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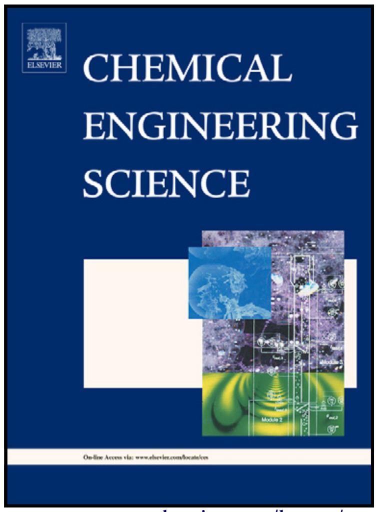

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Uncertainty Analysis and Robust Optimization of Multiscale Process Systems with Application to Epitaxial Thin Film Growth

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Abstract

Multiscale modeling of materials growth involves inherently coupled processes that span over a wide range of time and length scales. As a common practice, a multiscale model is adopted to simulate the thin film deposition process that augments Partial Differential Equations (PDEs), describing the macro-scale phenomena, with a high-order lattice-based kinetic Monte Carlo (KMC) simulator, which aims to capture thin film microstructure. Although such a model is a fair representation of the system, the evolution of thin film encompasses processes that are subject to model parameter uncertainty that can significantly affect the control and optimization objectives of this process, e.g. film's roughness and thickness. Thus, to provide a robust and more realistic strategy, it is crucial to perform an uncertainty analysis for this process. This work explores a systematic framework to analyze model parameter uncertainty for robust control and optimization of multiscale models. Such an analysis is extremely challenging due to i) the lack of a closed formulation between the process optimization objective (i.e. film thickness) and the model parameters and ii) the computational costs incurred to model the fine-scale events, typically performed using KMC simulation. To tackle these

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