# Physics-Informed Bayesian Optimization Framework for Etching Rate and Surface Roughness Co-optimization


Ziyi Hu
*State Key Laboratory of Fabrication Technologies for Integrated Circuits*
*Institute of Microelectronics, CAS*
Beijing, China

Junjie Li
*State Key Laboratory of Fabrication Technologies for Integrated Circuits*
*Institute of Microelectronics, CAS*
Beijing, China

Hua Shao
*State Key Laboratory of Fabrication Technologies for Integrated Circuits*
*Institute of Microelectronics, CAS*
Beijing, China
shaohua@ime.ac.cn

Rui Chen
*State Key Laboratory of Fabrication Technologies for Integrated Circuits*
*Institute of Microelectronics, CAS*
Beijing, China
chenrui1@ime.ac.cn

Lado Filipovic
*CDL for Multi-Scale Process Modeling of Semiconductor Devices and Sensors*
*Institute for Microelectronics, TU Wien*
Vienna, Austria
filipovic@iue.tuwien.ac.at

Ling Li
*State Key Laboratory of Fabrication Technologies for Integrated Circuits*
*Institute of Microelectronics, CAS*
Beijing, China



***Abstract*—Precise etching control, balancing etching rate (ER) and surface roughness (Ra), is critical yet challenging in advanced semiconductor manufacturing. Traditional co-optimization relies heavily on costly and time-consuming trial-and-error experiments. This study introduces a Physics-Informed Bayesian Optimization (PIBO) framework to efficiently optimize ER and Ra during silicon plasma etching. PIBO overcomes extrapolation limitations of conventional Gaussian Process Regression by integrating physical prior knowledge – specifically, qualitative relationships of source power (PW) and pressure (P) to the process metrics. It utilizes a 3D etching profile model to generate data across parameter spaces. The framework employs an iterative feedback loop: starting from limited experimental data, it recommends new parameter sets for evaluation; these results then refine the model and subsequent recommendations. This approach systematically minimizes the number of required experiments. By embedding engineering understanding of the PW and P effects and leveraging computational modeling, the PIBO framework bridges the gap between physical intuition and data-driven optimization. It significantly reduces reliance on extensive trial-and-error, enabling faster and more efficient acquisition of optimal etching parameters (PW, P) that achieve the desired ER/Ra balance, ultimately accelerating process development.**



***Index Terms*—Etch rate, Surface roughness, Physics-informed bayesian optimization, Process parameters.**


## I. INTRODUCTION

Precisely controlled etching is essential in advanced node semiconductor manufacturing, where key metrics such as etching rate (ER) and surface roughness (Ra) are critical for process quality and device performance. Fabs face a fundamental trade-off in achieving high ER while maintaining Ra within certain limits. Co-optimization is needed and traditionally relies heavily on expertise and extensive trial-and-error experiments, leading to long turnover, long design cycles, and high cost [1]. Thus, developing predictive methods based on limited experimental datasets is an urgent industry need.

Bayesian Optimization (BO), efficient in sampling and global optimization, employs historical data to recommend optimal parameters [2]. The physics-informed BO (PIBO) framework addresses conventional Gaussian Process Regression's extrapolation limits by integrating physical priors [3], offering new pathways for complex etching optimization.

In this study, we propose a PIBO framework for co-optimization of ER and Ra during plasma etching of silicon. The framework incorporates qualitative relationships of both source power (PW) and pressure (P) to process metric as prior knowledge, and uses a 3D etching profile model to generate data across the parameter spaces. Iterative feedback refines the recommendation mechanism, enabling efficient acquisition of optimized parameters with minimal experiments. This approach bridges engineering intuition and data-driven modeling, reducing reliance on trial-and-error while enhancing process optimization and development efficiency.

## II. PIBO FRAMEWORK

We applied the PIBO framework to optimize the ER and Ra of a planar Si substrate during Cl-based plasma etching. As shown in Fig. 1, the PIBO framework operates through four iterative stages to identify parameter combinations that satisfy the target specification: a) Perform 3D etching profile simulation using recommended parameters from PIBO; b) Analyze simulated data and calculate ER and Ra; c) Update the dataset correlating process parameters with target metrics; d) Execute PIBO algorithm to identify improved process condition for the next iteration.

