FEEDBACK CONTROL OF SURFACE ROUGHNESS IN A DEPOSITION PROCESS USING A STOCHASTIC PDE ⋆

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Abstract: This paper focuses on feedback control of surface roughness in a deposition process, based on a stochastic partial differential equation (PDE) which describes the fluctuation of surface height in the spatial domain. Specifically, we focus on control of surface roughness in a deposition process on a 1-dimensional lattice, whose fluctuation of surface height can be described by the Edwards-Wilkinson equation, a second-order stochastic PDE. We initially reformulate the stochastic PDE into a system of infinite stochastic ordinary differential equations by using modal decomposition. A finite-dimensional approximation of the Edwards-Wilkinson equation is then derived that captures the dominant mode contribution to the surface roughness. A state feedback controller is designed based on the finite-dimensional approximation to control the surface roughness. Analysis of the closed-loop system shows that the controller can drive the surface roughness governed by the infinite-dimensional system to desired levels. The effectiveness of the proposed method is demonstrated by numerical simulations.

Keywords: stochastic partial differential equations, feedback control, deposition processes, roughness control

1. INTRODUCTION

The surface roughness of thin films deposited from gas phase precursors is an important variable to control because it strongly affects the quality of such films. In a thin film growth process, the film is directly formed from microscopic random processes (e.g., particle adsorption, desorption, migration and surface reaction). Therefore, the stochastic nature of thin film growth processes must be fully considered in the modeling and control of the surface roughness of thin films. The desire to understand and control the thin film micro-structure has motivated extensive research on fundamental mathematical models describing the deposition processes, which include 1) kinetic Monte-Carlo methods (e.g., (Gillespie, 1976; Fichthorn and Weinberg, 1991; Lam and Vlachos, 2001)), and 2) stochastic partial differential equations (SPDEs) (e.g., (Edwards and Wilkinson, 1982; Villain, 1991)).

The kinetic Monte-Carlo simulation method can be used to predict properties of the thin film, by explicitly accounting for the micro-processes that directly shape thin film microstructure. Recently, a methodology for feedback control of thin film growth using kinetic Monte-Carlo models has been developed in (Lou and Christofides, 2003*a*; Lou and Christofides, 2003*b*). The methodology leads to the design of (a) real-time roughness estimators by using multiple small lattice kinetic Monte-Carlo simulators, adaptive filters and measurement error compensators and (b) feedback controllers based on the real-time roughness estimates. The method was successfully applied to control surface roughness in a *GaAs* deposition process using an experimentally determined kinetic Monte-Carlo process model (Lou and Christofides, 2004*b*).

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Other approaches have also been developed to: (a) identify linear models from outputs of kinetic Monte-Carlo simulators and perform controller design by using linear control theory (Siettos *et al.*, 2003), and (b) construct reduced-order approximations of the master equation (Gallivan and Murray, 2003).

However, the fact that kinetic Monte-Carlo models are not available in closed-form makes it very difficult to perform model-based controller design directly on the basis of kinetic Monte-Carlo models. To achieve better closed-loop performance, it is desirable to design feedback controllers on the basis of deposition process models. This motivates research on feedback control of deposition processes based on stochastic PDE models of thin film growth.

This paper focuses on feedback control of surface roughness in a deposition process, based on a stochastic partial differential equation (PDE) which describes the fluctuation of surface height in the spatial domain. Specifically, we focus on control of surface roughness in a deposition process on a 1-dimensional lattice, whose fluctuation of surface height can be described by the Edwards-Wilkinson equation, a second-order stochastic PDE. We initially reformulate the stochastic PDE into a system of infinite stochastic ordinary differential equations by using modal decomposition. A finite-dimensional approximation of the Edwards-Wilkinson equation is then derived that captures the dominant mode contribution to the surface roughness. A state feedback controller is designed based on the finite-dimensional approximation to control the surface roughness. Analysis of the closed-loop system shows that the controller can drive the surface roughness governed by the infinite-dimensional system to desired levels. The effectiveness of the proposed method is demonstrated by numerical simulations. Due to space limitations, we will present in this paper the main results of this research; further results and analysis can be found in (Lou and Christofides, 2004*c*).

