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Virtual metrology modeling of time-dependent spectroscopic signals by a fused lasso algorithm

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ABSTRACT

This paper proposes a fused lasso model to identify significant features in the spectroscopic signals obtained from a semiconductor manufacturing process, and to construct a reliable virtual metrology (VM) model. Analysis of spectroscopic signals involves combinations of multiple samples collected over time, each with a vast number of highly correlated features. This leads to enormous amounts of data, which is a challenge even for modern-day computers to handle. To simplify such complex spectroscopic signals, dimension reduction is critical. The fused lasso is a regularized regression method that performs automatic variable selection for the predictive modeling of highly correlated datasets such as those of spectroscopic signals. Furthermore, the fused lasso is especially useful for analyzing high-dimensional data in which the features exhibit a natural order, as is the case in spectroscopic signals. In this paper, we conducted an experimental study to demonstrate the usefulness of a fused lasso-based VM model and compared it with other VM models based on the lasso and elastic-net models. The results showed that the VM model constructed with features selected by the fused lasso algorithm yields more accurate and robust predictions than the lasso- and elastic net-based VM models. To the best of our knowledge, ours is the first attempt to apply a fused lasso to VM modeling.

1. Introduction

In semiconductor manufacturing, metrology is required to verify the quality of wafers after the completion of a certain process. As the device dimensions continue to decrease, the lot-to-lot process control is being increasingly replaced with the wafer-to-wafer control to achieve tighter process control [1]. However, wafer-to-wafer control requires metrology measurements from every wafer; this leads to an increase in the cost and in the production cycle time. To address these shortcomings, the concept of virtual metrology (VM; Fig. 1) has been developed in the recent years [2]. The metrology measurements should be related to the process conditions. A number of tool process variables that reflect these conditions, such as power, temperature, and flow rate, can be collected from the sensors attached to the tools. The quality variable (e.g., damage, depth, and uniformity) can be measured from the sampled wafers using the metrology equipment. From the relationship between the process variables and the quality variable, a VM model can be constructed to predict the outcomes of the quality variables from the unsampled wafers. Therefore, VM can be used for developing wafer-to-wafer control economically.

A typical semiconductor manufacturing process often involves several hundred operations among which, plasma etching has been recognized as one of the critical operations that directly affects the quality of a wafer [3]. Fig. 2 shows the plasma optical emission intensities that represent the plasma state of a wafer during the etching process. Spectroscopic signals usually consist of thousands of wavelengths, measured over hundreds of time points. This leads to a huge number of features per wafer—a situation that challenges analytical and computational capabilities. In some cases, there may be more observations than features in VM modeling problems. However, in spectroscopic signal used in this study, the number of features exceeds the number of observations in most cases [21,22,25]. To address this high-dimensionality problem, dimension reduction is critical. In other words, identification of important features that are most predictive of a given target value (metrology measurement of a wafer) is necessary. Furthermore, adjacent features are highly correlated with each other because of the natural sequence present in the signal. In this sense, VM modeling of spectroscopic signals can be challenging [4].

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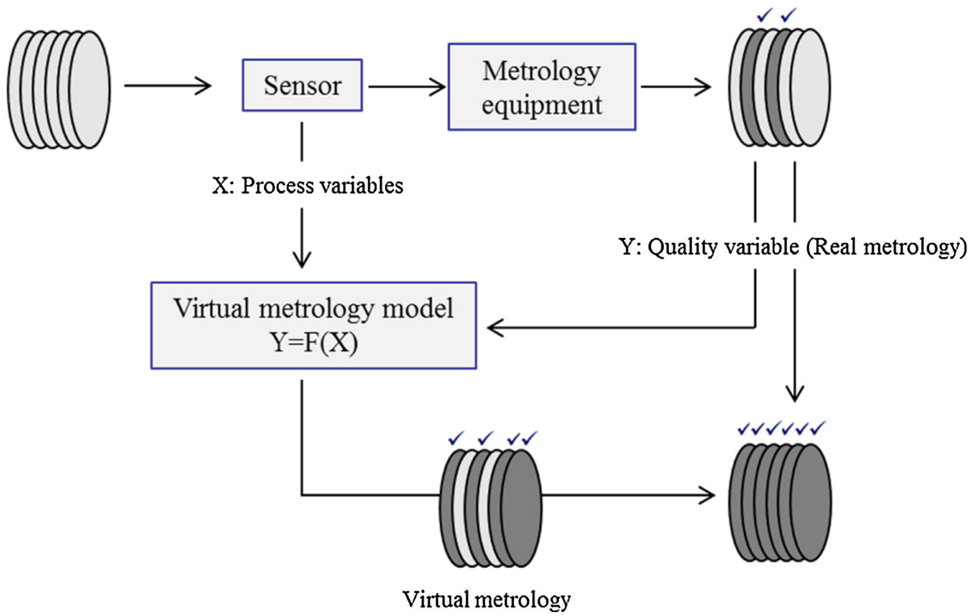

Fig. 1. Conceptual framework of virtual metrology.

