Feedback Control of Surface Roughness Using Stochastic PDEs

Yiming Lou and Panagiotis D. Christofides
Dept. of Chemical Engineering, University of California, Los Angeles, CA 90095

DOI 10.1002/aic.10299
Published online in Wiley InterScience (www.interscience.wiley.com).

Keywords: deposition processes, stochastic partial differential equations, kinetic Monte-Carlo simulation, feedback control, roughness control

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. The modern integrated circuit technology depends strongly on the uniformity and microstructure of deposited thin films (Granneman, 1993). Due to the increasingly stringent requirements on the quality of such films, on-line estimation and control of thin film deposition becomes important.

In a thin film growth process, the film is directly formed from microscopic random processes (for example, 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 (for example, Gillespie, 1976; Fichthorn and Weinberg, 1991; Lam and Vlachos, 2001), and (2) stochastic partial-differential equations (PDEs) (for example, Edwards and Wilkinson, 1982; Villain, 1991; Vvedensky et al., 1993).

The kinetic Monte-Carlo simulation method can be used to predict average properties of the thin film (which are of interest from a control point of view, for example, surface roughness), by explicitly accounting for the microprocesses 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, 2003a,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 estimators. 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, 2004b). 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 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.

Stochastic PDE models have been developed to describe the evolution of the height profile for surfaces in a variety of physical and chemical processes. Examples include deposition processes including adsorption and surface relaxation (Edwards and Wilkinson, 1982; Vvedensky, 2003), crystal growth from atomic-beams with and without desorption (Villain,

Correspondence concerning this article should be addressed to P. D. Christofides; e-mail: pdc@seas.ucla.edu.

1991), epitaxial growth processes with adsorption, desorption and surface migration (Vvedensky et al., 1993), surface erosion by ion sputtering (Cuerno et al., 1995), and ZrO_2 thin film growth by reactive ion beam sputtering (Qi et al., 2003).

This article presents a method for feedback control of surface roughness in deposition processes, based on stochastic PDEs which describe the fluctuation of surface height in the spatial domain. To demonstrate the method, we focus on control of surface roughness in a deposition process on a 1-dimensional (1-D) 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.

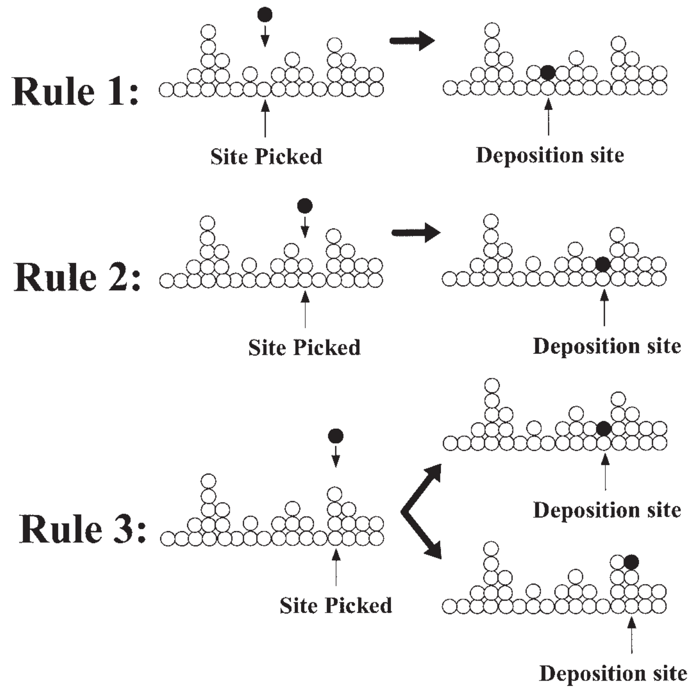

Figure 1. Rules of the deposition.

Preliminaries

We consider a deposition process on a one-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. The rules of the deposition are shown in Figure 1. There is no particle migration and desorption taking place on this process (see (Lou and Christofides, 2003a,b) for film growth processes that involve these phenomena).

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. Mathematically, kinetic Monte-Carlo simulation methods provide an unbiased realization of the master equation (Gillespie, 1976; Van Kampen, 1992), which describes the evolution of the probability that the surface is at a certain configuration. Kinetic Monte-Carlo simulation can predict average properties of the surface from a deposition process (which are of interest from a control point of view, like, for example, surface roughness). Since a kinetic Monte-Carlo simulation run constitutes a realization of a stochastic process, simulation results from different simulation runs are not identical. However, by averaging the results from different simulation runs, the averaged properties of the surface converge to the values obtained from the solution of the master equation.

