Prediction of Plasma CVD Process Data of a-Si:H Films via Machine Learning

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Abstract: Plasma processes demand many external parameters to be tuned. For the better tuning, process data of plasma CVD of hydrogenated amorphous silicon films is analysed by two methods: sparse principal component analysis and ensemble learning method. These analyses are useful not only for identifying key external parameters and suggesting better experimental conditions, but also for giving predictive insights into experimental results.

Keywords: machine learning, plasma CVD, ensemble learning, sparse principal component analysis

1. Introduction

In semiconductor manufacturing, plasma processes of CVD, sputtering, and etching, play central roles. These processes have dozens of tuning parameters and multiple objective variables for product evaluation. Relations between the tuning parameters and objective variables are highly complicated and thus are hard to be interpreted. Since plasma process has a non-linear relationship between these tuning parameters and plasma parameters and a complex relationship between the plasma and material interface/property of material, to identify important experimental tuning parameter for the quick production of the desired material requires considerable efforts by well-established researchers and can be a bottleneck of the research and development.

In general, plasma processes demand many external parameters to be tuned via trial-and-error, and the number of tuning parameters can be enormous in some practical cases. Physical and chemical parameters of reactive plasma in a reactor and products also have many characteristics. In such cases, data-based statistical or machine learning approach offers a novel way for tuning plasma processes in a short period.

In this study, the estimation of key tuning parameter in plasma process are partially overcome by utilizing a sparse principal component analysis (SPCA) [1,2] and an ensemble learning algorithm which is one of the machine learting method. We used one of the ensemble learning, gradient boosting regression trees (GBDT) [3], for estimating feature importance. In this study, we applied the method to plasma enhanced chemical vapor deposition for fabricating hydrogenated amorphous silicon (a-Si:H) solar cells [4] and present the demonstration of identification the key parameter thorough these two method.

2. Method

2.1 Film Deposition Process

First, we explain briefly the experimental setup used for the film deposition process [4]. This plasma CVD reactor employs a multi-hollow electrode, frequently together with a cluster eliminating filter. The external parameters are the SiH_4 flow rate, H2 flow rate, substrate temperature, gas pressure, film thickness, RF power, RF frequency, distance between electrode and substrate, presence/absence and type of the cluster eliminating filter, presence/absence of a 100 mesh, and type of multi-hollow electrode. The last three parameters are discrete, and the rest are continuous. Under each experiment conditions one film was deposited, and then the film was employed to fabricate16 or 7 solar cells.

2.2 Machine learning method

PCA(:principal component analysis) [1] is a method of linear transformation of high dimensional data. It transforms axes of data to new axes called principal components (PC1, PC2, …). PCs remain orthogonal and numbered in descending order of data variance along the axes. For example, if a shape of data is bread-like in 3D space, the variance along PC1 is very high, while ones along PC2 and PC3 are small. In such cases, we may ignore PC2 and PC3, and regard the data as one-dimensional. In this way, PCA can be used for dimensional reduction.

We describe sparse principal component analysis (SPCA) [2]. As the name suggests, SPCA is a family of PCA. The word “sparse” means “mostly zero”. For example, consider a linear combination $a_0x_0+ a_1x_1+\cdots+ a_nx_n$ and if the coefficients $a_0, a_1\ldots a_n$ are sparse, that means only a small number of them are non-zero. SPCA gives sparse estimations of PCs. This is helpful when you are trying to interpret principal components. Sparsity of loadings can be controlled by changing a regularization parameter.

We applied for estimating key plasma parameter using the gradient boosting regression trees (GBRT), which is one of ensemble learning. GBRT is an improved boosting algorithm for regression and classification problems.

3. Results and Discussion

3.1 Reslts of PCA/SPCA

Figure 1 shows the Eigenvalues of the normal PCs. Each of the first three components has an eigenvalues more than 1 and their sum is 91% of all variation of the data. The right side of Table 1 shows the loadings of the SPCA’s components. PC1 has high correlation with FF_{initial}, $\eta_{\mathrm{stabilized}}$, and “Degradation Ratio”. Thus, PC1 is interpreted as the film performance axis as a solar cell. PC2 has high correlation with η_{initial}, currents, and small correlation with *"Degradation Ratio"*, therefore PC2 is the initial performance axis. PC3 is the voltage related axis. Figure 2 shows PC1 distributions against four external parameters. These results show that, the cluster eliminating filter, SiH_4 flow rate, reactor pressure, and distance between substrate and electrode play key roles in determining the conversion efficiency of a-Si:H solar cells. From the viewpoint of physical mechanisms, these four parameters are reasonable as follows. First, clusters contribute mainly to SiH_2 bond formation in films and tend to enhance the light induced-degradation. The cluster eliminating filter reduces this contribution and hence PC1 depends on the filter type as in Fig. 2(a). Note that "filter type 0" is "w/o filter" and the rest numbers correspond to fineness of filter. Secondly, the SiH_4 flow rate is inversely proportional to the gas residence time in the plasma region, thus the cluster growth rate decreases with increasing the flow rate and hence PC1 depends on the SiH_4 flow rate as in Fig. 2(b). Thirdly, the distance between substrate and electrode affects cluster growth rate, leading to the results in Fig. 2(c). Finally, the pressure play at least two major roles: 1) the higher pressure gives the longer gas residence time leading to the faster growth of clusters, and 2) the higher pressures brings about the less diffusive transport of clusters to the substrate set in the upstream region. According to the balance between these two reverse effects, there is an appropriate pressure to obtain the highest PC1.