2. PRELIMINARIES

We consider a deposition process on a 1-dimensional lattice. In this process, particles land on the surface at a rate, r_a. The rules for the deposition are as follows: a site, l, is first randomly picked among the sites of the whole lattice and the deposition site is determined according to the following rules: 1) if the height of this site is lower than or equal to that of both each nearest neighbors, this site is picked as the deposition site; 2) if the height of only one of the two nearest neighbor sites is lower than that of the original site, deposition is on that site; 3) if the height of each one of the nearest neighbor sites is lower than that of the original site, the deposition site is randomly picked with equal probability between the two nearest neighbor sites. A schematic of the rules of the deposition is shown in Fig.1. There is no particle migration and desorption taking place on this process (see (Lou and Christofides, 2003*a*; Lou and Christofides, 2003*b*) for film growth processes that involve these phenomena).

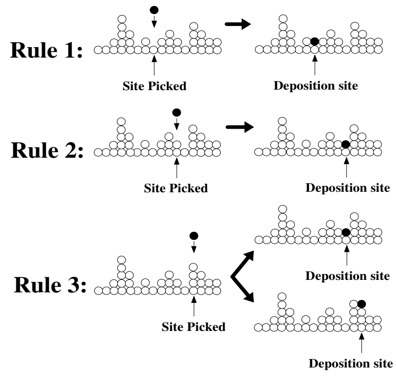

Fig. 1. Schematic of the rules of the deposition.

The deposition process is a stochastic process. Kinetic Monte-Carlo simulation can be used to predict the evolution of the surface configuration in this process. The kinetic Monte-Carlo model of the deposition process is a first-principle model in the sense that the deposition rules can be explicitly considered in the model. However, kinetic Monte-Carlo models are not available in closed-form, which prohibits their use for model-based control design. As an alternative, closed-form stochastic PDE models can be derived based on the deposition rules to describe the evolution of the surface configuration, which is consistent to that predicted by kinetic Monte-Carlo models. In this work, we focus on model-based feedback control design for surface roughness control using a stochastic PDE model of the deposition process described in Fig.1.

The equation for the height fluctuations of the surface in this deposition process was first developed by (Edwards and Wilkinson, 1982). Recently, the same equation was derived directly from the microscopic transition rules of the process (Vvedensky, 2003). Specifically, the height fluctuation of the surface is described by the following stochastic partial differential equation:

$$\frac{\partial h}{\partial t} = a^2 r_a \frac{\partial^2 h}{\partial x^2} + \xi(x,t) \tag{1}$$

where $x \in [-\pi, \pi]$ is the spatial coordinate, t is the time, $h(x,t)$ is the height of the surface at position x and time t, a is the lattice size and $\xi(x,t)$ is a Gaussian noise with zero mean and covariance:

$$\langle \xi(x,t)\xi(x',t') \rangle = \varsigma^2 \delta(x-x')\delta(t-t') \tag{2}$$

where $\varsigma^2 = a^3 r_a$, $\delta(\cdot)$ is the dirac function, and $\langle \cdot\cdot \rangle$ denotes the average. Note that the noise covariance depends on both space x and time t.

The surface roughness, r, is given by the following expression:

$$r(t) = \sqrt{\frac{1}{2\pi} \int_{-\pi}^{\pi} [h(x,t) - \bar{h}(t)]^2 dx} \tag{3}$$

where $\bar{h}(t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} h(x,t)dx$ is the average surface height.

Our objective is to control the surface roughness of the deposition process described by Fig.1. The controller design is based on the SPDE model of the process (Eqs.1 and 2). To do this, we formulate a distributed control problem in the spatial domain $[-\pi,\pi]$. The control problem is described by the following stochastic partial differential equation:

$$\frac{\partial h}{\partial t} = \nu \frac{\partial^2 h}{\partial x^2} + \sum_{i=1}^{p} b_i(x)u_i(t) + \xi(x,t) \tag{4}$$

subject to periodic boundary conditions:

$$\frac{\partial^j h}{\partial x^j}(-\pi,t) = \frac{\partial^j h}{\partial x^j}(\pi,t),\ j=0,1 \tag{5}$$

and the initial condition:

$$h(x,0) = h_0(x) \tag{6}$$

where $\nu = a^2 r_a$, u_i is the ith manipulated input, p is the number of manipulated inputs and b_i is the ith actuator distribution function (i.e., b_i determines how the control action computed by the ith control actuator, u_i, is distributed (e.g., point or distributed actuation) in the spatial interval $[-\pi,\pi]$)