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

Our objective is to control the surface roughness of the deposition process described by Figure 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

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

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 (that is, b_i determines how the control action computed by the ith control actuator u_i, is distributed (for example, 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

$$A\bar{\phi}_n(x) = \nu \frac{d^2\bar{\phi}_n(x)}{dx^2} = \lambda_n \bar{\phi}_n(x), \quad n = 1, \ldots, \infty$$

$$\frac{d^j\bar{\phi}_n}{dx^j}(-\pi) = \frac{d^j\bar{\phi}_n}{dx^j}(\pi), \quad j = 0, 1 \tag{7}$$

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 $n = 1, \ldots, \infty$. 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 (that is, 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 $\sigma(A) = \sigma_1(A) \cup \sigma_2(A)$, where $\sigma_1(A)$ contains the first m (with m finite) eigenvalues (that is, $\sigma_1(A) = \{\lambda_1, \ldots, \lambda_m\}$), and $\sigma_2(A)$ contains the remaining eigenvalues (that is, $\sigma_2(A) = \{\lambda_{m+1}, \ldots, \}$.

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

$$\frac{d\alpha_n}{dt} = -\nu n^2 \alpha_n + \sum_{i=1}^{p} b_{i\alpha_n} u_i(t) + \xi_\alpha^n(t)$$

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

where

$$b_{i\alpha_n} = \int_{-\pi}^{\pi} \phi_n(x)b_i(x)dx, \quad b_{i\beta_n} = \int_{-\pi}^{\pi} \psi_n(x)b_i(x)dx,$$

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

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

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

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 of the system of infinite stochastic ODEs of Eq. 9.

Remark 1. *Note that in practice, the control action u_i, can be implemented by manipulating the gas composition across the surface in a deposition process (Armaou and Christofides, 1999). Spatially controllable CVD reactors have been developed to enable across-wafer spatial control of surface gas composition during deposition (Adomaitis et al., 2003). In such a control problem formulation, the rate that particles land on the surface is spatially distributed and is computed by the controller. However, the value of r_a, which is used to calculate the values of ν and the covariance, ς in the system of Eq. 4, corresponds to the adsorption rate under open-loop operation, and, thus, it is a constant. The contribution of the spatially distributed adsorption rate to the fluctuations of the surface height profile (for example, the surface roughness) is captured by the term $\sum_{i=1}^{p} b_i(x)u_i(t)$. This control problem formulation is further supported by our simulation results that the controller designed, based on the stochastic PDE model of the deposition process can be applied to the kinetic Monte-Carlo model of the same deposition process to control the surface roughness to desired levels (see simulation results section).*

Feedback control

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

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 (that is, 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 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

$$x_s = [\alpha_1 \quad \cdots \quad \alpha_m \quad \beta_1 \quad \cdots \quad \beta_m]^T,$$

$$x_f = [\alpha_{m+1} \quad \beta_{m+1} \quad \cdots]^T,$$

$$\Lambda_s = diag[-\nu \quad \cdots \quad -m^2\nu \quad -\nu \quad \cdots \quad -m^2\nu],$$

$$\Lambda_f = diag[-(m+1)^2\nu - (m+1)^2\nu \cdots],$$

$$u = [u_1 \quad \cdots \quad u_p], \quad \xi_s = [\xi_\alpha^1 \quad \cdots \quad \xi_\alpha^m \quad \xi_\beta^1 \quad \cdots \quad \xi_\beta^m],$$

and

$$\xi_f = [\xi_\alpha^{m+1} \quad \xi_\beta^{m+1} \quad \cdots].$$

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

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.

