Autonomous Workflows and SHAP Interpretation of Deposition-Rates in Bipolar HiPIMS

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1. Introduction

1.1 Background

High-power impulse magnetron sputtering (HiPIMS) offers considerable control over ion energy and flux, making it invaluable for tailoring the microstructure and properties of advanced functional coatings. However, compared to conventional sputtering techniques, HiPIMS suffers from reduced deposition rates. Many groups have begun to evaluate complex pulsing schemes to improve upon this, leveraging multi-pulse schemes (e.g. pre-ionization or bipolar pulses). Unfortunately, the increased complexity of these pulsing schemes has led to high-dimensionality parameter spaces that are prohibitive to classic design of experiments. Our proposed workflow combines autonomous experimentation and interpretable machine learning and is broadly applicable to the discovery and optimization of complex plasma processes, paving the way for physics-informed, data-driven advancements in coating technologies.

1.2 Previous Work

Previous studies reported increased deposition rates in bipolar HiPIMS, attributing the improvement to an ion-reflecting sheath near the sputter target that suppressed back-attraction[1,2]. Based on this hypothesis, bipolar pulsing had been proposed as a promising route to overcome one of the main limitations of HiPIMS while preserving its high ionization benefits. In contrast, other experimental and plasma diagnostic studies observed no deposition-rate enhancement and instead identified changes in plasma potential and quenching of the afterglow plasma[3]. These conflicting results highlight the need for a systematic approach to sample datasets and analyse them to resolve coupled plasma–process interactions.

2. Methodology

In this work[4] we investigate multi-pulse HiPIMS for improving deposition rates of Al and Ti sputter targets. For this, we developed an autonomous experimental workflow combining Bayesian optimization (BO) with real-time control of a HiPIMS sputtering system. Over 3000 process conditions were collected via autonomous Bayesian sampling over a high dimensional parameter space (6 or more parameters). These process conditions were then interpreted using Shapley Additive Explanations (SHAP), to deconvolute complex process influences on deposition rates.

3. Results

In short, SHAP enable us to interpret the process conditions, to deconvolute complex process influences on deposition rates. This allows us to link observed variations in deposition rate to physical mechanisms such as back-attraction and plasma ignition. We find that deposition rates are primarily governed by unipolar pulse parameters, including power density, peak current density, and negative pulse width. In contrast, the positive pulse components of bipolar HiPIMS generally have a smaller influence. Short negative pulse widths reduce ion back-attraction but introduce losses associated with plasma ignition. In high-ionization regimes, we observe that applying a positive pulse immediately after the negative pulse may decrease deposition rates, which we attribute to quenching of the afterglow plasma. Any deposition-rate improvements from bipolar pulsing are small and typically within experimental uncertainty for both Al and Ti. Our results show that bipolar HiPIMS does not provide a systematic deposition-rate advantage under most conditions studied and can be detrimental when the positive pulse is poorly timed. By visualizing key physical mechanisms such as back-attraction and plasma ignition, our approach offers general applicability to other high-dimensional plasma and materials processing problems.

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