## Root Cause Analysis of Plasma Processes Perturbation using Optical Emission Spectroscopy Signals with Modified Autoencoder - Jaehteon Kim

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Plasma-assisted process is essential for nanoscale patterning of semiconductor and controlled with process variables. The mechanisms of particle generation, transportation and surface reaction enhance the non-linearity of plasma parameters and conceal the analytical causality of process result. The unclear causality serves as obstacle for detection of process perturbation and yield improvement.

In this work, modified autoencoder was developed for diagnosing the root causes of perturbation in a plasma process. Optical emission spectroscopy (OES) signals of size 11220x3648 were collected for training the autoencoder while varying four process conditions, such as RF power, pressure, Ar gas flow rate and CF<sub>4</sub> gas flow rate. The collected signals were normalized by dividing each signal vector's length and then fed into the autoencoder as input.

The encoder layers of the autoencoder consisted of two fully connected layers of size 3648x3648 and a fully connected layer of size 3648x4. The selectivity between the extracted features was improved by removing connections besides specific encoded features while the autoencoder is trained. The outputs of each layer passed hyperbolic tangent function as activation function for giving the non-linearity and batch normalization layer for solid training without gradient diminishing. Each layer can be expressed in below equation, where the x<sub>t</sub> means input vector of t<sup>th</sup> layer, W the parameter matrix, b the bias vector,  $\mu$ ,  $\sigma$ ,  $\gamma$ , and  $\beta$  means the parameters for batch normalization.

$$x_{t+1} = \gamma \frac{\tanh(W \cdot x + b) - \mu}{\sqrt{\sigma^2 + \epsilon}} + \beta$$

The loss function for training was consisted with reconstruction loss and selectivity loss. The reconstruction loss optimized the parameters to express the original data while extract the features well and selectivity loss was added to make the features react to only specific error while training. The loss function can be expressed as below, when the x means the input signals,  $\hat{x}$  reconstructed signals, z encoded features for x and the I means one-hot vector.

Loss function = CosEmbeddingLoss  $(x, \hat{x})$  + CosEmbeddingLoss (x, l)Constructed loss function optimized the parameters of modified autoencoder with backpropagation algorithm using adaptive moment estimation (ADAM) optimizer and learning rate was controlled with ReduceLROnPlateau algorithm. The train loss and validation loss was saturated to 0.01 and 0.06 just in 500 epoch.

As the validation step, OES signals of the size 2133x3648 were collected from standard processes and perturbated processes. The collected signals for test were inputted into the trained encoder layers to extract features. The perturbation of process and roots for each process perturbation were diagnosed with extracted feature scores. One of the extracted features, Z1 just reacted just for OES signals of power perturbated processes and detected the power perturbation. And the others also reacted to just specific features and detected the perturbation of pressure, Ar flow rate and CF<sub>4</sub> flow rate perfectly.

The relevance score means the contribution of each input for model to decide score. The relevance scores of each layer in this autoencoder model were expressed with summation of partial differentiation to input like below and were calculated to each wavelength. The relevance score of Ar line 589.35nm had the highest contribution to decision of Ar flow rate perturbation and pressure perturbation with 1.3% and 1.5% ratio to overall score. The relevance score of Ar line 750.45nm had the highest contribution to decision of CF<sub>4</sub> flow rate perturbation and power perturbation with 0.7% ratio to overall score.

$$\sum_{l} \frac{\partial x_{t+1,l}}{\partial x_{t,l}} = \sum_{l} \frac{\gamma_{t,l}}{\sqrt{\sigma^2 + \epsilon}} \cdot \left\{ 1 - \tanh^2(w_{t,(k,l)} x_{t,k}) \cdot w_{t,(k,l)} \right\}$$

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Figure 1. Perturbation detection algorithm scheme



Figure 2. Z features encoded from standard processes and RF power perturbated processes



Figure 3. Z features encoded from standard processes and pressure perturbated processes



Figure 4. Z features encoded from standard processes and Ar gas flow rate perturbated processes



Figure 5. Z features encoded from standard processes and CF4 perturbated processes

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