Simultaneous Regulation of Surface Roughness and Porosity in Thin Film Growth

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Abstract: This work focuses on simultaneous control of surface roughness and film porosity in a porous thin film deposition process modeled via kinetic Monte Carlo simulation on a triangular lattice. The microscopic model of the thin film growth process includes adsorption and migration processes. Vacancies and overhangs are allowed inside the film for the purpose of modeling thin film porosity. Appropriate closed-form dynamic models are first derived to describe the evolution of film surface roughness and porosity and used as the basis for the design of a model predictive control algorithm that includes penalty on the deviation of surface roughness and film porosity from their respective set-point values. Closed-loop simulations demonstrate that when simultaneous control of surface roughness and porosity is carried out, a balanced trade-off is obtained in the closed-loop system between the two control objectives of surface roughness and porosity regulation.

Keywords: thin film processing, roughness, porosity, model predictive control

1. INTRODUCTION

Thin film deposition processes play an important role in the semiconductor industry. Thin film microstructure, including surface roughness and film porosity, strongly affects the electrical and mechanical properties of thin films and of the resulting devices. Motivated by this, recent research efforts on modeling and control of thin film microstructure have focused mostly on thin film surface roughness on the basis of microscopic thin film growth models which utilize a square lattice. Specifically, kinetic Monte Carlo (kMC) models based on a square lattice and utilizing the solid-on-solid (SOS) approximation for deposition were initially employed to develop an effective methodology to describe the evolution of film microstructure and design feedback control laws for thin film surface roughness (Lou and Christofides (2003); Christofides et al. (2008)). This control methodology was successfully applied to surface roughness control of: a) a gallium arsenide (GaAs) deposition process (Lou and Christofides (2004)), and b) a multi-species deposition process with long range interactions (Ni and Christofides (2005a)). Furthermore, a method that couples partial differential equation (PDE) models and kMC models was developed for computationally efficient multiscale optimization of thin film growth (Varshney and Armaou (2005)). However, kMC models are not available in closed-form and this limitation restricts the use of kMC models for system-level analysis and design of model-based feedback control systems. To overcome this problem, model identification of linear deterministic models from outputs of kMC simulators was used for controller design using linear control theory (Siettos et al. (2003); Armaou et al. (2004)). However, deterministic models are only effective in controlling the expected values of macroscopic variables, i.e., the first-order statistical moments of the microscopic distribution. For higher statistical moments of the microscopic distributions such as the surface roughness (the second moment of height distribution on a lattice), deterministic models are not sufficient, and stochastic differential equation (SDE) models may be needed.

SDEs arise naturally in the modeling of surface morphology of ultra thin films in a variety of thin film preparation processes (Edwards and Wilkinson (1982); Villain (1991); Vvedensky et al. (1993)). Advanced control methods based on SDEs have been developed to address the need of model-based feedback control of thin film microstructure. Specifically, methods for state feedback control of surface roughness based on linear (Lou and Christofides (2005); Ni and Christofides (2005b)) and nonlinear (Lou and Christofides (2008)) SDE models have been developed. However, state feedback control assumes full knowledge of the surface morphology at all times, which may be a restrictive requirement in certain practical applications. To this end, output feedback control of surface roughness was recently developed (Hu et al. (2008)) by incorporating a Kalman-Bucy type filter, which utilizes information from a finite number of noisy measurements.

In the context of modeling of thin film porosity, kMC models have been widely used to model the evolution of porous thin films in many deposition processes and to investigate the influence of the macroscopic parameters on the porous thin film microstructure (Wang and Clancy (1998); Zhang et al. (2004)). Deterministic and stochastic ordinary differential equation (ODE) models of film porosity were recently developed (Hu et al. (2009a)) to model the evolution of film porosity and its fluctuation and design model predictive control (MPC) algorithms to control film porosity to a desired level and reduce run-to-run porosity variability. Despite recent significant efforts on modeling and control of surface roughness and film porosity, simultaneous regulation of surface roughness and film porosity within a unified control framework has not been investigated.