Feedback controller 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; $\Lambda_{cs} = diag[\lambda_{c\alpha 1} \quad \cdots \quad \lambda_{c\alpha m} \quad \lambda_{c\beta 1} \quad \cdots \quad \lambda_{c\beta m}]$, $\lambda_{c\alpha i}$ 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 $(n = 1, \ldots, m)$ on the poles of the finite-dimensional system of Eq. 13. Then, we will show in the next subsection that the surface roughness of the infinite-dimensional system of Eq. 9 can be controlled to a 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

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

where $X_s(k) = \tilde{x}_s(k\Delta t)$, $G_{cs} = e^{\Lambda_{cs}\Delta t}$, $\zeta_s(k) = \int_{k\Delta t}^{(k+1)\Delta t} e^{\Lambda_{cs}((k+1)\Delta t - t)}\xi_s(t)dt$. 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 $R_1 = \langle \zeta_s\zeta_s^T\rangle$. Equation 17 cannot 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 $P_\alpha(\infty) = diag[\langle\alpha_1(\infty)^2\rangle \quad \cdots \quad \langle\alpha_m(\infty)^2\rangle$, $P_\beta(\infty) = diag[\langle\beta_1(\infty)^2\rangle \quad \cdots \quad \langle\beta_m(\infty)^2\rangle]$. Using Result 1, $\langle\alpha_n(\infty)^2\rangle$ and $\langle\beta_n(\infty)^2\rangle$ $(n = 1, \ldots, m)$ can be computed by using the following expressions

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

From Eq. 19, we can see that by assigning the closed-loop poles $\lambda_{c\alpha_n}$, and $\lambda_{c\beta_n}$ $(n = 1, \ldots, m)$ at desired locations, the covariances of the states α_n and β_n $(n = 1, \ldots, m)$ 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.

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 and Daoutidis, 1997; 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 $\Lambda_\varepsilon x_s$ term can be made very small compared to the $\Lambda_f x_f$ term and thus, the closed-loop system of Eq. 20 can be adequately described by the following system

$$\frac{dx_s}{dt} = \Lambda_{cs}x_s + \xi_s$$

$$\frac{dx_f}{dt} = \Lambda_f x_f + \xi_f \tag{21}$$

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

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

Therefore, for m sufficiently large, 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 $m \rightarrow \infty$, 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

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

where

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

Remark 2. Note that in order to regulate the surface roughness to a desired level, $\langle\sqrt{r_d^2}\rangle$, the number of actuators should be large enough so that the value of $\langle\sqrt{r_d^2}\rangle$ is achievable. Specifically, the number of actuators, m should be selected such that the following inequality holds

$$\sqrt{\langle r_d^2\rangle} > \varsigma\sqrt{\frac{1}{2\pi}\left(\sum_{n=m+1}^{\infty}\frac{1}{\nu n^2}\right)} \tag{25}$$

This is because the closed-loop stability requires that $\lambda_{c\alpha_i} < 0$ and $\lambda_{c\beta_i} < 0$ (for $i = 1, \ldots, m$), and thus, $\lambda^* > 0$ in Eq. 24.

Remark 3. 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 so that the following equation holds*

$$\lambda^* = \frac{2\pi(\langle r_d^2\rangle - \langle r_f^2\rangle)}{\varsigma^2} \tag{26}$$

The controller which assigns the poles of the system of Eq. 15 to satisfy Eq. 26 is not unique. Consequently, for a fixed number of actuators p, the controller that can regulate the closed-loop surface roughness to a desired level is also not unique. Furthermore, we note that robust control methods (Christofides, 1998; Christofides and Baker, 1999), which utilize bounds of the noise terms, can be employed to design controller that can achieve arbitrary degree of attenuation of the effect of noise on the PDE system state.

Remark 4. Note that the expected value of the open-loop surface roughness converges to its steady-state value $\sqrt{\langle r_{ol}^2\rangle}$, which can be computed as follows

$$\sqrt{\langle r_{ol}^2\rangle} = \sqrt{\frac{\varsigma^2}{2\pi\nu}\left(\sum_{k=1}^{\infty}\frac{1}{k^2}\right)} \tag{27}$$

If the closed-loop poles of the finite-dimensional system of Eq. 15 are written as $\lambda_{c\alpha_k} = -\nu n_{\alpha_k}^2$ and $\lambda_{c\beta_k} = -\nu n_{\beta_k}^2$ for $k = 1, \ldots, m$, the ratio of the expected value of the steady-state closed-loop surface roughness, $\sqrt{\langle r_{cl}^2\rangle}$ to that of the steady-state open-loop surface roughness, $\sqrt{\langle r_{ol}^2\rangle}$ can be computed as follows

$$\frac{\sqrt{\langle r_{cl}^2\rangle}}{\sqrt{\langle r_{ol}^2\rangle}} = \sqrt{\frac{\sum_{k=1}^{m}\left(\frac{1}{n_{\alpha_k}^2}+\frac{1}{n_{\beta_k}^2}\right)+\sum_{k=m+1}^{\infty}\frac{1}{k^2}}{\sum_{k=1}^{\infty}\frac{1}{k^2}}} \tag{28}$$

This ratio is independent of the lattice size of the deposition system. Therefore, if the control objective is to achieve a certain percentage of reduction of the value of surface roughness from that under open-loop operation, the number of actuators needed is independent of the lattice size of the deposition process.

