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Robust multivariable estimation and control in an epitaxial thin film growth process under uncertainty

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ABSTRACT

This study presents a multivariable robust estimator that predicts the controlled outputs in a thin film growth process for online applications. The evolution of the epitaxial growth process on a substrate is modeled based on a multiscale approach, coupling a continuum gas phase model and a kinetic Monte Carlo (KMC) model that describes the evolution of the thin film surface. In the estimator, the issue of computationally intensive KMC simulations is circumvented by developing reduced-order models that are identified offline based on data obtained from the multiscale model. This approach significantly reduces the simulation time over KMC and makes the online control and optimization feasible. The estimator evaluates the surface roughness and growth rate based on the substrate temperature and the bulk precursor mole fraction during the growth process. To provide robust estimations, the estimator is designed to evaluate the upper and lower bounds on the outputs under model parameter uncertainties. To assess the uncertainty propagation into the system's outputs, power series expansion (PSE) is employed in the presence of distributional parametric uncertainties. The sensitivities of the outputs with respect to the uncertain parameters are assessed offline at different substrate temperatures and bulk precursor mole fractions. Accordingly, upper and lower bounds on the outputs are determined at a specific confidence level and employed to identify a reduced-order model for online applications. To assess the efficiency of the estimator, proportional integral (PI) controllers are coupled with the estimator to control surface roughness and growth rate while manipulating the substrate temperature and the bulk precursor mole fraction, respectively. The robust control of the process under parameter uncertainties is investigated using the bounds estimated on the controlled outputs.

1. Introduction

Thin film deposition from gas phase precursors is a key unit operation to manufacture high quality semiconductors [1]. The film microstructure is determined by the surface microscopic events that strongly depend on the macroscopic behavior of this process. As such, highly efficient control and optimization frameworks are needed to achieve specific thin film's characteristics by manipulating the macroscopic variables of the process [2]. Although optical *in-situ* devices can be employed to measure the system's micro-scale properties, they mostly cannot provide frequent measurements, which are required to develop an effective feedback control strategy [3]. Hence, real-time estimators are needed to estimate the controlled outputs at a time scale comparable to the real thin film growth process while online measurements are not available. To model this process, the thin film growth, and its interaction with the surroundings, needs to be studied by coupling the chemical and physical phenomena occurring over different temporal and spatial scales [4]. Multiscale modeling provides a framework to describe the effect of macroscopic variables on microscopic phenomena of thin film surface configuration [5,6]. In [7], the inherent multiscale nature of the epitaxial growth was investigated through coupling of a deterministic continuum model representing the macroscopic scale events and a stochastic lattice-based kinetic Monte Carlo (KMC) model, which describes the microscopic surface morphology. Despite the fact that multiscale modeling is regarded as an attractive alternative tool compared to the application of molecular modeling techniques for the entire process domain, this approach often requires computationally intensive simulations. This issue results in profound limits in the development of real-time online control for these systems and therefore has motivated significant research efforts toward the development of efficient reduced models [8]. A methodology for real-time estimation and control of roughness during thin film growth process

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has been proposed based on multiple reduced-order lattices in KMC simulations, an adaptive filter and measurement error compensator [9]. Thus, the reduce-order models can either be used as an estimator for feedback control in the absence of measurement, or as a basis for the design of a model predictive control (MPC) framework [10–12]. In most of these approaches, the precision of the estimator depends upon the output measurement provided by the sensor.

Although KMC models have been adopted for estimation and control in a few cases, the unavailability of a closed-form model constrains their applications in model-based approaches. Methodologies for multivariable predictive control approaches have been developed through identification of linearized stochastic partial differential equation (PDE) models, used to describe the microscopic phenomena [13]. Those closed-form models describe the evolution of the surface height in certain processes such as epitaxial growth [14]. Likewise, model reduction can be achieved through direct identification of the underlying master equation [15,16]. To reduce the number of configurations in the master equation, similar configurations can be grouped into specific classes [17]. To estimate the surface roughness using those reduced models, a linear least-squares-based observer is developed that can be utilized for control and optimization applications [18]. A comprehensive optimization and control strategy requires the simultaneous modeling of fluid phase and surface morphology. Accordingly, a closed-form model has been obtained by deriving low-dimensional approximations through proper orthogonal decomposition for both microscopic and macroscopic scales [19]. In [20], the receding horizon control of surface roughness is accomplished via identification of a state-space model for a set of coarse observables employing proper orthogonal decomposition and Carleman linearization. The microstructure of the thin film surface is described through identification of a set of spatially coarse invariant parameters [21]. In [22], a low-order model was developed based on the data collected from a coupled KMC-finite difference code for the robust control of a copper electrodeposition process.