To study the dynamics of Eq.4, we initially consider the eigenvalue problem of the linear operator of Eq.4, which takes the form:

$$\begin{aligned} A\bar{\phi}_n(x) &= \nu \frac{d^2\bar{\phi}_n(x)}{dx^2} = \lambda_n \bar{\phi}_n(x),\ n=1,\cdots,\infty, \\ \frac{d^j\bar{\phi}_n}{dx^j}(-\pi) &= \frac{d^j\bar{\phi}_n}{dx^j}(\pi), \qquad j=0,1 \end{aligned} \tag{7}$$

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 eigenvalues of multiplicity two) with eigenfunctions $\phi_n = (1/\sqrt{\pi})\sin(nx)$ and $\psi_n = (1/\sqrt{\pi})\cos(nx)$ for $n=1,\cdots,\infty$. From the solution of the eigenvalue problem shown in Eq.7, it follows that for a fixed value of $\nu > 0$ the distance between two consecutive eigenvalues (i.e., λ_n and λ_{n+1}) increases as n increases. Furthermore, the eigenspectrum of operator A in Eq.7, $\sigma(A)$ can be partitioned as $\sigma(A) = \sigma_1(A)\bigcup\sigma_2(A)$, where $\sigma_1(A)$ contains the first m (with m finite) eigenvalues (i.e. $\sigma_1(A) = \{\lambda_1,\ldots,\lambda_m\}$) and $\sigma_2(A)$ contains the remaining eigenvalues (i.e., $\sigma_2(A) = \{\lambda_{m+1},\ldots,\}$.

To present the method that we use to control the stochastic PDE of Eq.4, we first derive stochastic ODE approximations of Eq.4 using modal decomposition. To this end, we first expand the solution of Eq.4 in an infinite series in terms of the eigenfunctions of the operator of Eq.7 as follows:

$$h(x,t) = \sum_{n=1}^{\infty} \alpha_n(t)\phi_n(x) + \sum_{n=0}^{\infty} \beta_n(t)\psi_n(x) \tag{8}$$

where $\alpha_n(t)$, $\beta_n(t)$ are time-varying coefficients. Substituting the above expansion for the solution, $h(x,t)$, into Eq.4 and taking the inner product with the adjoint eigenfunctions, $\phi_n^*(z) = (1/\sqrt{\pi})\sin(nz)$ and $\psi_n^*(z) = (1/\sqrt{\pi})\cos(nz)$, the following system of infinite stochastic ODEs is obtained:

$$\begin{aligned} \frac{d\alpha_n}{dt} &= -\nu n^2 \alpha_n + \sum_{i=1}^{p} b_{i\alpha_n} u_i(t) + \xi_\alpha^n(t) \\ \frac{d\beta_n}{dt} &= -\nu n^2 \beta_n + \sum_{i=1}^{p} b_{i\beta_n} u_i(t) + \xi_\beta^n(t);\ n=1,\ldots,\infty \end{aligned} \tag{9}$$

where $b_{i\alpha_n} = \int_{-\pi}^{\pi} \phi_n(x)b_i(x)dx$, $b_{i\beta_n} = \int_{-\pi}^{\pi} \psi_n(x)b_i(x)dx$, $\xi_\alpha^n(t) = \int_{-\pi}^{\pi}\xi(x,t)\phi_n(x)dx$, $\xi_\beta^n(t) = \int_{-\pi}^{\pi}\xi(x,t)\psi_n(x)dx$.

The covariances of $\xi_\alpha^n(t)$ and $\xi_\beta^n(t)$ can be computed by using the following result (Åström, 1970):

Result 1: If (1) $f(x)$ is a deterministic function, (2) $\eta(x)$ is a random variable with $\langle\eta(x)\rangle = 0$ and covariance $\langle\eta(x)\eta(x')\rangle = \sigma^2\delta(x-x')$, and (3) $\varepsilon = \int_a^b f(x)\eta(x)dx$, then ε is a random number with $\langle\varepsilon\rangle = 0$ and covariance $\langle\varepsilon^2\rangle = \sigma^2\int_a^b f^2(x)dx$.

