro/nanoscale manufacturing, due to increasing demand on the fabrication yield and throughput, applying VM on the process brings several advantages. Advanced process control (APC) can be enhanced by replacing traditional lot-to-lot control with wafer-to-wafer control [1]. In addition, VM can inform and modify the sampling mechanism of the physical measurement. Current approach relies on physical metrology of randomly sampled products, which is not time and cost-efficient, since non-defective wafers are also measured, while defective ones are easily missed. With the assistance of VM, only wafers with undesirable predicted qualities need to be further inspected. However, plasma processes, such as reactive ion etching (RIE) involve complex physical and chemical process which inherently makes VM difficult to apply. Furthermore, due to fluctuation in process conditions and the tool aging, roots causes or key variables for VM models are hard to define.

In this work, a novel scheme for extracting predictive features from optical emission spectroscopy (OES) signals in RIE is demonstrated. The OES spectra contain qualitative information of the chemical species and are useful for etching end-point detection. However, the amount of OES signal data is overwealming for VM modeling, with signal often being noisy and fluctuating with chamber conditions, which greatly complicates OES analysis. The proposed scheme is divided into two parts, namely dimensionality reduction and dynamic-inspired features extraction. For dimensionality reduction, principal component analysis (PCA) is used to analyze and select key wavelengths of the OES signal [2]. Combining contiguous key wavelengths to form integration bands further reduces the dimensionality of the feature set obtained from the OES signals. Dynamic-inspired features extraction [3] can then be applied to the integration bands and key wavelengths, yielding statistics-inspired and dynamics-based features from the transient and steady state portions of those bands. Finally, after the feature selection process, these features are combined with other data, including tool settings, system readings and non-numerical data are used to build a VM model by partial least squares (PLS) or support vector regression (SVR). Compared with deep learning techniques such as long short-term memory (LSTM), this approach is highly explainable and able to provide further information for the process control.

The initial results examining the end-point detection of a single RIE step indicate that the proposed approach is viable and performs better compared with traditional feature identification by user experience. Table I lists the newly-proposed features in this work, as well as the traditional feature set. In the transient states, 8 types of features in the raw data and the gradient of the raw data are extracted. In the steady states, 10 types of features are typically obtained by identifying key wavelengths and relevant feature types based on user experience and domain knowledge. Figure 1 shows successful separations between transients and steady states in the OES signal at 440 nm wavelength. Table II summarizes the root mean square error (RMSE) and R-squared of two PLS models. The results demonstrate that although R-squared of the PLS model based on dynamic-

inspired features is quite low, only 0.35, it still outperforms the traditional features PLS model by 270%. The RMSE also reduces by around 14% when the newly proposed features are applied. We will present the application of PCA for key wavelength selection and dynamic-inspired features extraction for multiple RIE steps, which can improve the prediction accuracy since more information is involved when building the VM model.

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	Traditional Features			
Steady State		Transient		
Raw Data	The Gradient of The Raw Data	Raw Data	The Gradient of The Raw Data	Mean, maximum and minimum of
Median Duration Standard deviation Pulse counts Amplitude	Median Standard deviation Minimum Maximum Range	Amplitude Duration Rise time Pre overshooting Post overshooting Area under curve	Maximum Minimum	several specific regions in 6 key wavelengths (Pre-defined by user)

Table I. List of dynamic-inspired features and traditional features



Figure 1. Transients and steady states in the OES signal at 440 nm wavelength.

Table II. VM results

	PLS Model (Dynamic-inspired Features)	PLS Model (Traditional Features)	
R-squared	0.35	0.13	
RMSE	0.113	0.131	

References:

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[2] H. H. Yue et al., Journal of Vacuum Science & Technology A, 2001, 19, 66-75.

[3] A. A. U. Haq & D. Djurdjanovic, Journal of Industrial Information Integration, 2019, 13, 22-31