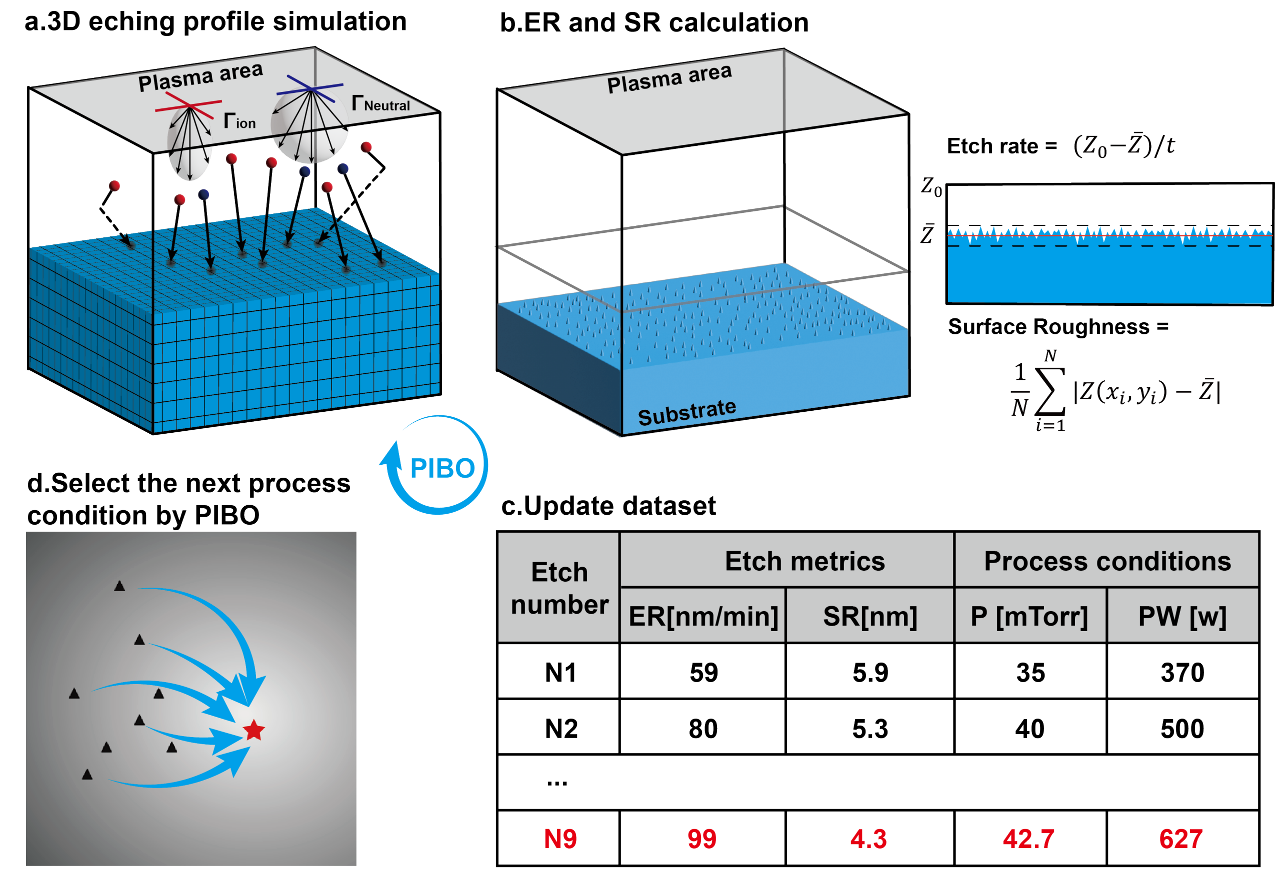


Fig. 1. PIBO framework for co-optimization of ER and Ra. (a) Data acquisition by 3D etching profile simulation, (b) ER & Ra calculation, (c) Etch metrics for 9 runs (N1-N9), (d) Select the next process condition by PIBO.

