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PARAMETER IDENTIFICATION FOR NONLINEAR STOCHASTIC PDE MODEL OF A SPUTTERING PROCESS

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Abstract: This work focuses on identification of the parameters of the nonlinear stochastic Kuramoto-Sivashinsky equation (KSE), a fourth order nonlinear stochastic partial differential equation (PDE), that describes the fluctuation of surface height of a sputtering process including two surface micro-processes, diffusion and erosion. To perform the system identification, we initially formulate the nonlinear stochastic KSE into a system of infinite nonlinear stochastic ordinary differential equations (ODEs) by using Galerkin's method. A finite-dimensional approximation of the stochastic KSE is then constructed that captures the dominant mode contribution to the state and the evolution of the state covariance of the stochastic ODE system is derived. Then, a kinetic Monte-Carlo (kMC) simulator is used to generate surface snapshots during process evolution to obtain values of the state vector of the stochastic ODE system. Subsequently, the state covariance of the stochastic ODE system that corresponds to the sputtering process is computed based on the kMC simulation results. Finally, the model parameters of the nonlinear stochastic KSE are obtained by using least-squares fitting so that the state covariance computed from the stochastic KSE process model matches that computed from kMC simulations. Simulations are performed to demonstrate the effectiveness of the proposed parameter identification approach. *Copyright ©2007 IFAC*

Keywords: system identification, nonlinear stochastic PDEs, sputtering processes, kinetic Monte-Carlo simulations

1. INTRODUCTION

Modeling and control of thin film micro-structure in deposition and sputtering processes has attracted significant research efforts to improve the quality of thin films of advanced materials used in a wide range of applications, e.g., microelectronic devices, optics, micro-electro-mechanical systems (MEMS) and biomedical products. Sputtering processes are widely used in the thin film and semiconductor fabrication to remove material from the surface of solids through the impact of energetic particles. In a sputtering process, the surface is directly shaped by the microscopic surface processes (e.g., erosion, diffusion and surface reaction), which are stochastic processes. Therefore, the stochastic nature of sputtering processes must be fully considered in the modeling and control of such processes. The desire to understand and control the thin film micro-structure has motivated extensive research on fundamental mathematical models describing the microscopic features of surfaces formed by surface micro-processes, which include 1) dynamical Monte-Carlo methods, and 2) stochastic partial differential equations (PDEs).

Using fundamental process models, systematic methods for real-time control and optimization of thin film growth processes to achieve desired material micro-structure have been developed. Specifically, a methodology for feedback control of thin film surface roughness using kinetic Monte-Carlo (kMC) models was developed in (Lou and Christofides, 2003). However, the need to perform system-level analysis and the design and implementation of model-based feedback control systems calls for closed-form stochastic process models. This has motivated recent re-

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search on the development of methods for feedback control of surface roughness based on linear (Lou and Christofides, 2005; Ni and Christofides, 2005) and nonlinear (Lou and Christofides, 2006) stochastic PDE process models. Also, methods for multiscale optimization to achieve both macroscopic and microscopic objectives have been developed (Varshney and Armaou, 2005).

Although stochastic PDE models are suitable for model-based controller design, the construction of stochastic PDE models for thin film growth processes directly based on microscopic process rules is, in general, a very difficult task. Motivated by this, a systematic identification approach was developed for linear stochastic PDEs (Lou and Christofides, 2005). Furthermore, a method for construction of linear stochastic PDE models for thin film growth using first principles-based microscopic simulations was developed and applied to construct stochastic PDE models for thin film deposition processes in 2-dimensional lattices (Ni and Christofides, 2005). However, nonlinearities exist in many material preparation processes in which surface evolution can be modeled by stochastic PDEs. A typical example of such processes is the sputtering process whose surface evolution is described by the nonlinear stochastic Kuramoto-Sivashinsky equation (KSE). In a simplified setting, the sputtering process includes two types of surface micro-processes, erosion and diffusion. The nonlinearity of the sputtering process originates from the dependence of the rate of erosion on a nonlinear sputtering yield function (Cuerno *et al.*, 1995). A method for nonlinear control of stochastic PDEs was recently developed (Lou and Christofides, 2006). However, Available methods for identification and construction of linear stochastic PDEs require the analytical solutions of state covariances (Lou and Christofides, 2005; Ni and Christofides, 2005), which prevent their direct applications to nonlinear stochastic PDEs. This motivates the research on development of methods for identification of nonlinear stochastic PDE process models.