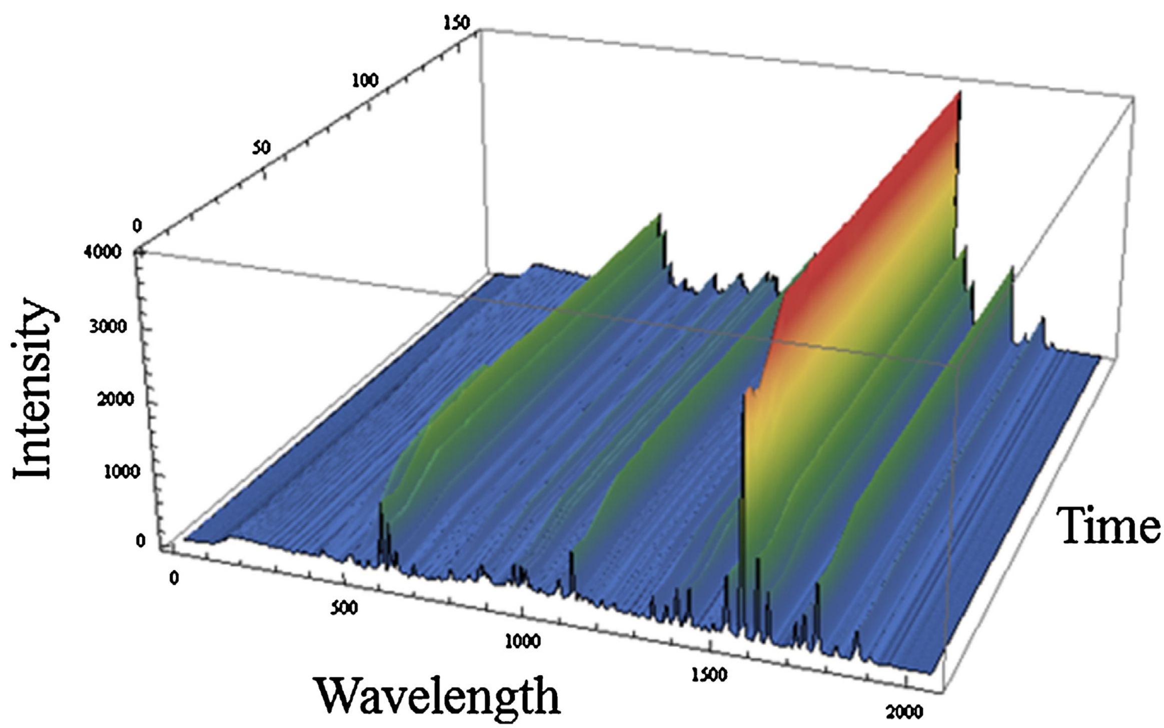

Fig. 2. Time-dependent spectroscopic signals.

To achieve high prediction accuracy for VM, selecting a near-optimal set of features of the process data that can capture the actual characteristics of the product quality is crucial [5]. If we select too many features, irrelevant ones such as noise may be included and they may adversely affect the prediction accuracy of VM [6]. However, selecting too few features may prevent us from capturing important structures of the data [7]. Hence, the identification of the best subset of the features is important for not only developing an accurate model but also facilitating its interpretation. We consider interpretability to be an important issue because engineers who actually operate the semiconductor tools prefer a model that can be easily understood.

Principal component regression (PCR) and partial least squares (PLS) are common regression methods for extracting significant features in a high-dimensional dataset. Both PCR and PLS extract new features by transforming the original features. Generally, the first few features extracted by PCR or PLS are sufficient to satisfy the objective of an analysis; hence, these methods have been widely applied in the VM modeling of high-dimensional data such as spectroscopic signals. Wan et al. investigated a Gaussian process regression-based VM model for predicting etch rate using spectroscopic signals [9]. Prior to training the VM model, they mapped the large input space to a reduced latent feature space using PLS. Park et al. built a PCR-based VM model for etching-rate prediction