Remark 5. Note that it is possible to apply the proposed method to control the surface roughness of deposition processes taking place in 2-D surfaces. In a 2-D process, the feedback control design and the analysis of the closed-loop system will be based on the model of Eq. 11. Moreover, Eq. 11 will be obtained by solving the eigenvalue/eigenfunction problem of the operator A in the 2-D spatial domain with appropriate boundary conditions. After Eq. 11 is obtained, the method for control design and closed-loop analysis presented earlier can be applied to control the surface roughness for 2-D surfaces described by stochastic PDEs.

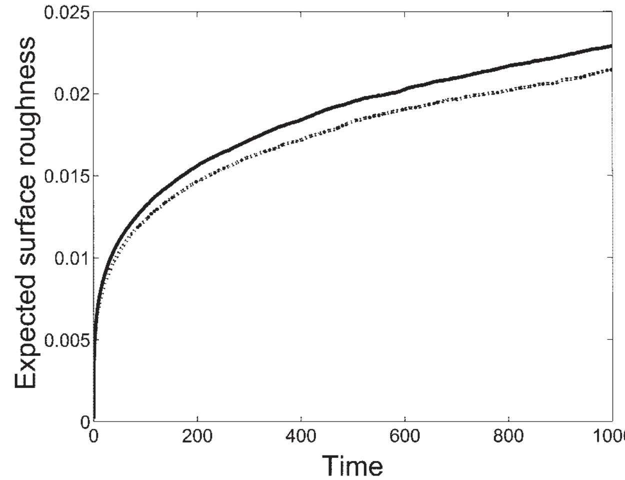

Figure 2. Comparison of the open-loop profile of the expected surface roughness from the kinetic Monte-Carlo simulator (solid line) and that from the solution of the SPDE using 1,000 modes (dotted line).

Simulation results

In this section, we present an application of the proposed state feedback controller to the deposition process described in Figure 1 to regulate the surface roughness to a desired level. Specifically, the deposition occurs on a lattice containing 1,000 sites. Therefore, $a = 0.00628$. The open-loop deposition rate for each site is $\bar{r}_a = 1s^{-1}$. A 1,000th 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 $1/\delta t$.

In the first simulation, we compare the expected value of the open-loop surface roughness 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 (Gillespie, 1976) 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 $dt = (-\ln \zeta)/(N \times r_a)$, 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 expected surface roughness are obtained by averaging surface roughness profiles (either from the stochastic PDE or the kinetic Monte-Carlo simulations) from 1,000 independent simulation runs by using the same simulation parameters. Figure 2 shows the simulation results. The two profiles

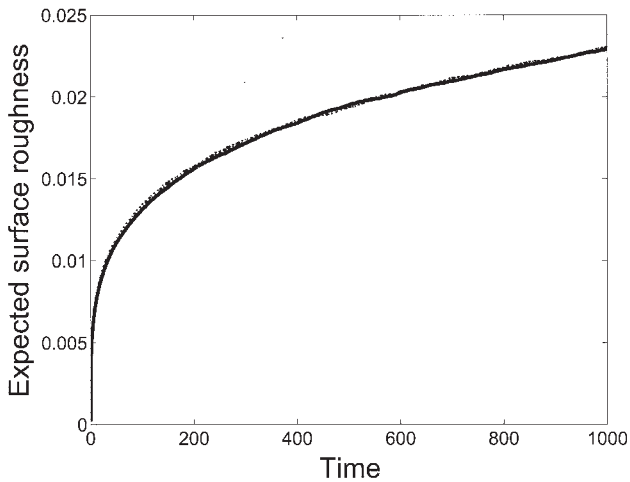

Figure 3. Comparison of the open-loop profile of the expected surface roughness from the kinetic Monte-Carlo simulator (solid line) and that from the solution of the SPDE, with adjusted covariance, using 1000 modes (dotted line).