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Motivated by these considerations, the present work focuses on simultaneous regulation of surface roughness and film porosity in a porous thin film deposition process modeled via kMC simulation on a triangular lattice. The definition of surface height profile is first introduced and the dynamics of surface height of the thin film are described by an Edwards-Wilkinson (EW)-type equation. Subsequently, an appropriate definition of film site occupancy ratio (SOR) is introduced to represent the porosity and a deterministic ODE model is derived to describe the time evolution of film SOR. The model parameters are estimated on the basis of data obtained from the kMC simulator of the deposition process using least-square methods. The developed dynamic models are used as the basis for the design of a model predictive control algorithm that includes penalty on the deviation of surface roughness square and film SOR from their respective set-point values. Simulation results demonstrate the applicability and effectiveness of the proposed modeling and control approach in the context of the deposition process under consideration.

2. PROCESS DESCRIPTION AND MODELING

2.1 On-lattice kinetic Monte Carlo model of film growth

The thin film growth process considered in this work includes two microscopic processes: an adsorption process, in which particles are incorporated into the film from the gas phase, and a migration process, in which surface particles move to adjacent sites (Wang and Clancy (1998); Levine and Clancy (2000); Yang et al. (1997)). Specifically, the film growth model used in this work is an on-lattice kMC model in which all particles occupy discrete lattice sites. The on-lattice kMC model is valid for temperatures $T < 0.5T_m$, where T_m is the melting point of the crystal. At high temperatures ($T \lesssim T_m$), the particles cannot be assumed to be constrained on the lattice sites and the on-lattice model is not valid. In this work, a triangular lattice is selected to represent the crystalline structure of the film, as shown in Fig.1. All particles are modeled as identical hard disks and the centers of the particles deposited on the film are located on the lattice sites. The diameter of the particles equals the distance between two neighboring sites. The width of the lattice is fixed so that the lattice contains a fixed number of sites in the lateral direction. The new particles are always deposited vertically from the top side of the lattice where the gas phase is located; see Fig.1. Particle deposition results in film growth in the direction normal to the lateral direction. The direction normal to the lateral direction is thus designated as the growth direction. The number of sites in the lateral direction is defined as the lattice size and is denoted by L. The lattice parameter, a, which is defined as the distance between two neighboring sites and equals the diameter of a particle (all particles have the same diameter), determines the lateral extent of the lattice, La.

The number of nearest neighbors of a site ranges from zero to six, the coordination number of the triangular lattice. A site with no nearest neighbors indicates an unadsorbed particle in the gas phase (i.e., a particle which has not been deposited on the film yet). A particle with six nearest neighbors is associated with an interior particle that is fully surrounded by other particles and cannot migrate. A particle with two to five nearest neighbors is possible to diffuse to an unoccupied neighboring site with a probability that depends on its local environment. In the triangular lattice, a particle with only one nearest neighbor is considered unstable and is subject to instantaneous surface relaxation.

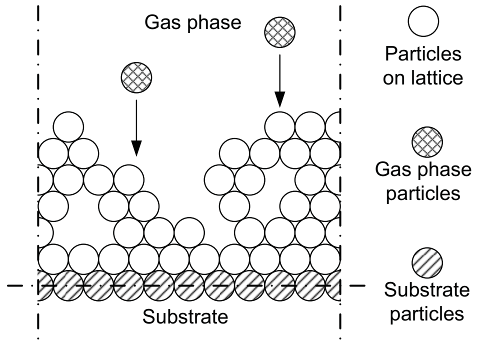

Fig. 1. Thin film growth process on a triangular lattice.

In the simulation, a bottom layer in the lattice is initially set to be fully packed and fixed, as shown in Fig.1. There are no vacancies in this layer and the particles in this layer cannot migrate. This layer acts as the substrate for the deposition and is not counted in the computation of the number of the deposited particles, i.e., this fixed layer does not influence the film surface roughness and porosity (see Section 2.2 below). All microscopic processes (Monte Carlo events) are assumed to be Poisson processes. These Monte Carlo events occur randomly with probabilities proportional to their respective rates. The events are executed instantaneously upon selection and the state of the lattice remains unchanged between two consecutive events. The specific rules used to carry out the adsorption and migration processes and their simulation are discussed in detail in Hu et al. (2009b) and are not presented here due to space limitations.

2.2 Definitions of surface roughness and site occupancy ratio

Utilizing the continuous-time Monte Carlo algorithm, simulations of the kMC model of a porous silicon thin film growth process can be carried out. Snapshots of film microstructure, i.e., the configurations of particles within the triangular lattice, are obtained from the kMC model at various time instants during process evolution. To quantitatively evaluate the thin film microstructure, two variables, surface roughness and film porosity, are introduced in this subsection.

