Materials Day

Abstract Guide

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Develop a Bayesian molecular beam epitaxy (BaMBE) interface for AI guided design of synthesis experiments

*M. Y. Yu, R. Trice, M. Hilse, W. Reinhart, and S. Law

Over the past few decades, chalcogenide compounds have garnered significant attention as topological insulators, semiconductors, and two-dimensional materials. The synthesis of chalcogenide thin films has made critical breakthroughs leveraging molecular beam epitaxy (MBE) technology. However, the optimization of processing conditions is time-consuming and costly and, due to the complex interactions between parameters, not guaranteed to result in the best conditions. This project focuses on developing machine learning models based on Bayesian optimization to predict and guide MBE synthesis experiments to achieve optimal samples with minimal time and cost. We started building the model using GaSe, and used reflection high-energy electron diffraction (RHEED), X-ray diffraction ω scans, and atomic force microscopy (AFM) measurements to characterize the samples. We have developed a preliminary model based on the full-width at half maximum (FWHM) of the ω curves. It shows an R^2 correlation of 0.631 between the predicted FWHM and the empirical FWHM, indicating a good possibility of predicting trends in how growth conditions affect crystallinity. The model also successfully identified "outlier" samples and have experimentally verified. For further optimization, we created a low-dimensional embedding of the RHEED patterns and connected it to process conditions and FWHM. We found that Se:Ga flux ratio is closely related to RHEED while growth rates and temperatures are not, and we confirmed that poor crystallinity is reflected by poor RHEED patterns. We performed surrogate process modeling on FWHM to evaluate the correlation between the predicted and empirical data and improved the R^2 from -0.011 to 0.686. We found that incorporating RHEED conditions into the surrogate process model can refine the FWHM predictions. Now we are expanding the processes to AFM features and have preliminary findings: unsupervised learning on AFM shows some distinct morphologies and correlates with surface roughness metric, while roughness is weakly correlated with RHEED embedding.

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