### A. *Data acquisition by 3D etching profile simulation*

We simulate the etching process of planar Si substrate during Cl-based plasma using a 3D etch profile simulation model based on Monte Carlo and voxel methods. This model includes the incident distribution of particles, Monte Carlo ray tracing, and profile evolution based on the voxel method. As illustrated in Fig. 1(a), we divided the 3D structure into a grid of $x{\times}y{\times}z$ voxels, defining a simulation window of $length{\times}width{\times}height$ in $nm^3$. We assign different number to represent the presence of different types of materials in each voxel. The model also includes the relationship between the process conditions and the properties of incident particles. Particles are emitted from the plasma region at fixed positions and angles derived from the specified process parameters. They travel in straight lines until they reach the substrate surface and interact with it. We incorporate physically reasonable reaction probabilities into the model based on prior literature [4]–[6]. As particles strike and react with the surface, affected substrate voxels are gradually converted to vacuum, simulating material removal. Thus, this model provides real-time simulation of the etching profile. The model mainly considers two kinds of incident particles: isotropic incident particles and anisotropic incident particles. The incidence angle distribution of isotropic incident particles follows the cosine distribution. The incidence angle distribution of anisotropic incident particles obeys Gaussian distribution and mean $\mu$ represents the center incident angle, which is normal to the substrate, while standard deviation $\sigma$ represents the degree of the incident angle dispersion around the normal direction. In this study, $\mu$ is equal to 0 and $\sigma$ is equal to 0.035, this corresponds to 99.7% of anisotropic incident particles within ±5.73°. The influence of particle incident energy is ignored in this study.

### B. *ER & Ra calculation and dataset update*

Following the etching simulation, the etching model can automatically calculate the ER and Ra through global statistics, and update the dataset for PIBO. The ER is calculated as the average etching depth, while Ra is evaluated using the arithmetic average deviation metric shown in Fig. 1(b). These values are then used to update the dataset (Fig. 1(c)), which links process parameters with the corresponding metric outcomes. This updated dataset is used in the subsequent PIBO-driven parameter optimization step.

### C. *Process parameter selection via PIBO*

The goal of the optimization is to simultaneously tune ER and Ra towards their respective target values. Source power

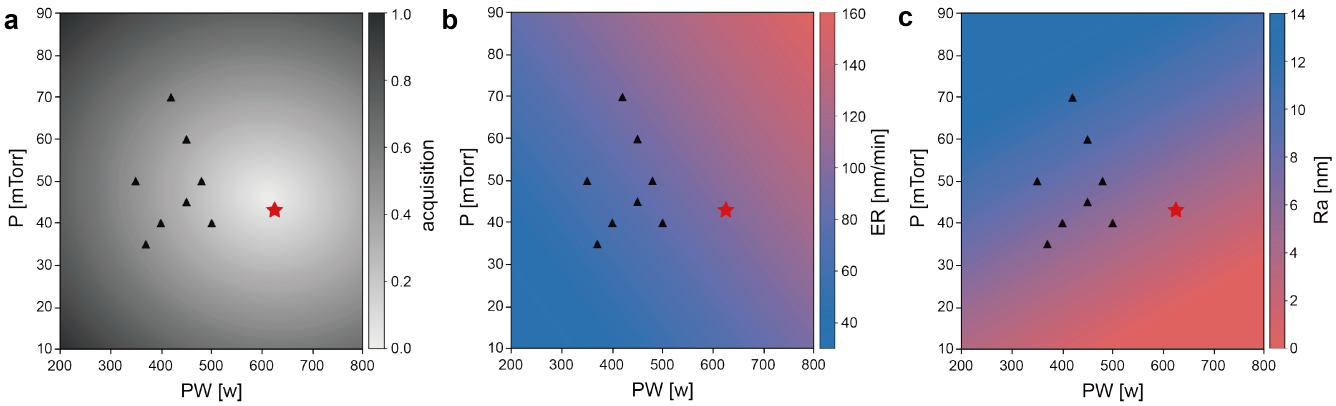


Fig. 2. Prediction results from PIBO (star) with 8 samples (triangles). Two-dimensional plots of (a) acquisition values, (b) ER values, and (c) Ra values as a function of P and PW

and pressure are widely identified as the two most influential process parameters [7]. Therefore, we adjust PW and P, while keeping other conditions fixed, to find combinations that best satisfy the target performance. We use the following predictive functions to model the relationships between PW, P, ER, and Ra:

$$ER = a_1 * P * PW + b_1 + r_1(P, PW) \tag{1}$$

$$Ra = a_2 * P/PW + b_2 + r_2(P, PW) \tag{2}$$

where we impose $a_1 \geqslant 0$ and $a_2 \geqslant 0$.

A Gaussian process (GP) is used to model the residual components $r_1$ and $r_2$. Since the interaction of PW and P may be complex, GP better fits the residual terms on top of the linearity relationship between PW/P and ER/Ra. This predictive model is used to compute acquisition values that ultimately recommend a new process condition ($PW^{N+1}$, $P^{N+1}$) for the next process. Simply put, a low acquisition value indicates that the rescaled distance between the predicted values and their respective targets is likely to be close to zero. Therefore, we choose the next experimental conditions with the lowest acquisition value, cf. Fig. 1(d).