Surface roughness, which measures the texture of thin film surface, is represented by the root mean square (RMS) of the surface height profile of the thin film. Determination of surface height profile is slightly different in the triangular lattice model compared to a SOS model. In the SOS model, the surface of thin film is naturally described by the positions of the top particles of each column. In the triangular lattice model, however, due to the existence of vacancies and overhangs, the definition of film surface needs further clarification. Specifically, taking into account practical considerations of surface roughness measurements, the surface height profile of a triangular lattice model is defined based on the particles that can be reached from abobe in the vertical direction, as shown in Fig.2. In this definition, a particle is considered as a surface particle only if it is not blocked by the particles in both neighboring columns. Therefore, the surface height profile of a porous thin film is the line that connects the sites that are occupied by the surface particles. With this definition, the surface height profile can be treated as a function of the spatial coordinate. Surface roughness, as a measurement of the surface texture, is defined as the standard deviation of the surface height profile from its average height. The definition expression of surface roughness is given later in Section 3.1.

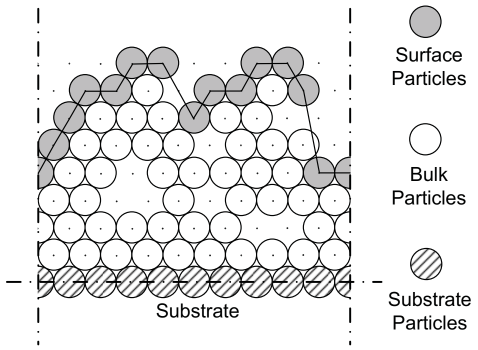

Fig. 2. Definition of surface height profile. A surface particle is a particle that is not blocked by particles from both of its neighboring columns in the vertical direction.

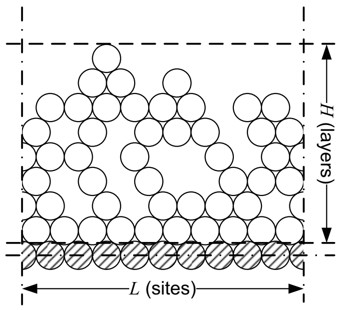

Fig. 3. Illustration of the definition of film SOR of Eq.1.

In addition to film surface roughness, the film site occupancy ratio (SOR) is introduced to represent the extent of the porosity inside the thin film. The mathematical expression of film SOR is defined as follows:

$$\rho = \frac{N}{LH} \tag{1}$$

where ρ denotes the film SOR, N is the total number of deposited particles on the lattice, L is the lattice size, and H denotes the number of deposited layers. Note that the deposited layers are the layers that contain only deposited particles and do not include the initial substrate layers. The variables in the definition expression of Eq.1 can be found in Fig.3. Since each layer contains L sites, the total number of sites in the film that can be contained within the H layers is LH. Thus, film SOR is the ratio of the occupied lattice sites, N, over the total number of available sites, LH. Film SOR ranges from 0 to 1. Specifically, $\rho = 1$ denotes a fully occupied film with a flat surface. The value of zero is assigned to ρ at the beginning of the deposition process since there are no particles deposited on the lattice.

3. DYNAMIC MODEL CONSTRUCTION AND PARAMETER ESTIMATION

3.1 Edwards-Wilkinson-type equation of surface height

An Edwards-Wilkinson (EW)-type equation can be used to describe the surface height evolution in many microscopic processes that involve thermal balance between adsorption (deposition) and migration (diffusion). In this work, an EW-type equation is chosen to describe the dynamics of the fluctuation of surface :

$$\frac{\partial h}{\partial t} = r_h + \nu \frac{\partial^2 h}{\partial x^2} + \xi(x,t) \tag{2}$$

subject to PBCs:

$$h(-\pi,t) = h(\pi,t), \quad \frac{\partial h}{\partial x}(-\pi,t) = \frac{\partial h}{\partial x}(\pi,t) \tag{3}$$

and the initial condition:

$$h(x,0) = h_0(x) \tag{4}$$

where $x \in [-\pi,\pi]$ is the spatial coordinate, t is the time, r_h and ν are the model parameters, and $\xi(x,t)$ is a Gaussian white noise with the following expressions for its mean and covariance:

$$\begin{aligned} \langle \xi(x,t) \rangle &= 0 \\ \langle \xi(x,t)\xi(x',t') \rangle &= \sigma^2 \delta(x-x')\delta(t-t') \end{aligned} \tag{5}$$

where σ^2 is a parameter which measures the intensity of the Gaussian white noise and $\delta(\cdot)$ denotes the standard Dirac delta function.