Using Result 1, we obtain $\langle\xi_\alpha^n(t)\xi_\alpha^n(t')\rangle = \varsigma^2\delta(t-t')$ and $\langle\xi_\beta^n(t)\xi_\beta^n(t')\rangle = \varsigma^2\delta(t-t')$.

In this work, the controlled variable is the expected value of surface roughness, $\sqrt{\langle r^2\rangle}$. According to Eq.8, we have $\bar{h}(t) = \beta_0(t)\psi_0$. Therefore, $\sqrt{\langle r^2\rangle}$ can be rewritten in terms of α_n and β_n as follows:

$$\begin{aligned} \sqrt{\langle r^2\rangle} &= \sqrt{\frac{1}{2\pi}\langle\int_{-\pi}^{\pi}(h(x,t)-\bar{h}(t))^2dx\rangle} \\ &= \sqrt{\frac{1}{2\pi}\sum_{i=1}^{\infty}\left[\langle\alpha_i^2\rangle + \langle\beta_i^2\rangle\right]} \end{aligned} \tag{10}$$

Therefore, the surface roughness control problem for the stochastic PDE system of Eq.4 is formulated as the one of controlling the covariance of the states α_n and β_n in the stochastic ODE system of Eq.9.

3. FEEDBACK CONTROL

In this section, we design a linear state feedback controller for the system of Eq.9 so that the surface roughness defined in Eq.10 can be controlled to a desired level.

3.1 Model reduction

Owing to its infinite-dimensional nature, the system of Eq.9 cannot be directly used for the design of controllers that can be implemented in practice (i.e., the practical implementation of controllers which are designed on the basis of this system will require the computation of infinite sums which cannot be done by a computer). Instead, we will base the controller design on finite-dimensional approximations of this system. Subsequently, we will show that the resulting controller will enforce the desired control objective in the closed-loop infinite-dimensional system.

Specifically, we rewrite the system of Eq.9 as follows:

$$\frac{dx_s}{dt} = \Lambda_s x_s + B_s u + \xi_s$$
$$\frac{dx_f}{dt} = \Lambda_f x_f + B_f u + \xi_f \tag{11}$$

where $x_s = [\ \alpha_1\ \cdots\ \alpha_m\ \beta_1\ \cdots\ \beta_m\ ]^T$, x_f=$[\alpha_{m+1}\ \beta_{m+1}\ \cdots\ ]^T$, $\Lambda_s = diag[\ -\nu\ \cdots\ -m^2\nu\ -\nu\ \cdots\ -m^2\nu\ ]$, $\Lambda_f = diag[-(m+1)^2\nu\ -(m+1)^2\nu\ \cdots]$, $u = [\ u_1\ \cdots\ u_p\ ]$, $\xi_s = [\ \xi_\alpha^1\ \cdots\ \xi_\alpha^m\ \xi_\beta^1\ \cdots\ \xi_\beta^m\ ]$, and $\xi_f = [\xi_\alpha^{m+1}\ \xi_\beta^{m+1}\ \cdots]$.

$$B_s = \begin{bmatrix} b_{1_{\alpha_1}} & \cdots & b_{p_{\alpha_1}} \\ \vdots & \ddots & \vdots \\ b_{1_{\alpha_m}} & \cdots & b_{p_{\alpha_m}} \\ b_{1_{\beta_1}} & \cdots & b_{p_{\beta_1}} \\ \vdots & \ddots & \vdots \\ b_{1_{\beta_m}} & \cdots & b_{p_{\beta_m}} \end{bmatrix} \quad B_f = \begin{bmatrix} b_{1_{\alpha_{m+1}}} & \cdots & b_{p_{\alpha_{m+1}}} \\ b_{1_{\beta_{m+1}}} & \cdots & b_{p_{\beta_{m+1}}} \\ b_{1_{\alpha_{m+2}}} & \cdots & b_{p_{\alpha_{m+2}}} \\ b_{1_{\beta_{m+2}}} & \cdots & b_{p_{\beta_{m+2}}} \\ \vdots & \vdots & \vdots \end{bmatrix} \tag{12}$$

We note that the subsystem x_f in Eq.11 is infinite-dimensional.

Neglecting the x_f subsystem, the following $2m$-dimensional system is obtained:

$$\frac{d\tilde{x}_s}{dt} = \Lambda_s \tilde{x}_s + B_s u + \xi_s \tag{13}$$

where the tilde symbol in $\tilde{x}_s$ denotes that this state variable is associated with a finite-dimensional system.

