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Predictions for High Mobility Amorphous ITO(In_2O_3:Sn) Films via Hybrid Machine Learning Model

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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.

Recently, there has been growing interest in amorphous In_2O_3:Sn (a-ITO) due to its unique advantages, including surface smoothness, good short-range uniformity, low internal stress, and high etching rate, which all stem from its amorphous structures [1]. However, conventional a-ITO films have much lower mobility than polycrystalline ITO (pc-ITO) films, limiting their practical use. Moreover, the instability of amorphous phases of ITO thin films and their tendency to crystallize at substrate temperatures around 150-200 °C pose additional limitations on the practical utilization of a-ITO films in various devices. To address these challenges, we have recently developed a novel fabrication method called nitrogen-mediated amorphization (NMA) method that can produce a-ITO films with higher mobility and improved thermal stability than conventional methods [2,3]. However, since the NMA method for a-ITO thin film fabrication is a new control one of crystal growth that is not restricted by the crystallization temperature. There is not much information available on the experimental conditions required for amorphization and boundary conditions between amorphous and crystalline materials. Thus, in this study, we propose the hybrid model incorporating machine learning techniques, such as classification and regression models, as an efficient approach for determining the boundary conditions and optimal sputtering conditions to achieve high mobility a-ITO thin films.

2. Method

This hybrid model that was consisted of support vector machine (SVM)[4] as a classification model and gradient boosting regression tree (GBRT)[5] as a regression model. SVM is a powerful classification model that is particularly useful when working with high-dimensional data. It works by finding the hyperplane that maximally separates the two classes in the feature space. GBRT is an ensemble learning technique that leverages multiple decision trees to create a more accurate predictive model. In GBDT, decision trees are trained in a sequential manner, with each subsequent tree aiming to correct the errors made by the previous tree. ITO films were fabricated on quartz glass substrates by radio-frequency (RF) magnetron sputtering with nitrogen-mediated amorphization (NMA) method.[8-10] N_2/Ar flow ratio, which is the feature of nitrogen mediated amorphization method, ranges from 0 % to 12.5 %. The vertical position of the substrate is controllable in 55-105 mm of target-substrate distance (gap). The substrate temperature varies from room temperature (~30 °C) to 300 °C. The sputtering target was ITO (In_2O_3:Sn) or In_2O_3. These four parameters (N_2/Ar flow ratio, gap, substrate temperature, type of target) are used as the features which means the variables for training predictive models and performing predictions. Among the 203 thin film datasets examined in this study, 26% correspond to crystalline thin films, while 74% represent amorphous ones.

3. Results and Discussion

The hybrid results between SVM and GBRT models for the fabrication of ITO thin films show the boundary conditions between amorphous and crystalline crystallinity and optimal thin film deposition conditions that resulted in a-ITO films with 27% higher mobility near the boundary than previous research results. Thus, this prediction model identified key parameters and optimal sputtering conditions necessary for producing high mobility a-ITO films. The identification of such boundary conditions through machine learning is crucial in the exploration of thin film properties and enables the development of high-throughput experimental designs.

References

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