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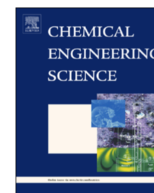

Stochastic nonlinear model predictive control applied to a thin film deposition process under uncertainty

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HIGHLIGHTS

- A thin film deposition process is simulated using the multiscale approach.
- Models are developed to predict the statistical moments of thin film properties.
- An uncertainty analysis of the process is performed using PSEs.
- Sensitivities are obtained from data collected offline using the multiscale model.
- The model is applied as a basis of a stochastic NMPC framework.

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ABSTRACT

This paper investigates the application of stochastic nonlinear model predictive control (NMPC) to a thin film deposition process in the presence of model-plant mismatch while ensuring constraints at a specific probability limit. To capture the multiscale nature of the process, the evolution of the thin film is modelled using nonlinear partial differential equations (PDEs) embedded with lattice-based kinetic Monte Carlo (KMC) simulations. To provide a computationally tractable closed-form expression for online predictive control applications, model identification is performed using data collected from the multiscale deposition model. The closed-form model predicts the expected value and the variance of the thin film properties based on the substrate temperature during the deposition process. The parameters of the closed-form model are determined offline employing power series expansion (PSE). The closed-form model allows the reformulation of probabilistic constraints into their corresponding deterministic expressions thus enabling the design of a computationally tractable stochastic NMPC. To show the effectiveness of the approach, a shrinking horizon stochastic NMPC framework is devised to minimize the final surface roughness while complying with actuator constraints and a probabilistic constraint on the final film thickness.

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1. Introduction

Thin film deposition is a key unit operation in the microelectronics industry where advanced control strategies are required to improve product quality specifications (Braatz et al., 2006a; Nagy and Allgöwer, 2007). Model predictive control (MPC) provides an effective framework employing the system model to predict the control actions which optimize a performance index in the presence of constraints (Allgöwer et al., 2004; García et al., 1989; Qin and Badgwell, 2003). Hence, in practice, a closed-form model is essential for efficient and accurate forecasting of the process behaviour (Morari and Lee, 1999). Unlike conventional feedback controllers, the main advantage of the MPC formulation is the ability to cope with the safety, operational or economic constraints in the presence of model-plant mismatch (Mayne et al., 2000). Robust formulations have been proposed to guarantee the closed-loop performance under deterministic parameter uncertainty in MPC frameworks (Bemporad and Morari, 1999; Mayne et al., 2006; Zeilinger et al., 2014). Robust MPC addresses the optimal control problems with hard constraints that should be satisfied for all realizations of the parameter uncertainty (Lee and Yu, 1997; Zafiriou, 1990). Such a control design, however, can be overly conservative for realizations in the uncertainties that are more likely to occur (Nagy and Braatz, 2004). Therefore, distributional uncertainty analyses have been proposed where the restriction

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imposed by the bounded uncertainty description is relaxed using probabilistic-based uncertainties (Nagy and Braatz, 2003a, 2003b). To analyse the effect of different uncertainty descriptions on the thin film deposition, offline optimization of the process has been performed under bounded and probabilistic uncertainties (Rasoulian and Ricardez-Sandoval, 2015a). In addition to distributional parameter uncertainties, the MPC formulation can be solved with probabilistic constraints (Cannon et al., 2009; Lee, 2014; Li et al., 2002; Mesbah et al., 2014). Adopting a chance constrained approach, stochastic MPC allows an acceptable level of risk where the constraints are satisfied with a specific probability of occurrence (Cannon et al., 2011; Li et al., 2008; Schwarm and Nikolaou, 1999).

In essence, an effective MPC framework for the deposition process requires a closed-form model that represents the complex dynamics of the process. A comprehensive modelling of this process requires expressions that describe the evolution of the material at the molecular level due to interactions with the corresponding surroundings. The pertinent model that captures the multiscale nature of this process typically couples lattice-based kinetic Monte Carlo (KMC) simulations capturing the microscopic variations with nonlinear partial differential equations (PDEs) that describe the macro-scale phenomena (Lam and Vlachos, 2001). Due to embedded KMC simulations, this multiscale model does not provide a closed-form expression that is needed for real-time model-based strategies (Christofides and Armaou, 2006). This limitation has motivated the development of low-order models for online control and optimization applications. Reduced-order lattices have been employed in the KMC simulations to develop an estimator for feedback control in the absence of measurements at the micro-scale level, or as a basis to design an MPC framework (Christofides et al., 2008; Lou and Christofides, 2004). Attention has also been directed towards data-driven identification of low-order models to approximate the KMC simulations for real-time control applications (Gallivan and Murray, 2004; Middlebrooks and Rawlings, 2007; Raimondeau and Vlachos, 2000; Varshney and Armaou, 2008). The input–output behaviour of a coupled KMC and finite-difference code has been employed to develop a low-order model for a copper electrodeposition process (Rusli et al., 2006). In another approach, the evolution of the surface morphology in the deposition process is modelled by stochastic PDEs where the parameters of the model are identified using data collected from KMC simulations (Hu et al., 2009; Lou and Christofides, 2006; Ni and Christofides, 2005). Moreover, coarse time-steppers have been proposed that apply macroscopic system level tasks to multiscale systems without explicitly developing a closed-form expression (Armaou et al., 2004; Siettos et al., 2003). That approach is applicable to low statistical moments of microscopically evolving properties.