## III. Results and Discussion

To examine the effectiveness of the PIBO method for etching process optimization, we prepared an initial dataset comprising 8 sets of process parameters. Their ER ranged from 59 nm/min to 94 nm/min, while the Ra ranged between 5.3 nm and 11.4 nm. Subsequently, we used PIBO to obtain optimized process conditions for an ER of 100 nm/min (±3 nm/min) and a Ra of less than 5 nm. Fig. 2 shows the acquisition of 8 initial data (black triangle) and the data after optimization (red star) in the parameter space of PW and P. It is noteworthy that the optimized parameter values are not within the range of the existing data, indicating that this prediction method can extrapolate beyond the original data range. Fig. 3 shows the ER and Ra as functions of the number of etching runs, respectively. The parameters after optimization yield an ER of

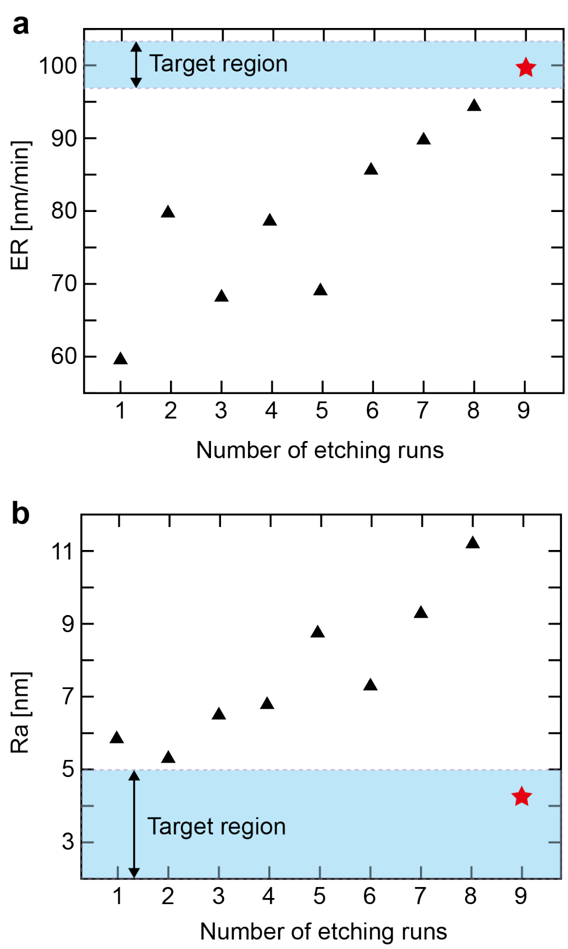


Fig. 3. (a) ER value for the N9 is within the target region of 100 ± 3 nm/min, (b) Ra value for the N9 is within the target region of $\leq$ 5 nm.

99 nm/min and an Ra of 4.3 nm, which meet the optimization targets. Fig. 4 shows the etched surface of one sample from the initial dataset and one after optimization, respectively. It is quite evident that the etched surface after optimization is smoother, confirming the framework's capabilities.

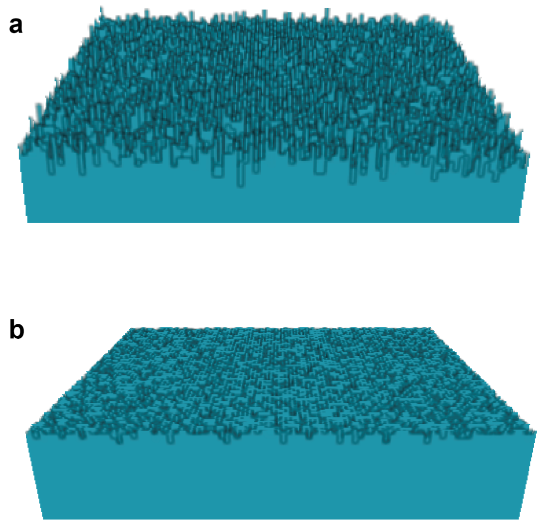


Fig. 4. 3D etch simulation results. The surface of the (b) N9 is smoother than that of the (a) N1.

## ACKNOWLEDGMENT

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