Another complication in controlling the thin film growth process is model-plant mismatch [23,24]. The evaluation of accurate model parameters at molecular scale is not trivial [25], and accordingly experimental design methodologies have gained attention to determine the process optimal parameters in molecular models [26,27]. In those works, to avoid high computational intensity encountered with molecular simulations, the model is approximated using low-order power series expansion (PSE) [28]. These approaches apply sensitivity analysis not only to determine the key parameters affecting the outputs of the process, but to analyze model uncertainty. Sensitivity analysis of the KMC models involves computationally intensive simulations that are inherently stochastic; thus, efficient gradient estimations method have been proposed in the literature to analyze such processes [29,30]. Quantifying the influence of parameter uncertainties on the process states and outputs is essential to improve productivity in industrial applications. Although Monte Carlo sampling-based method can be used to propagate the uncertainty into the outputs via the primary model, it is computationally intensive compared to PSE and polynomial chaos expansion (PCE). In the expansion-based approaches, the actual process model is approximated with a simple representation that can be evaluated at minimum computational cost [31]. Uncertainty analysis using these expansions has initiated significant advances in the robust optimal control of batch processes [32–34], and optimal design of large-scale chemical processes [35]. Likewise, robust control of thin film microstructure requires estimation of the distribution of the performance index. In [36], a second-order PSE was adopted to propagate the parameter uncertainty into the final surface roughness in order to show the advantage of applying nonlinear model predictive control (NMPC) approach in microelectronics industries under uncertainty. The model employed in that work to describe the thin film surface properties is a reduced-order closed-form model presented in [15]. In our previous work, high-order PSEs have been employed to analyze the uncertainty propagation into the rates of the microscopic events in multiscale process systems [37]. Upper and lower bounds estimated on the outputs from the distributions of the states were used for robust optimization of a thin film growth process. In that work, upper and lower bounds were estimated using KMC simulations and that approach was appropriate for offline optimization. However, the implementation of that framework for online applications is still challenging due to the computational costs associated with the simulations of the KMC model.

Although the controllability of the thin film growth process has been studied in the literature, model parameter uncertainty has been usually neglected in those methodologies. Moreover, most of the advanced microstructure controllers proposed in the literature for thin film deposition require measurements at fine scale, while in practice, thin film depositions are typically operated in open-loop. Thus, control approaches that can operate regardless of the measurements are essential for the efficient operation of these processes. In this study, to address the issue of the lack of frequent measurements, an estimator has been developed that is able to provide estimates of the controlled outputs based on the key manipulated variables typically available for these systems. Since the uncertainties at the microscopic scale can lead to drastic loss in the control objective, the estimator is extended to provide a robust estimate of the outputs of interest under parametric uncertainties. In order to reduce the computational burden, the estimator is designed via offline identification. This approach enables the estimator to predict the controlled outputs for online purposes. To investigate the effectiveness of the estimator, the control of surface roughness and growth rate in a thin film growth process is performed under different scenarios. This paper is organized as follows: in Section 2, the multiscale modeling framework used in this study to describe the thin film growth process is provided. Section 3 presents the PSE-based approach to propagate the model parameter uncertainty into system's outputs. Also, an algorithm to construct the multivariable robust estimator is presented in this section. In Section 4, the performance of the estimator is evaluated by coupling the estimator with PI controllers to simultaneously control the surface roughness and the growth rate under different scenarios. Concluding remarks are presented at the end of this article.

2. Thin film growth model

In this work, the thin film growth process in a stagnation-point flow chamber has been studied. The gas flow transfers precursor atoms to the substrate and forms a uniform boundary layer of gas adjacent to the surface of the film. As shown in Fig. 1, these atoms are deposited on the substrate through microscopic events. A multiscale integration hybrid technique has been employed to capture the disparity in the scales of this system. The entire domain is decomposed and continuum description is used to model the aforementioned boundary layer while the surface of the film is described using a two-dimensional lattice-based KMC simulation model. Each of these models is described next.

2.1. *Gas phase macroscopic model*

At the macroscopic level, continuum descriptions of fluid flow, heat and mass transfer can be employed. Creating an axially uniform high velocity flow in the inlet of the chamber avoids the development of velocity, temperature and concentration gradients