A Data-Driven Computational Workflow For The Growth Of Porous Anodized Aluminum Oxide: Integration Of Surrogate Modeling And Uncertainty Quantification

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Introduction

The electrochemical growth of anodic aluminum oxide (AAO) is governed by complex coupled physical, chemical, and transport phenomena. We present a **quantified computational framework** that simulates the AAO **growth** process, integrating physics-based modelling, data-driven modeling, surrogate modeling, and uncertainty quantification (**UQ**) to enhance predictive accuracy and computational efficiency. The model captures four distinct phases of anodization—compact oxide formation, pore nucleation, pore growth, and steady-state honeycomb structure development.

Computational workflow of AAO

To ensure the reliability of the developed computational workflow, the models must account for key physical, electrochemical, and transport processes governing anodization. Accordingly, the developed model considers four distinct mechanisms across four phases during the growth process of anodized aluminium. More specifically, these phases are connected based on time, applied voltage, and current density. The proposed phases are illustrated in Figure 1.

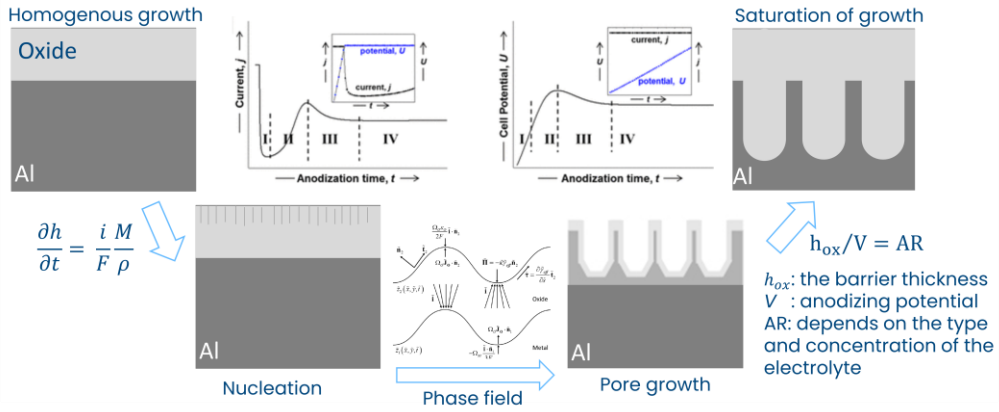

Figure 1: the proposed phases to simulate the AAO layer growth

To **reduce computational cost and complexity**, **Kriging surrogate models** are constructed at each stage of the workflow, enabling **efficient parameter exploration and uncertainty-aware predictions**. The stochastic nature of the pore nucleation phase is modeled using a **Weibull distribution**, ensuring a realistic representation of surface heterogeneity. Additionally, a **phase-field model** is incorporated to describe pore coalescence and the self-assembly of hexagonal structures in later growth phases.

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Validation and Sensitivity Analysis

The developed workflow is tested under different anodization conditions, demonstrating its capability to **simulate current transients, ion migration, and oxide layer evolution** with high fidelity. By integrating an **uncertainty quantification framework**, illustrated in Figure 2, we perform **sensitivity analysis** to identify key governing parameters such as applied voltage, electrolyte composition, and electric field strength. This approach enables **robust predictions and optimized process control**, ensuring the model's reliability in different anodization scenarios.

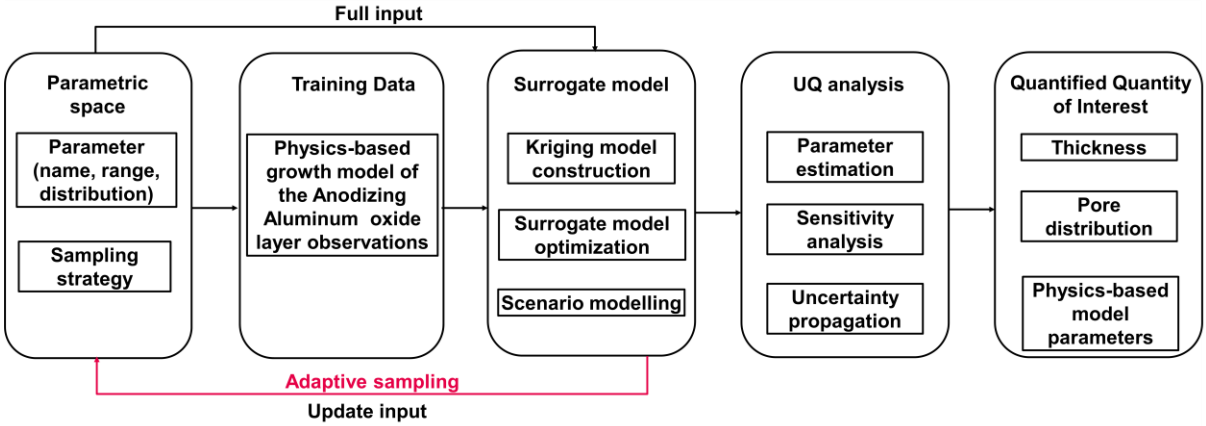

Figure 2: uncertainty quantification workflow using surrogate models. (adapted with change from 1).

Initial Results and Outlook

The initial results of the developed quantified workflow showed good agreement with experimental measurement using FIB, as can be seen in Figure 3. Moreover, the proposed methodology contributes to the development of computationally efficient, uncertainty-aware models for **electrochemical material processing**, advancing the integration of physics-based and data-driven approaches.

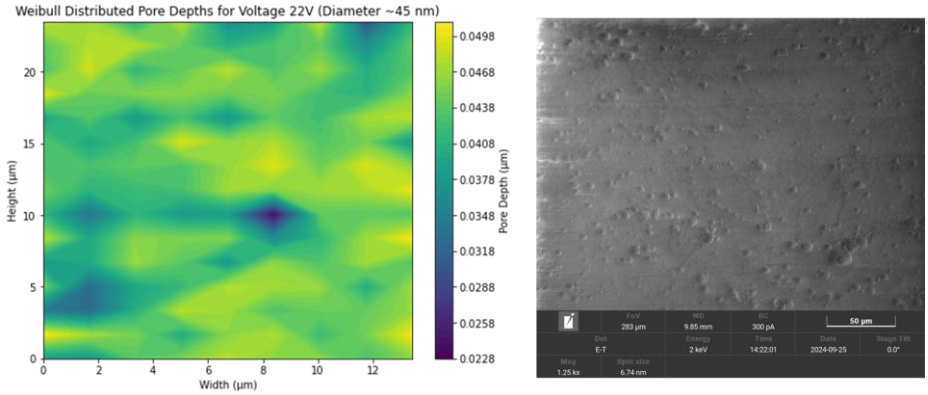

Figure 3: Sample of validation imaging, to the right is the distribution of pores and their depth by Weibull function and to the left is the FIB image at the same applied voltage of 22V.

References

[1] T. AlBaraghtheh, R. Willumeit-Römer, B. Zeller-Plumhoff,(2024). Best Practices in Developing a Workflow for Uncertainty Quantification for Modeling the Biodegradation of Mg-Based Implants. Adv. Sci., 11, 2403543.