To proceed with model parameter estimation and control design, a stochastic ODE approximation of Eq.2 is first derived using Galerkin's method. Consider the eigenvalue problem of the linear operator of Eq.2, which takes the form:

$$\begin{gathered} A\bar{\phi}_n(x) = \nu \frac{d^2\bar{\phi}_n(x)}{dx^2} = \lambda_n \bar{\phi}_n(x) \\ \bar{\phi}_n(-\pi) = \bar{\phi}_n(\pi), \quad \frac{d\bar{\phi}_n}{dx}(-\pi) = \frac{d\bar{\phi}_n}{dx}(\pi) \end{gathered} \tag{6}$$

where λ_n denotes an eigenvalue and $\bar{\phi}_n$ denotes an eigenfunction. A direct computation of the solution of the above eigenvalue problem yields $\lambda_0 = 0$ with $\psi_0 = 1/\sqrt{2\pi}$, and $\lambda_n = -\nu n^2$ (λ_n is an eigenvalue of multiplicity two) with eigenfunctions $\phi_n = (1/\sqrt{\pi})\sin(nx)$ and $\psi_n = (1/\sqrt{\pi})\cos(nx)$ for $n = 1,\cdots,\infty$. Note that the $\bar{\phi}_n$ in Eq.6 denotes either ϕ_n or ψ_n. For fixed positive value of ν, all eigenvalues (except the zero-th eigenvalue) are negative and the distance between two consecutive eigenvalues (i.e. λ_n and λ_{n+1}) increases as n increases.

To this end, the solution of Eq.2 is expanded in an infinite series in terms of the eigenfunctions as follows:

$$h(x,t) = \sum_{n=1}^{\infty} \alpha_n(t)\phi_n(x) + \sum_{n=0}^{\infty} \beta_n(t)\psi_n(x) \tag{7}$$

where $\alpha_n(t)$, $\beta_n(t)$ are time-varying coefficients. Substituting the above expansion for the solution, $h(x,t)$, into Eq.2 and taking the inner product with the adjoint eigenfunctions, $\phi_n^*(x) = (1/\sqrt{\pi})\sin(nx)$ and $\psi_n^*(x) = (1/\sqrt{\pi})\cos(nx)$, the following system of infinite stochastic ODEs is obtained:

$$\begin{gathered} \frac{d\beta_0}{dt} = \sqrt{2\pi} r_h + \xi_\beta^0(t) \\ \frac{d\alpha_n}{dt} = \lambda_n \alpha_n + \xi_\alpha^n(t), \frac{d\beta_n}{dt} = \lambda_n \beta_n + \xi_\beta^n(t), n = 1,\ldots,\infty \end{gathered} \tag{8}$$

where

$$\xi_\alpha^n(t) = \int_{-\pi}^{\pi} \xi(x,t)\phi_n^*(x)dx, \quad \xi_\beta^n(t) = \int_{-\pi}^{\pi} \xi(x,t)\psi_n^*(x)dx. \tag{9}$$

The covariances of $\xi_\alpha^n(t)$ and $\xi_\beta^n(t)$ can be computed as follows: $\langle \xi_\alpha^n(t)\xi_\alpha^n(t') \rangle = \sigma^2\delta(t-t')$ and $\left\langle \xi_\beta^n(t)\xi_\beta^n(t') \right\rangle = \sigma^2\delta(t-t')$.

Since the stochastic ODE system is linear, the analytical solution of state variance can be obtained from a direct computation as follows:

$$\begin{gathered} \left\langle \alpha_n^2(t) \right\rangle = \frac{\sigma^2}{2\nu n^2} + \left(\left\langle \alpha_n^2(t_0) \right\rangle - \frac{\sigma^2}{2\nu n^2} \right) e^{-2\nu n^2(t-t_0)} \\ \left\langle \beta_n^2(t) \right\rangle = \frac{\sigma^2}{2\nu n^2} + \left(\left\langle \beta_n^2(t_0) \right\rangle - \frac{\sigma^2}{2\nu n^2} \right) e^{-2\nu n^2(t-t_0)} \\ n = 1,2,\ldots,\infty \end{gathered} \tag{10}$$

where $\langle \alpha_n^2(t_0) \rangle$ and $\langle \beta_n^2(t_0) \rangle$ are the state variances at time t_0. The analytical solution of state variance of Eq.10 will be used in the parameter estimation and the MPC design.