Additional complexity in modelling the thin film deposition process arises due to limited experimental data available at the fine-scale level (Ricardez-Sandoval, 2011; Vlachos, 2005). Development of first-principle models using *ab initio* methods or density functional theory (DFT) calculations requires high computational costs (Li et al., 2015). DFT calculations, however, can provide the prior estimates of the parameters in the optimal experimental design (Braatz et al., 2006b). In parameter optimization approaches, highly expensive molecular simulations can be circumvented using low-order models developed based on power series expansion (PSE) (Prasad and Vlachos, 2008; Raimondeau et al., 2003). Despite the efforts made for parameter optimization, model-plant mismatch has mostly been overlooked in control and optimization of thin film deposition processes, mainly due to the computational costs of uncertainty analysis in multiscale process systems. The common approach for distributional uncertainty propagation is the application of a sampling-based technique on the process model. In a thin film deposition process, however, the current multiscale models are computationally prohibitive to assess product variability using the traditional sampling-based methods. Analytical techniques such as PSE and polynomial chaos expansion provide a practical approach to this problem since the complex multiscale model can be approximated with a mathematical expansion (Bahakim et al., 2014; Kumar and Budman, 2014; Mandur and Budman, 2014; Nagy and Braatz, 2007). In the PSE, the coefficients of the expansion consist of the sensitivities of the outputs with respect to the uncertain parameters. Since the KMC simulations are inherently stochastic and are not available as a closed-form expression, the sensitivities have to be determined numerically using average of responses from multiple simulations (Drews et al., 2004; McGill et al., 2012). Therefore, uncertainty analysis of multiscale system using PSEs can still be computationally intensive. Nagy and Allgöwer (2007) adopted PSEs to develop a nonlinear model predictive control (NMPC) framework that minimizes the end-point thin film properties in a deposition process. In that work, the first and second-order sensitivities were calculated using the closed-form state-space model provided by Gallivan (2003). In our previous work, the robust optimization of thin film epitaxial growth is performed through a PSE-based algorithm that approximates the distribution of rates of microscopic events under uncertainty. Then, using the probability distribution function (PDF) of the rates, probabilistic bounds on the outputs are estimated (Rasoulian and Ricardez-Sandoval, 2014). For online applications, however, that method is computationally intractable and a closed-form model is required to predict the controlled outputs efficiently (Rasoulian and Ricardez-Sandoval, 2015b). Therefore, an algorithm has been proposed for offline identification of a closed-from model that predicts the controlled outputs at a predefined probability for a robust NMPC application (Rasoulian and Ricardez-Sandoval, 2015c). In that work, to ensure the robust performance, hard constraints were imposed on the MPC framework. The internal model used in the MPC algorithm is a closed-form model that was identified offline to represent the dynamic behaviour of system under uncertainty in the model parameters. The identification of this model was performed such that it predicts bounds on the outputs according to a narrow confidence level, which must be specified a priori. To that end, new offline identification is required in that approach to be able to estimate the outputs at a different confidence level.

In this paper, a systematic framework is presented that enables the identification of a closed-form model to estimate the first and second-order statistical moments of the thin film properties. The parameters of the closed-form model are determined offline through PSEs developed for the multiscale model under uncertainty in the model parameters. This improves on our previous work since the conservatism imposed by the hard constraints is reduced by imposing probabilistic (soft) constraints in the MPC. The closed-form model identified from the algorithm proposed in this work enables the prediction of outputs at any probability limit. Moreover, employing this model the probabilistic constraints in the stochastic MPC framework can be reformulated as deterministic constraints, thus allowing the implementation of this control framework for the thin film deposition process under uncertainty in the model parameters.

The remainder of the paper is organized as follows. In Section 2, the multiscale model of the thin film deposition process is presented. The PSE-based uncertainty propagation employed for this process, and the required computational costs, are also presented in this section to motivate the identification of a closed-form model for real-time applications. Section 3 presents the algorithm used in this work to develop a closed-form model that predicts the statistical moments of the controlled outputs as a function of the control actions during the deposition process.

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