This work focuses on identification of the parameters of the nonlinear stochastic KSE process model that describes the fluctuation of surface height of a sputtering process including two surface micro-processes, diffusion and erosion. To perform the system identification, we initially formulate the nonlinear stochastic KSE into a system of infinite nonlinear stochastic ODEs by using Galerkin's method. A finite-dimensional approximation of the stochastic KSE is then derived that captures the dominant mode contribution to the state. The evolution of the state covariance of the stochastic ODE system is subsequently derived. Then, we use a kMC simulator to generate surface snapshots for different instants during process evolution to obtain values of the state vector of the stochastic ODE system. Subsequently, the state covariance of the stochastic ODE system that corresponds to the sputtering process is computed based on the kMC simulation results. Finally, the model parameters of the nonlinear stochastic KSE are obtained by using least-squares fitting so that the state covariance computed from the stochastic KSE process model matches that computed from kMC simulations. Computer simulations are performed to demonstrate the effectiveness of the proposed parameter identification approach.

2. PROCESS DESCRIPTION

We consider a 1-D-lattice representation of a crystalline surface in a sputtering process, which includes two surface micro-processes, erosion and diffusion. The solid-on-solid assumption is made which means that no defects or overhangs are allowed in the process. The microscopic rules are as follows: a site, i, is first randomly picked among the sites of the whole lattice and the particle at the top of this site is subject to: a) erosion with probability $0 < f < 1$, or b) diffusion with probability $1 - f$.

If the particle at the top of site i is subject to erosion, the particle is removed from the site i with probability $P_e \cdot Y(\phi_i)$. P_e is determined as $\frac{1}{7}$ times the number of occupied sites in a box of size 3×3 centered at the site i, which is shown in Fig. 1. There is a total of 9 sites in the box. The central one is the particle to be considered for erosion (the one marked by $\bullet$). Among the remaining 8 sites, the site above the central site of interest must be vacant since the central site is a surface site. Therefore, only 7 of the 8 sites can be occupied and the maximum value of P_e is 1. $Y(\phi_i)$ is the sputtering yield function defined as follows:

$$Y(\phi_i) = y_0 + y_1\phi_i^2 + y_2\phi_i^4 \tag{1}$$

where y_0, y_1 and y_2 are process dependent constants and ϕ_i is the local slope defined as follows:

$$\phi_i = \tan^{-1}\left(\frac{h_{i+1} - h_{i-1}}{2a}\right) \tag{2}$$

where a is the lattice parameter and h_{i+1} and h_{i-1} are the values of surface height at sites $i+1$ and $i-1$, respectively.

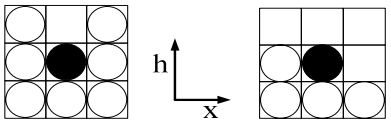

Fig. 1. Schematic of the rule to determine P_e. P_e is defined as $\frac{1}{7}$ times the number of occupied sites in a box of size 3×3 centered at the particle on the top of site i; $P_e = 1$ in the left figure and $P_e = \frac{4}{7}$ in the right figure, where the particle marked by $\bullet$ is on the top of site i.

If the particle at the top of site i is subject to diffusion, one of its two nearest neighbors, j ($j = i+1$ or $i-$

1) is randomly chosen and the particle is moved to the nearest neighbor column with probability $w_{i\to j}$ as follows:

$$w_{i\to j} = \frac{1}{1+\exp(\beta \Delta H_{i\to j})} \tag{3}$$

where $\Delta H_{i\to j}$ is the energy difference between the final and initial states of the move, $\beta = \frac{1}{k_B T}$ and H is defined through the Hamiltonian of an unrestricted solid-on-solid model as follows:

$$H = \left(\frac{J}{a^2}\right) \sum_{k=1}^{L} (h_k - h_{k+1})^n \tag{4}$$

where J is the bond energy, L is the total number of sites in the lattice and n is a positive number. In the simulations presented in this paper, we use $n = 2$ and $\beta J = 2.0$.