Based on these results, we have designed new experiments focusing on the SiH_4 flow rate dependence [5]. SiH_2 bond density in a-Si:H films nonlinearly decreases with increasing the SiH_4 flow rate. Eventually, the experiments realized a lower SiH_2 bond density than previous ones. It should be noted that a-Si:H films with the lower SiH_2 bond density tends to show lower light-induced degradation.

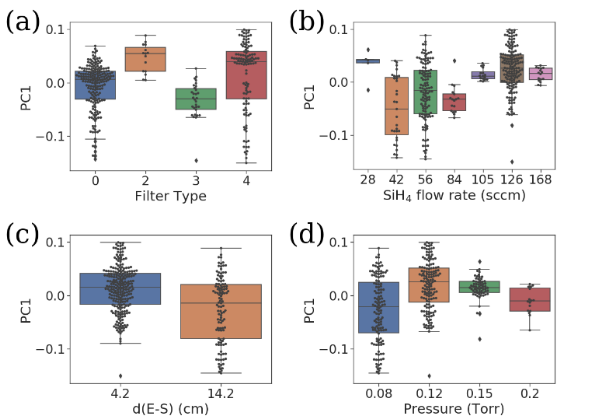

Fig. 2. Box plots showing changes of distributions regards to varying specific external parameters along PC1 obtained with SPCA. Dots represent data points. Each x-axis is (a) filter type, (b) silane flow rate, (c) distance between electrode-substrate, (d) pressure of reactor respectively.

PCA and SPCA analyses are useful not only for identifying key external parameters and suggesting better experimental conditions, but also for giving new insights into experimental results.

3.2 Reslts of GBDT

Figure 3 shows the feature importance of plasma CVD of a-Si:H films. The target value is the stabilized efficiency. These results are consistent with our previous findings that nanoparticles and high order silane related radicals tend to reduce the stabilized efficiency. Based on these results we have selected new experimental conditions and have succeeded in realizing highly stable a-Si:H solar cells.

4. References

[1] I. T. Jolliffe, Springer Ser. Stat. **98**, 487 (2002).
[2] S. Yi, et al., Pattern Recognit. 61, 524 (2017).
[3] J. H. Friedman, The Annals of Satistics, **29**, 5 1189 (2001).
[4] K. Keya, *et. al.*, Jpn. J. Appl. Phys. **55**, 07LE03 (2016).
[5] T. Kojima, *et al.*, Plasma Fusion Res., **13**, 1406082 (2018).

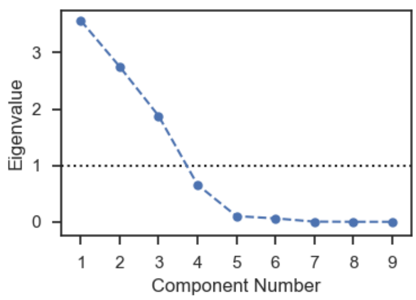

Fig. 1. Eigenvalues of normal PCA's components.

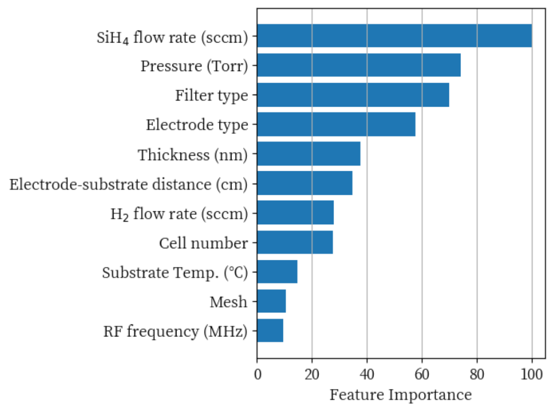

Fig. 3. Feature importance of plasma CVD of a-Si:H estimated by GBRT model.