When the dynamic model of surface height profile is determined, surface roughness of the thin film is defined as the standard deviation of the surface height profile from its average height and is computed as follows:

$$r(t) = \sqrt{\frac{1}{2\pi}\int_{-\pi}^{\pi}[h(x,t)-\bar{h}(t)]^2 dx} \tag{11}$$

where $\bar{h}(t) = \dfrac{1}{2\pi}\displaystyle\int_{-\pi}^{\pi} h(x,t)dx$ is the averaged surface height. According to Eq.7, we have $\bar{h}(t) = \beta_0(t)\psi_0$. Therefore, $\langle r^2(t) \rangle$ can be rewritten in terms of $\langle \alpha_n^2(t) \rangle$ and $\langle \beta_n^2(t) \rangle$ as follows:

$$\begin{aligned}\langle r^2(t) \rangle &= \frac{1}{2\pi}\left\langle \int_{-\pi}^{\pi}(h(x,t)-\bar{h}(t))^2 dx \right\rangle \\ &= \frac{1}{2\pi}\left\langle \sum_{i=1}^{\infty}(\alpha_i^2(t)+\beta_i^2(t)) \right\rangle = \frac{1}{2\pi}\sum_{i=1}^{\infty}\left[\langle \alpha_i^2(t) \rangle + \langle \beta_i^2(t) \rangle\right]\end{aligned} \tag{12}$$

where $\bar{h} = \dfrac{1}{2\pi}\displaystyle\int_{-\pi}^{\pi} h(x,t)dx = \beta_0(t)\psi_0$ is the average of surface height. Thus, Eq.12 provides a direct link between the state variance of the infinite stochastic ODEs of Eq.8 and the expected surface roughness of the thin film. Note that the model parameter r_h does not appear in the expression of surface roughness, since only the zeroth state, β_0, is affected by r_h but this state is not included in the computation of the expected surface roughness square of Eq.12.

3.2 Deterministic dynamic model of film site occupancy ratio

Since film porosity is another control objective, a dynamic model is necessary in the MPC formulation to describe the evolution of film porosity, which is represented by the film SOR of Eq.1. The dynamics of the expected value of the film SOR evolution are approximately described by a linear first-order deterministic ODE as follows:

$$\tau \frac{d\langle \rho(t) \rangle}{dt} = \rho^{ss} - \langle \rho(t) \rangle \tag{13}$$

where t is the time, τ is the time constant and ρ^{ss} is the steady-state value of the film SOR. The deterministic ODE system of Eq.13 is subject to the following initial condition:

$$\langle \rho(t_0) \rangle = \rho_0 \tag{14}$$

where t_0 is the initial time and ρ_0 is the initial value of the film SOR. Note that ρ_0 is a deterministic variable, since ρ_0 refers to the film SOR at $t = t_0$. From Eqs.13 and 14, it follows that

$$\langle \rho(t) \rangle = \rho^{ss} + (\rho_0 - \rho^{ss})\, e^{-(t-t_0)/\tau}. \tag{15}$$

3.3 Parameter estimation

Referring to the EW equation of Eq.2 and the deterministic ODE model of Eq.13, there are several model parameters, ν, σ^2, ρ^{ss} and τ, that need to be determined as functions of the substrate temperature. These parameters describe the dynamics of surface height and of film SOR and can be estimated by comparing the predicted evolution profiles from the dynamic models of Eqs.2 and 13 and the ones from the kMC simulation of the deposition process in a least-square sense (Hu et al. (2009a,b)).

Since surface roughness is a control objective, we choose the expected surface roughness square of Eq.12 as the output for the parameter estimation of the EW equation of Eq.2. Thus, the model coefficients, ν and σ^2, can be obtained by solving the minimization problem as follows:

$$\min_{\nu,\sigma^2}\sum_{i=1}^{n_1}\left[\langle r^2(t) \rangle - \frac{1}{2\pi}\sum_{i=1}^{\infty}\left(\langle \alpha_i^2(t) \rangle + \langle \beta_i^2(t) \rangle\right)\right]^2 \tag{16}$$

where n_1 is the number of the data samplings of surface height profile and surface roughness from the kMC simulations. The predictions of model state variance, $\langle \alpha_i^2(t) \rangle$ and $\langle \beta_i^2(t) \rangle$, can be solved from the analytical solution of Eq.10.