3. STOCHASTIC PDE MODEL OF THE SPUTTERING PROCESS

The sputtering process is a stochastic process. The equation for the height fluctuations of the surface in this sputtering process was derived in (Lauritsen *et al.*, 1996) and is a stochastic Kuramoto-Sivashinsky equation of the following form:

$$\frac{\partial h}{\partial t} = -\nu \frac{\partial^2 h}{\partial x^2} - \kappa \frac{\partial^4 h}{\partial x^4} + \frac{\lambda}{2}\left(\frac{\partial h}{\partial x}\right)^2 + \xi(x,t) \tag{5}$$

subject to periodic boundary conditions:

$$\frac{\partial^j h}{\partial x^j}(-\pi,t) = \frac{\partial^j h}{\partial x^j}(\pi,t),\ j = 0,\cdots,3 \tag{6}$$

and the initial condition:

$$h(x,0) = h_0(x) \tag{7}$$

where ν, κ, and λ are parameters related to surface mechanisms (Lauritsen *et al.*, 1996), $x \in [-\pi,\pi]$ is the spatial coordinate, t is the time, $h(x,t)$ is the height of the surface at position x and time t. $\xi(x,t)$ is a Gaussian noise with the following expressions for its mean and covariance:

$$\begin{aligned} \langle \xi(x,t) \rangle &= 0 \\ \langle \xi(x,t)\xi(x',t') \rangle &= \sigma^2 \delta(x-x')\delta(t-t') \end{aligned} \tag{8}$$

where σ is a constant, $\delta(\cdot)$ is the dirac function, and $\langle\cdot\rangle$ denotes the expected value. Note that the noise covariance depends on both space x and time t.

To study the dynamics of Eq.5, we initially consider the eigenvalue problem of the linear operator of Eq.5, which takes the form:

$$\begin{aligned} A\bar{\phi}_n(x) = -\nu \frac{d^2\bar{\phi}_n(x)}{dx^2} - \kappa \frac{d^4\bar{\phi}_n(x)}{dx^4} = \lambda_n \bar{\phi}_n(x) \\ n = 1,\cdots,\infty \\ \frac{d^j\bar{\phi}_n}{dx^j}(-\pi) = \frac{d^j\bar{\phi}_n}{dx^j}(+\pi);\ j = 0,\cdots,3; \end{aligned} \tag{9}$$

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 $\lambda_n = \nu n^2 - \kappa n^4$ (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.9 denotes either ϕ_n or ψ_n. From the expression of the eigenvalues, it follows that for fixed values of $\nu > 0$ and $\kappa > 0$, the number of unstable eigenvalues of the operator A in Eq.9 is finite and the distance between two consecutive eigenvalues (i.e. λ_n and λ_{n+1}) increases as n increases.

In the stochastic KSE model of Eq.5, there are four model parameters, ν, κ, λ, and σ^2 to be determined. To present the method that we use to identify the parameters of Eq.5, we first derive a nonlinear stochastic ODE approximation of Eq.5 using Galerkin's method. To this end, we first expand the solution of Eq.5 in an infinite series in terms of the eigenfunctions of the operator of Eq.9 as follows:

$$h(x,t) = \sum_{n=1}^{\infty} \alpha_n(t)\phi_n(x) + \sum_{n=0}^{\infty} \beta_n(t)\psi_n(x) \tag{10}$$

where $\alpha_n(t)$, $\beta_n(t)$ are time-varying coefficients. Substituting the above expansion for the solution, $h(x,t)$, into Eq.5 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 nonlinear stochastic ODEs is obtained:

$$\begin{aligned} \frac{d\alpha_n}{dt} &= (\nu n^2 - \kappa n^4)\alpha_n + \lambda \cdot f_{n\alpha} + \xi_\alpha^n(t) \\ & n = 1,\ldots,\infty \\ \frac{d\beta_n}{dt} &= (\nu n^2 - \kappa n^4)\beta_n + \lambda \cdot f_{n\beta} + \xi_\beta^n(t) \end{aligned} \tag{11}$$

where the expressions for $f_{n\alpha}$ and $f_{n\beta}$ can be found in (Lou and Christofides, 2006) and are omitted here for brevity.