reflect the same tendency of the evolution of the surface roughness. However, the expected surface roughness from the solution of the stochastic PDE model of Eq. 1 is about 9% lower than that from the kinetic Monte-Carlo simulation. This difference of expected surface roughness from the two models is due to approximations made during the derivation of the stochastic PDE model of the deposition process based on the master equation and the transition rules (see Remark 6 for a discussion on this issue). However, this model error can be compensated by appropriately adjusting the value of covariance of Eq. 2. In the second simulation run, we increase the value of ς in Eq. 2 by 9% (ς is increased from 4.98×10^{-4} to 5.43×10^{-4}), and show the comparison of the profiles of expected surface roughness from the kinetic Monte-Carlo simulation and from the solution of the stochastic PDE model in Figure 3. We can see that with this adjustment of ς, the two profiles are almost identical. Therefore, by slightly adjusting the covariance of the stochastic PDE model of Eq. 1, the model can adequately capture the evolution of surface roughness of the deposition process described in Figure 1 obtained by the kinetic Monte-Carlo simulations. Therefore, our control design will be based on the stochastic PDE model of the process with adjusted ς.

Subsequently, we design a state feedback controller based on a 40th order stochastic ODE approximation constructed by using the first 40 eigenmodes of the system of Eq. 9 with adjusted value of the covariance. 40 control actuators are used to control the system. The ith actuator distribution function is taken to be

$$b_i(x) = \begin{cases} \dfrac{1}{\sqrt{\pi}} \sin(ix); & i = 1, \ldots, 20 \\ \dfrac{1}{\sqrt{\pi}} \cos[(i-20)x]; & i = 21, \ldots, 40 \end{cases} \tag{29}$$

The expected open-loop surface roughness converges to 0.045, which can be computed using Eq. 27. The desired closed-loop surface roughness is 0.01 in this simulation, which is a 78% reduction compared to the open-loop surface roughness. Using Eq. 24, we design the state feedback controller such that $\lambda_{c\alpha_i} = \lambda_{c\beta_i} = -0.023$, for $i = 1, \ldots, 20$. Then, we apply the designed controller to the kinetic Monte-Carlo model of the deposition process to control the surface roughness to the desired level. In this simulation, the controller is implemented by manipulating the adsorption rate of particles across the surface. Specifically, the adsorption rate on site i at time t is determined according to the following expression

$$r_a(i, t) = \bar{r}_a + \left(\sum_{j=1}^{40} b_j(x_i) u_j(t) \right) / a \tag{30}$$

The following simulation algorithm is used to run the kinetic Monte-Carlo simulations for the closed-loop system. First, a random number is generated to pick a site among all the sites on the 1-D lattice; the probability that a surface site is picked is proportional to the adsorption rate on this site, which is computed using Eq. 30. 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 $dt = -\ln \zeta / (\sum_{i=1}^{N} r_a(i))$, where ζ is a random number in the (0, 1) interval, and N is the total number of sites on the lattice. Once a particle is deposited, the first 40 states ($\alpha_1, \ldots, \alpha_{20}$ and $\beta_1, \ldots, \beta_{20}$) are updated and new control actions are computed to update the spatially distributed adsorption rate across the

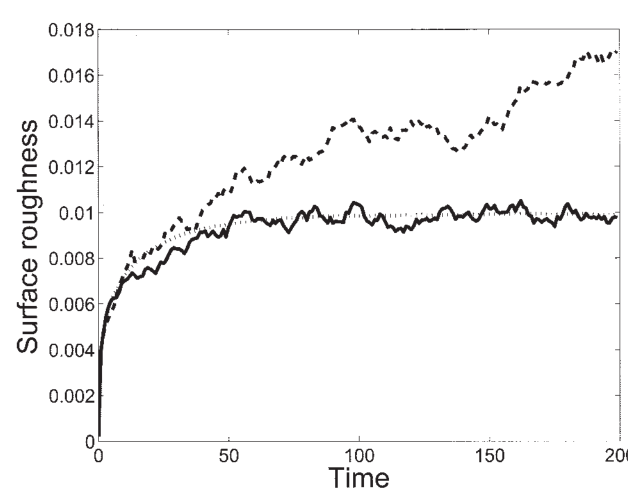

Figure 4. Closed-loop simulation results by applying the controller designed based on the first 40 modes of the SPDE model to the kinetic Monte-Carlo model.