With respect to the parameters of the equation for film porosity, ρ^{ss} and τ can be estimated similarly from the solutions of Eq.15 as follows:

$$\min_{\rho^{ss},\tau}\sum_{i=1}^{n_2}\left[\langle \rho(t_i) \rangle - \left(\rho^{ss} + (\rho_0 - \rho^{ss})\, e^{-(t-t_0)/\tau}\right)\right]^2 \tag{17}$$

where n_2 is the number of the data samplings of film SOR from the kMC simulations. We note that since the dynamic models of film surface height and film SOR may have different dynamics, different numbers of data samplings at different time instants may be used to estimate the parameters of the dynamic models.

The data used for the parameter estimation are obtained from the open-loop kMC simulation of the thin film growth process. The process parameters, i.e., the substrate temperature and the adsorption rate, are fixed during each open-loop simulation. The predictions from the dynamic models with the estimated parameters are close to the open-loop simulation profiles. Detailed data and plots can be found in Hu et al. (2009b).

The parameters that are estimated from fixed operating conditions are suitable for the feedback control design in this work. This is because the control input in the MPC formulation is piecewise, i.e., the manipulated substrate temperature remains constant between two consecutive sampling times, and thus, the dynamics of the microscopic process can be predicted from the dynamic models with estimated parameters. The dependence of the model parameters on substrate temperature is used in the formulation of the model predictive controller in the next section. Thus, parameter estimation from open-loop kMC simulation results of the thin film growth process for a variety of operation conditions is performed to obtain the dependence of the model coefficients on substrate temperature. In this work, the deposition rate for all simulations is fixed at 1 layer/s. The range of T is between 300 K and 800 K, which is from room temperature to the upper limit of the allowable temperature for a valid on-lattice kMC model of silicon film. The dependence of the model parameters on the substrate temperature can be found in Hu et al. (2009b).

4. MODEL PREDICTIVE CONTROL DESIGN

We consider the problem of regulation of surface roughness and of film SOR to desired levels within a model predictive control framework. State feedback control is considered in this work, i.e., the surface height profile and the value of film SOR are assumed to be available to the controller. Real-time film roughness and SOR can be estimated from in-situ thin film thickness measurements (Buzea and Robbie, 2005) in combination with off-line film porosity measurements. Since surface roughness and film SOR are stochastic variables, the expected values, $\langle r(t)^2 \rangle$ and $\langle \rho \rangle$, are chosen as the control objectives. The substrate temperature is used as the manipulated input and the deposition rate is fixed at a certain value, W_0, during the entire closed-loop simulation. To account for a number of practical considerations, several constraints are added to the control problem. First, there is a constraint on the range of variation of the substrate temperature. This constraint ensures validity of the on-lattice kMC model. Another constraint is imposed on the rate of change of the substrate temperature to account for actuator limitations. The control action at a time t is obtained by solving a finite-horizon optimal control problem. The cost function in the optimal control problem includes penalty on the deviation of $\langle r^2 \rangle$ and $\langle \rho \rangle$ from their respective set-point values. Different weighting factors are assigned to the penalties of the surface roughness and of the film SOR. Surface roughness and film SOR have very different magnitudes, ($\langle r^2 \rangle$ ranges from 1 to 10^2 and $\langle \rho \rangle$ ranges from 0 to 1). Therefore, relative deviations are used in the formulation of the cost function to make the magnitude of the two terms comparable. The optimization problem is subject to the dynamics of the surface height of Eq.2 and of the film SOR of Eq.13. The optimal temperature profile is calculated by solving a finite-dimensional optimization problem in a receding horizon fashion. Specifically, the MPC problem is formulated as follows:

$$\begin{aligned} \min_{T_1,\ldots,T_i,\ldots,T_p} J &= \sum_{i=1}^{p} \Big\{ q_{r^2,i} \left[(r^2_{set} - \langle r^2(t_i) \rangle)/r^2_{set} \right]^2 \\ &\quad + q_{\rho,i} \left[(\rho_{set} - \langle \rho(t_i) \rangle)/\rho_{set} \right]^2 \Big\} \\ &\quad \text{subject to} \\ \frac{\partial h}{\partial t} &= r_h + \nu \frac{\partial^2 h}{\partial x^2} + \xi(x,t), \tau \frac{d\langle \rho(t) \rangle}{dt} = \rho^{ss} - \langle \rho(t) \rangle \\ &T_{min} < T_i < T_{max}, |(T_{i+1} - T_i)/\Delta| \leq L_T \\ &i = 1, 2, \ldots, p \end{aligned} \tag{18}$$