3.2 Feedback control design

We design the state feedback controller on the basis of the finite-dimensional system of Eq.13. To simplify our development, we assume that $p = 2m$ and pick the actuator distribution functions such that B_s^{-1} exists. The state feedback control law then takes the form:

$$u = B_s^{-1}(\Lambda_{cs} - \Lambda_s)\tilde{x}_s \tag{14}$$

where the matrix Λ_{cs} contains the desired poles of the closed-loop system; $\Lambda_{cs} = diag[\lambda_{c\alpha 1} \cdots \lambda_{c\alpha m}\ \lambda_{c\beta 1} \cdots \lambda_{c\beta m}]$, $\lambda_{c\alpha i}$ and $\lambda_{c\beta i}$ $(1 \le i \le m)$ are desired poles of the closed-loop finite-dimensional system, which can be computed from the desired closed-loop surface roughness level.

We first analyze the dependence of the covariances of the states α_n and β_n $(n = 1, \cdots, m)$ on the poles of the finite-dimensional system of Eq.13. Then, we will show in subsection 3.3 that the surface roughness of the infinite-dimensional system of Eq.9 can be controlled to the desired level by using the state feedback controller of Eq.14, which only uses a finite number of actuators.

By applying the controller of Eq.14 to the system of Eq.13, the closed-loop system takes the form:

$$\frac{d\tilde{x}_s}{dt} = \Lambda_{cs}\tilde{x}_s + \xi_s(t) \tag{15}$$

To analyze the effect of the feedback controller on the covariance of the state $\tilde{x}_s$, we discretize Eq.15 in the time domain, using Δt as time step, as follows:

$$X_s(k+1) = G_{cs}X_s(k) + \zeta_s(k);\ k = 0, \cdots, \infty \tag{16}$$

where $X_s(k) = \tilde{x}_s(k\Delta t)$, $G_{cs} = e^{\Lambda_{cs}\Delta t}$, $\zeta_s(k) = \int_{k\Delta t}^{(k+1)\Delta t} e^{\Lambda_{cs}(t-k\Delta t)}\xi_s(t)dt$. According to (Åström, 1970, Chapter 3), if all eigenvalues of G_{cs} are within the unit circle on the complex plane, the covariance matrix of $X_s(k)$, $P(k) = \langle X_s(k)X_s(k)^T\rangle$ converges to $P(\infty)$, which is the solution of the following equation:

$$P(\infty) = G_{cs}P(\infty)G_{cs}^T + R_1 \tag{17}$$

where $R_1 = \langle \zeta_s \zeta_s^T \rangle$. Eq.17 can not be solved, in general, analytically. However, for the specific deposition system considered in this work, the analytical solution for $P(\infty)$ can be obtained as follows:

$$P(\infty) = \begin{bmatrix} P_\alpha(\infty) & 0 \\ 0 & P_\beta(\infty) \end{bmatrix} \tag{18}$$

where $P_\alpha(\infty) = diag[\ \langle \alpha_1(\infty)^2\rangle\ \cdots\ \langle \alpha_m(\infty)^2\rangle\ ]$, $P_\beta(\infty) = diag[\ \langle \beta_1(\infty)^2\rangle\ \cdots\ \langle \beta_m(\infty)^2\rangle\ ]$. Using Result 1, $\langle \alpha_n(\infty)^2\rangle$ and $\langle \beta_n(\infty)^2\rangle$ $(n = 1, \cdots, m)$ can be computed by using the following expressions:

$$\langle \alpha_n(\infty)^2\rangle = -\frac{\varsigma^2}{2\lambda_{c\alpha_n}};\ \langle \beta_n(\infty)^2\rangle = -\frac{\varsigma^2}{2\lambda_{c\beta_n}} \tag{19}$$

From Eq.19, we can see that by assigning the closed-loop poles $\lambda_{c\alpha_n}$ and $\lambda_{c\beta_n}$ $(n = 1, \cdots, m)$ at desired locations, the covariances of the states α_n and β_n $(n = 1, \cdots, m)$ can be controlled to desired levels. Therefore, according to Eq.10, the contribution to the surface roughness from the finite-dimensional system of Eq.13 can be controlled to the desired level.