(a) The closed-loop surface roughness profile from one simulation run (solid line), (b) the expected closed-loop surface roughness profile (dotted line), and (c) the open-loop surface roughness profile from one simulation run (dashed line).

surface. The closed-loop system simulation results are shown in Figure 4. The dotted line shows the expected surface roughness, which is the average of surface roughness profiles obtained from 200 independent runs, under feedback control. We can see that the controller successfully drives the expected surface roughness to the desired level. The solid line shows the surface roughness profile under feedback control from one simulation run; due to the stochastic nature of the deposition process, stochastic fluctuations can be observed in the closed-loop surface roughness profile, but the surface roughness is very close to the set-point value under feedback control. For the sake of comparison, the dashed-line shows a surface roughness profile from one open-loop simulation run. We can see that under feedback control, a much lower surface roughness can be achieved. Finally, we note that the proposed approach for controller design can be, in principle, applied to larger scale deposition processes to control surface roughness. In such a case, the stochastic PDE model can be constructed by initially deriving a stochastic PDE model, based on the transition rules and then fitting the model parameters, based on experimental roughness data of the specific deposition process (see also the discussion in Remark 4).

Remark 6. The stochastic PDE models for many deposition processes can be derived, based on the corresponding master equations, which describe the evolution of the probability that the surface is at a certain configuration. Two major assumptions are made to derive the stochastic PDE models, based on the master equation. Specifically, if $\boldsymbol{H} = \{h_1, h_2, \cdots\}$ *represents the surface configuration,* $\boldsymbol{r} = \{r_1, r_2, \cdots\}$ *is the array of jump lengths at each site and* $W(\boldsymbol{H}; r,)$ *is the transition rate from* $\boldsymbol{H}$ *to* $\boldsymbol{H} + r$*, it is assumed that there exists a quantity* δ *such that (1)* $W(\boldsymbol{H}; r) \approx 0$*, for* $|\boldsymbol{r}| > \delta$*, and (2)* $W(\boldsymbol{H} + \Delta\boldsymbol{H}; r) \approx W(\boldsymbol{H}; r)$*, for* $|\Delta\boldsymbol{H}| < \delta$ *(Van Kampen, 1992). Because the difference in successive configurations is one height unit on a single site, the first assumption can be satisfied by increasing the number of lattice sites in the deposition process (equivalently, reducing the size of a single lattice on a fixed spatial domain as considered in this work). However, due to the dependence of the final deposition site on the local surface configuration, a change in a surface site by one height unit can produce a step change in W, which violates the second assumption; increasing the number of sites in the deposition process cannot alleviate this problem (Haselwandter and Vvedensky, 2002). Therefore, increase of the lattice sites can reduce the error of the solution of the stochastic PDE and of the kinetic Monte-Carlo simulation due to the first assumption, however, it cannot completely eliminate the model error between the expected roughness value obtained from the discrete microscopic kMC simulation and from the stochastic PDE (which is a continuous approximation of the discrete process), due to the fact that the second assumption cannot be fully satisfied. As a result, to design feedback controllers based on stochastic PDE models, it is necessary to adjust the model parameters to compensate for this model error.*

Remark 7. Note that the controller design method developed in this work can be applied to other processes modeled by stochastic PDEs (see, for example, (Lou and Christofides, 2004a) for an application of this method to control the stochastic Kuramoto-Sivashinsky equation which describes the evolution of the height profile for surfaces in a variety of physical and chemical processes including surface erosion by ion sputtering (Cuerno et al., 1995), and ZrO_2 *thin film growth by reactive ion beam sputtering (Qi et al., 2003)).*

Literature Cited

Armaou, A., and P. D. Christofides, “Plasma-Enhanced Chemical Vapor Deposition: Modeling and Control,” *Chem. Eng. Sci.*, **54,** 3305 (1999).

Åström, K. J., *Introduction to Stochastic Control Theory,* Academic Press, New York (1970).

Adomaitis, R. A., J. O. Choo, G. W. Rubloff, L. Henn-Lecordier, and Y. Liu, Spatially Controllable CVD: The Programmable Reactor Project. In *AIChE Meeting, paper 177f,* San Francisco, CA (2003).

Christofides, P. D., “Robust Control of Parabolic PDE Systems.” *Chem. Eng. Sci.,* **53,** 2449 (1998).