where t is the current time, Δ is the sampling time, p is the number of prediction steps, $p\Delta$ is the specified prediction horizon, t_i, $i = 1, 2, \ldots, p$, is the time of the ith prediction step ($t_i = t + i\Delta$), respectively, T_i, $i = 1, 2, \ldots, p$, is the substrate temperature at the ith step ($T_i = T(t + i\Delta)$), respectively, W_0 is the fixed deposition rate, $q_{r^2,i}$ and $q_{\rho,i}$, $i = 1, 2, \ldots, p$, are the weighting penalty factors for the deviations of $\langle r^2 \rangle$ and $\langle \rho \rangle$ from their respective set-points at the ith prediction step, T_{min} and T_{max} are the lower and upper bounds on the substrate temperature, respectively, and L_T is the limit on the rate of change of the substrate temperature.

The optimal set of control actions, ($T_1, T_2, \ldots, T_p$), is obtained from the solution of the multi-variable optimization problem of Eq.18, and only the first value of the manipulated input trajectory, T_1, is applied to the deposition process during the time interval $(t, t + \Delta)$. At time $t + \Delta$, a new measurement of ρ and h is received and the MPC problem of Eq.18 is solved for the next control input trajectory.

The MPC formulation proposed in Eq.18 is developed on the basis of the EW equation of surface height and the deterministic ODE model of the film SOR. The EW equation, which is a distributed parameter dynamic model, contains infinite dimensional stochastic states. Therefore, it leads to a model predictive controller of infinite order that cannot be realized in practice (i.e., the practical implementation of such a control algorithm will require the computation of infinite sums which cannot be done by a computer). To this end, a finite dimensional approximation of the EW equation of order $2m$, derived using modal decomposition, is used in the simulations below.

5. SIMULATION RESULTS

In this section, the model predictive controller is applied to the kMC model of the thin film growth process described in Section 2. The value of the substrate temperature is obtained from the solution of the MPC problem at each sampling time and is applied to the closed-loop system until the next sampling time. The optimization problem is solved using a local constrained minimization algorithm using a broad set of initial guesses.

The constraint on the rate of change of the substrate temperature is imposed onto the optimization problem, which is realized in the optimization process in the following way:

$$\begin{aligned} \left| \frac{T_{i+1} - T_i}{\Delta} \right| \leq L_T \Rightarrow T_i - L_T\Delta \leq T_{i+1} \leq T_i + L_T\Delta \\ i = 1, 2, \ldots, p. \end{aligned} \tag{19}$$

The desired values (set-point values) in the closed-loop simulations are $r^2_{set} = 10.0$ and $\rho_{set} = 0.95$. The order of finite-dimensional approximation of the EW equation in the MPC formulation is $m = 20$. The deposition rate is fixed at 1 layer/s and initial temperature of 600 K. The variation of temperature is from 400 K to 700 K. The maximum of change of the temperature is $L_T = 10$ K/s. The sampling time is fixed at $\Delta = 1$ s. The number of prediction steps is set to be $p = 5$. The simulation duration is determined on the basis of a desired film thickness and the fixed adsorption rate and is chosen as 1000 s for the closed-loop simulations in this work. All expected values are obtained from 1000 independent simulation runs.

Closed-loop simulations of separately regulating film surface roughness and porosity are first carried out. In these control problems, the control objective is to only regulate one of the control variables, i.e., either surface roughness or film SOR, to a desired level. The cost functions of these problems contain only penalty on the error either of the expected surface roughness square, or of the expected film SOR, from their set-point values. The corresponding MPC formulations can be realized by assigning different values to the penalty weighting factors, $q_{r^2,i}$ and $q_{\rho,i}$.

In the roughness-only control problem, the weighting factors take the following values: $q_{r^2,i} = 1$ and $q_{\rho,i} = 0$, $i = 1, 2, \ldots, p$. Fig.4 shows the closed-loop simulation results of the roughness-only control problem. From Fig.4, we can see that the expected surface roughness square is successfully regulated at the desire level, 10. Since no penalty is included on the error of the expected film SOR, the final value of expected film SOR at the end of the simulation, $t = 1000$ s, is 0.988, which is far from the desired film SOR, 0.95.