3.3 Analysis of the closed-loop infinite-dimensional system

In this subsection, we show that when the state feedback controller of Eq.14 is used to manipulate the poles of the finite-dimensional system of Eq.13, the contribution to the surface roughness from the α_f and β_f subsystem of the system of Eq.11 is bounded and can be made arbitrarily small by increasing the dimension of the x_s subsystem.

By applying the feedback controller of Eq.14 into the infinite-dimensional system of Eq.11, we obtain the following closed-loop system:

$$\frac{dx_s}{dt} = \Lambda_{cs}x_s + \xi_s$$
$$\frac{dx_f}{dt} = \Lambda_\varepsilon x_s + \Lambda_f x_f + \xi_f \tag{20}$$

where $\Lambda_\varepsilon = B_f B_s^{-1}(\Lambda_{cs} - \Lambda_s)$.

The boundedness of the state of the above system follows directly from the stability of the matrices Λ_{cs} and Λ_f and the structure of the system, where the x_s subsystem is independent of the x_f state (see

(Christofides, 2001) for results and techniques for analyzing the stability properties of such systems).

Due to the structure of the eigenspectrum of operator A (Section 2), the effect of the control action computed from Eq.14 to the poles of the x_f subsystem can be reduced by increasing m. Therefore, by picking m sufficiently large, the $\Lambda_\varepsilon x_s$ can be made very small compared to $\Lambda_f x_f$ and thus, the closed-loop system of Eq.20 can be adequately described by the following system:

$$\begin{aligned} \frac{dx_s}{dt} &= \Lambda_{cs} x_s + \xi_s \\ \frac{dx_f}{dt} &= \Lambda_f x_f + \xi_f \end{aligned} \tag{21}$$

On the basis of the above system, it can be shown that the covariance of the state of the x_f subsystem converges to $[\ \langle \alpha_{m+1}(\infty)^2 \rangle\ \ \langle \beta_{m+1}(\infty)^2 \rangle\ \ \cdots\ \cdots]$, where

$$\langle \alpha_n(\infty)^2 \rangle = \frac{\varsigma^2}{2n^2\nu};\ \langle \beta_n(\infty)^2 \rangle = \frac{\varsigma^2}{2n^2\nu};\ n > m \tag{22}$$

Therefore, the overall contribution to the surface roughness from the x_f subsystem in Eq.11 can be computed as follows:

$$\frac{\varsigma}{\sqrt{2\pi(m+1)\nu}} < \sqrt{\frac{1}{2\pi}\sum_{n=m+1}^{\infty}\left[\frac{\varsigma^2}{\nu n^2}\right]} < \frac{\varsigma}{\sqrt{2\pi m \nu}} \tag{23}$$

Clearly, as $m \to \infty$, the contribution to the surface roughness from the α_f and β_f subsystem goes to zero.

In summary, under the controller of Eq.14, the closed-loop surface roughness, for m sufficiently large, can be adequately described by the following expression:

$$\sqrt{\langle r^2 \rangle} = \varsigma\sqrt{\frac{1}{2\pi}[\lambda^* + \sum_{n=m+1}^{\infty}\frac{1}{\nu n^2}]} \tag{24}$$

where

$$\lambda^* = \sum_{i=1}^{m}(-\frac{1}{2\lambda_{c\alpha_i}} - \frac{1}{2\lambda_{c\beta_i}}) \tag{25}$$

Remark 1. Note that to control the closed-loop surface roughness to $\sqrt{\langle r_d^2 \rangle}$, we need to design a controller to assign the poles of the finite-dimensional system of Eq.15 to appropriate values. The controller which assigns the poles of the system of Eq.15 to satisfy Eq.25 is not unique. Consequently, for a fixed number of actuators, p, the controller that can drive the closed-loop surface roughness to a desired level is also not unique.

4. SIMULATION RESULTS

In this section, we present an application of the proposed state feedback controller to the deposition process described in Fig.1 to regulate the surface roughness to a desired level. Specifically, the deposition occurs on a lattice containing 1000 sites. Therefore, $a = 0.00628$. The deposition rate for each site is $r_a = 1s^{-1}$. A $600th$ order stochastic ordinary differential equation approximation of the system of Eq.4 is used to simulate the process (the use of higher-order approximations led to identical numerical results, thereby implying that the following simulation runs are independent of the discretization). The δ function involved in the covariances of ξ_α^n and ξ_β^n is approximated by $\frac{1}{\delta t}$.

