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Predicting Plasma-Deposited Thin Film Properties Using Machine Learning based on Optical Emission Spectroscopy

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Traditionally, thin film fabrication using plasma processes has relied on a trial-and-error approach driven by experience and intuition due to the complexity of plasma reactions. This method often results in inefficiencies, leading to wasted energy, materials, and resources. To address this challenge, optical emission spectroscopy (OES) is used in plasma-based manufacturing for real-time process monitoring and control without disrupting the plasma. However, tetraethylorthosilicate (TEOS)-based plasma deposition presents additional difficulties due to its complex emission spectrum. Additionally, when oxygen is present in the deposition process, oxygen atom density and ion flux become critical parameters [1]. In this study, we propose a data-driven approach to express the SiO_2 deposition rate using a mathematical model informed by plasma emission spectra and machine learning.

The data sets ware prepared by fabricating SiO_2 thin film using capacitively coupling plasma with RF of 13.56 MHz and a mixture of TEOS, oxygen and argon as gas sources. The total of 31 deposition conditions were collected under different parameters of plasma power, pressure, and gaseous ratio. In addition, the optical emission spectrum was measured in similar conditions with deposition processes. Supervised and unsupervised learning were used for predicting deposition rate of SiO_2. A gradient boosting regression tree (GBRT) model was employed to predict the deposition rate based on plasma emission data, with the results interpreted using SHapley Additive exPlanations (SHAP) [2, 3]. For unsupervised learning, we utilized principal component analysis (PCA).

The deposition rate prediction of GBRT model result showed an agreement with the measured deposition rate, owning a coefficient determination R^2 of 0.93 ± 0.04 and 0.54 ± 0.32 for train data and test data, respectively (Figure 1). The SHAP result revealed that the deposition rate is significantly influenced by the following species, OH, CO, OI, ArI and ArII as shown in Figure 2. It is suggested that these species are correlated to the TEOS dissociation process through electron impact, reaction with oxygen atoms and argon metastable. On the other hand, the PCA showed that at least 6 principal components were required to obtain prediction coefficient determination R^2 above 0.90.

The model provides insights into the contributions and correlations of different plasma species to the SiO_2 deposition process. Furthermore, we leverage these findings to derive a mathematical model for predicting the deposition rate, demonstrating that OES can serve as a valuable tool for monitoring plasma output under varying process conditions [4]. This approach holds significant potential for industrial applications, particularly in semiconductor manufacturing.

References
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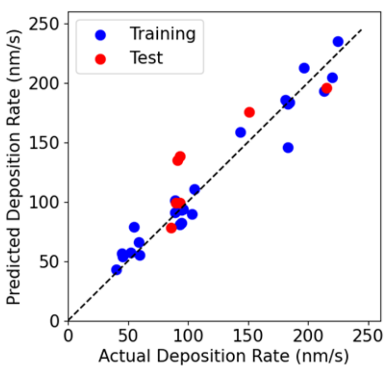

Figure 1 ML model performance of the SiO_2 film deposition rate.

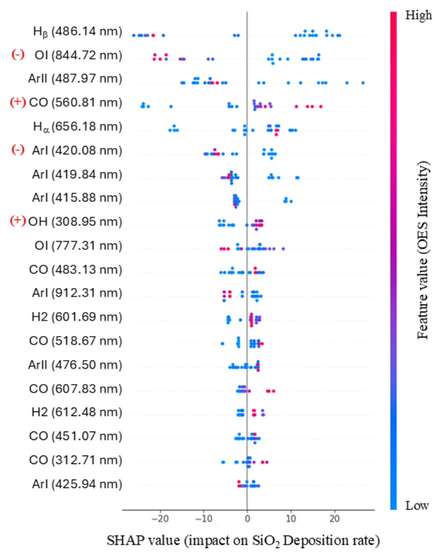

Figure 2 SHAP summary plot of OES to the SiO_2 film deposition rate.