In the SOR-only control problem, the weighting factors are assigned as: $q_{r^2,i} = 0$ and $q_{\rho,i} = 1$, $i = 1, 2, \ldots, p$. Fig.5 shows the closed-loop simulation results of the SOR-only control problem. Similar to the results of the roughness-only control problem, the desired value of expected film SOR, 0.95, is approached at large times. However, since the error from the expected surface roughness square is not considered in the cost function, $\langle r^2 \rangle$ reaches a very high level around 125 at the end of the simulation.

Finally, closed-loop simulations of simultaneous regulation of surface roughness and film SOR are carried out by assigning non-zero values to both penalty weighting factors. Specifically, $q_{r^2,1} = q_{r^2,2} = \cdots = q_{r^2,p} = 1$ and $q_{\rho,1} = q_{\rho,2} = \cdots = q_{\rho,p} = q_{SOR}$ and q_{SOR} varies from 1 to 10^4. Since substrate temperature is the only manipulated input, the desired-values of r^2_{set} and ρ_{set} cannot be achieved simultaneously. With different assignments of penalty weighting factors, the MPC evaluates and strikes a balance between the two set-points. Fig.6 shows the expected

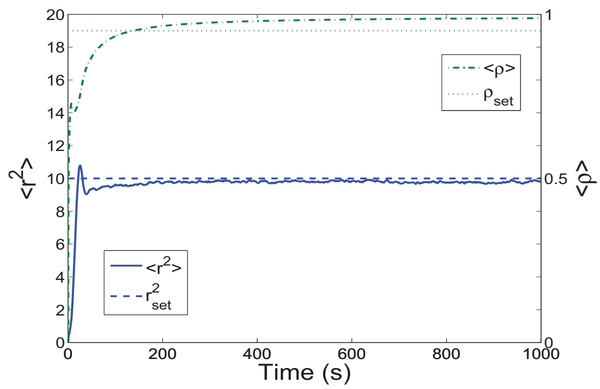

Fig. 4. Profiles of the expected values of surface roughness square (solid line) and of the film SOR (dash-dotted line) under closed-loop operations with cost function including only penalty on surface roughness.

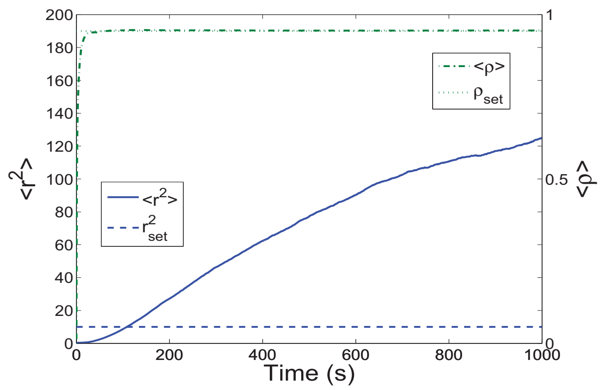

Fig. 5. Profiles of the expected values of surface roughness square (solid line) and of the film SOR (dash-dotted line) under closed-loop operation with cost function including only penalty on the film SOR.

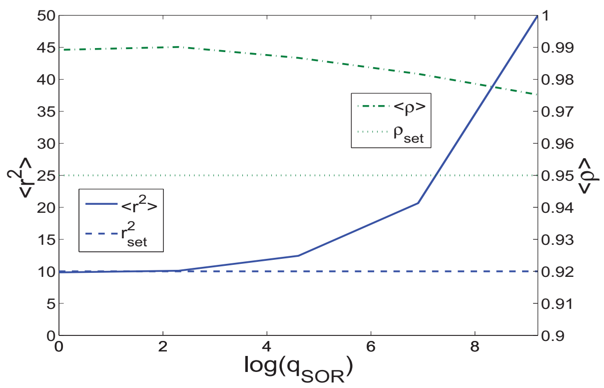

Fig. 6. Profiles of the expected values of surface roughness square (solid line) and of the film SOR (dash-dotted line) at the end of the closed-loop simulations ($t = 1000$ s) with the following penalty weighting factors: $q_{r^2,i}$ fixed at 1 for all i and for different values of q_{SOR}.

values of r^2_{set} and ρ_{set} at the end of closed-loop simulations of the simultaneous control problem with respect to different weighting factors. It is clear from Fig.6 that as the weighting on expected film SOR increases, the expected film SOR approaches its set-point value of 0.95, while the expected surface roughness square deviates from its set-point value of 10.

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