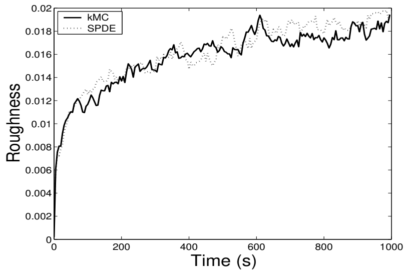

Fig. 2. Comparison of the open-loop profile of surface roughness from the kinetic Monte-Carlo simulator (solid line) and that from the solution of the SPDE using 300 modes (dotted line).

In the first simulation, we compare the open-loop surface roughness profile of the deposition process from the solution of the stochastic PDE model of Eq.1 to that from a kinetic Monte-Carlo simulation. We use the kinetic Monte-Carlo algorithm developed in (Vlachos, 1997) to simulate the process. First, a random number is generated to pick a site among all the sites on the 1-D lattice. If the height of this site is lower than or equal to that of both each nearest neighbors, this site is picked as the deposition site and the height of this site increases by a; if the height of only one of the two nearest neighbor sites is lower than that of the original site, deposition is on that site and the height of that site increases by a; if the height of each one of the nearest neighbor sites is lower than that of the original site, a second random number is generated to randomly pick one of the two nearest neighbors with equal probability and the height of the picked site increases by a. Upon an executed event, a time increment, dt, is computed by $dt = \frac{-\ln\zeta}{N \times r_a}$, where ζ is a random number in the $(0,1)$ interval and N is the total number of sites on the lattice.

The profiles of surface roughness from the kinetic Monte-Carlo simulation and the solution of the stochastic PDE model are shown in Fig.2. The two profiles are very close, which means that the stochastic PDE model of Eq.4 can adequately (see Remark 2 below for a discussion on this issue) simulate the evolution of surface roughness of the deposition process described in Fig.1.

Subsequently, we design a state feedback controller based on a $60th$ order stochastic ODE approximation constructed by using the first 60 eigenmodes of the system of Eq.9. 60 control actuators are used to control the system. The ith actuator distribution function is taken to be:

$$b_i(z) = \frac{1}{\sqrt{\pi}}[\sin(iz) + \cos(iz)];\ i = 1, \cdots, 60 \quad (26)$$

Our desired roughness is around 0.0058. Using Eq.24, we design the state-feedback controller such that $\lambda_{c\alpha_i} = \lambda_{c\beta_i} = -3.55$, for $i = 1, \cdots, 30$. Under this state feedback controller, the closed-loop surface roughness is in the range $[0.0057, 0.0058]$. Fig.3 shows a comparison between the closed-loop roughness profile (solid line) and the open-loop roughness profile (dotted line). We can see the controller successfully drives the surface roughness to the desired level, which is much lower than that corresponding to open-loop operation ($u_i(t) = 0$, $i = 1, \ldots, 60$).

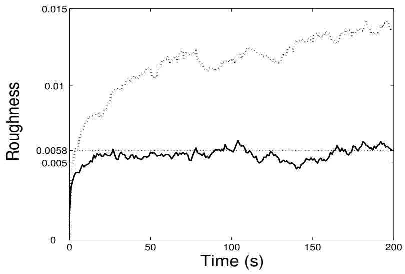

Fig. 3. Closed-loop roughness profile (solid line) when the controller is designed based on the first 60 modes vs. the open-loop roughness profile (dotted line).

Remark 2. Note that all simulation results of roughness profiles shown in this section are realizations of a stochastic process. Therefore, fluctuations can be observed in all simulation results. Our control objective is to drive the expected roughness to the desired level, so roughness profiles from each simulation fluctuate around this desired level due to the stochastic nature of the process. Conceptually, if we run infinite number of simulations with the same parameters, and average the roughness profiles obtained from each simulation run, the desired expected roughness profile can be obtained.

Remark 3. Note that the controller design method developed in this work can be applied to other processes described by stochastic PDE models. For example, it can be used to control the stochastic Kuramoto-Sivashinsky equation (Lou and Christofides, 2004*a*), which describes evolution of surface microstructure in a variety of physical and chemical processes including ZrO_2 thin film growth by reactive ion beam sputtering (Qi *et al.*, 2003).

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