Christofides, P. D., *Nonlinear and Robust Control of PDE Systems: Methods and Applications to Transport-Reaction Processes,* Birkhäuser, Boston (2001).

Christofides, P. D., and J. Baker, “Robust Output Feedback Control of Quasi-Linear Parabolic PDE Systems,” *Syst. & Contr. Lett.,* **36,** 307 (1999).

Christofides, P. D., and P. Daoutidis, “Finite-Dimensional Control of Parabolic PDE Systems Using Approximate Inertial Manifolds,” *J. Math. Anal. Appl.,* **216,** 398 (1997).

Cuerno, R., H. A. Makse, S. Tomassone, S. T. Harrington, and H. E. Stanley, “Stochastic Model for Surface Erosion Via Ion Sputtering: Dynamical Evolution from Ripple Morphology to Rough Morphology,” *Phy. Review Lett.,* **75,** 4464 (1995).

Edwards, S. F., and D. R. Wilkinson, “The Surface Statistics of a Granular Aggregate,” *Proc. R. Soc. Lond. A,* **381,** 17 (1982).

Fichthorn, K. A., and W. H. Weinberg, “Theoretical Foundations of Dynamical Monte Carlo Simulations,” *J. of Chem. Phys.,* **95,** 1090 (1991).

Gallivan, M. A., and R. M. Murray, Model Reduction and System Identification of Master Equation Control Systems. *Proc. of A. Control Conf.* Denver, Colorado, pp. 3561–3566 (2003).

Gillespie, D. T., “A General Method for Numerically Simulating the Stochastic Time Evolution of Coupled Chemical Reactions,” *J. of Comp. Phy.,* **22,** 403 (1976).

Granneman, E. H., “Thin Films in the Integrated Circuit Industry: Requirements and Deposition Methods,” *Thin Solid Films,* **228,** 1 (1993).

Haselwandter, C., and D. D. Vvedensky, “Fluctuations in the Lattice Gas for Burgers’ Equation,” *J. of Phy. A: Math. and General,* **35,** L579 (2002).

Lam, R., and D. G. Vlachos, “Multiscale Model for Epitaxial Growth of Films: Growth Mode Transition,” *Physical Review,* **64,** 035401 (2001).

Lou, Y., and P. D. Christofides, “Estimation and Control of Surface Roughness in Thin Film Growth Using Kinetic Monte-Carlo Models,” *Chem. Eng. Sci.,* **58,** 3115 (2003a).

Lou, Y., and P. D. Christofides, “Feedback Control of Growth Rate and Surface Roughness in Thin Film Growth,” *AIChE J.,* **49,** 2099 (2003b).

Lou, Y., and P. D. Christofides, “Feedback Control of Surface Roughness in a Sputtering Process Using the Stochastic Kuramoto-Sivashinsky Equation,” *Comp. & Chem. Eng.,* **24,** 225 (2005).

Lou, Y., and P. D. Christofides, “Feedback Control of Surface Roughness of GaAs (001) Thin Films Using Kinetic Monte-Carlo Models,” *Comp. & Chem. Eng.,* in press (2004b).

Qi, H. J., L. H. Huang, Z. S. Tang, C. F. Cheng, J. D. Shao, and F. X. Fan, “Roughness Evolution of ZrO_2 Thin Films Grown by Reactive Ion Beam Sputtering,” *Thin Solid Films,* **444,** 146 (2003).

Siettos, C. I., A. Armaou, A. G. Makeev, and I. G. Kevrekidis, “Microscopic/Stochastic Timesteppers and “Coarse” Control: a kMC Example,” *AIChE J.,* **49,** 1922 (2003).

Van Kampen, N. G., *Stochastic Processes in Physics and Chemistry,* North-Holland, Amsterdam (1992).

Villain, J., “Continuum Models of Crystal Growth from Atomic Beams With and Without Desorption,” *J. Phys. I,* **1,** 19 (1991).

Vvedensky, D. D., “Edwards-Wilkinson Equation from Lattice Transition Rules,” *Physical Review E,* **67,** 025102 (2003).

Vvedensky, D. D., A. Zangwill, C. N. Luse, and M. R. Wilby, “Stochastic Equations of Motion for Epitaxial Growth,” *Physical Review E,* **48,** 852 (1993).

Manuscript received Dec. 16, 2003, and revision received May 14, 2004.