$$\xi_\alpha^n(t) = \int_{-\pi}^{\pi} \xi(x,t)\phi_n(x)dx\ ;\ \xi_\beta^n(t) = \int_{-\pi}^{\pi} \xi(x,t)\psi_n(x)dx \tag{12}$$

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

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 $\langle\varepsilon^2\rangle = \sigma^2\int_a^b f^2(x)dx$ (Åström, 1970).

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

4. PARAMETER IDENTIFICATION OF THE NONLINEAR STOCHASTIC PDE MODEL

While the parameters of stochastic PDE models for many deposition processes and sputtering 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; for all practical purposes, the stochastic PDE model parameters should be identified by matching the prediction of the stochastic PDE model to that of kinetic Monte-Carlo simulations due to the approximations made in the derivation of the stochastic PDE model from the master equation (Haselwandter and Vvedensky, 2002; Lou and Christofides, 2005).

In this section, we present a method to identify the parameters of the nonlinear stochastic PDE model of the sputtering process by using the data from the kinetic Monte-Carlo simulations of the same process.

4.1 *Model reduction*

Owing to its infinite-dimensional nature, the system of Eq.11 cannot be directly used as a basis to design a parameter identification algorithm that can be implemented in practice (i.e., the practical implementation of such algorithms designed on the basis of this system will require the computation of infinite sums which cannot be done by a computer). Instead, we will identify model parameters using a finite-dimensional approximation of this system. Subsequently, we rewrite the system of Eq.11 as follows:

$$\begin{aligned} \frac{dx_s}{dt} &= \Lambda_s x_s + f_s(x_s,x_f) + \xi_s \\ \frac{dx_f}{dt} &= \Lambda_f x_f + f_f(x_s,x_f) + \xi_f \end{aligned} \tag{13}$$

where $x_s = [\alpha_1 \cdots \alpha_m \ \beta_1 \cdots \beta_m]^T$, x_f=[α_{m+1} β_{m+1} $\cdots$ $]^T$, Λ_s=$diag[\lambda_1 \cdots \lambda_m \ \lambda_1 \cdots \lambda_m]$, Λ_f = $diag[\lambda_{m+1}$ λ_{m+1} λ_{m+2} λ_{m+2} $\cdots]$, $f_s(x_s,x_f)$ = $[f_{1\alpha}(x_s,x_f)$ $\cdots$ $f_{m\alpha}(x_s,x_f)$ $f_{1\beta}(x_s,x_f)$ $\cdots$ $f_{m\beta}(x_s,x_f)]^T$, $f_f(x_s,x_f)$ = $[f_{m+1\alpha}(x_s,x_f)$ $f_{m+1\beta}(x_s,x_f)$ $\cdots$ $]^T$, ξ_s = $[\xi_\alpha^1 \cdots \xi_\alpha^m \ \xi_\beta^1$ $\cdots$ $\xi_\beta^m]$, ξ_f = $[\xi_\alpha^{m+1}$, and ξ_β^{m+1} $\cdots]$. The dimension of the x_s subsystem is $2m$ and the x_f subsystem is infinite-dimensional.

We note that the subsystem x_f in Eq.13 is infinite-dimensional. Neglecting the x_f subsystem, the following $2m$-dimensional system is obtained:

$$\frac{d\tilde{x}_s}{dt} = \Lambda_s \tilde{x}_s + f_s(\tilde{x}_s,0) + \xi_s \tag{14}$$

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

4.2 *System of deterministic ODEs for state covariance*

The system of Eq.14 is a finite-dimensional nonlinear stochastic ODE system including all four parameters, ν, κ, λ, and σ^2 of the of stochastic PDE model of Eq.5. We derive the system of deterministic ODEs that describes the dynamics of the covariance matrix of x_s, which is defined as $P_s = \langle x_s x_s^T \rangle$.

Consider the evolution of the state of Eq.14 in a small time interval, $[t, t+\Delta t]$ as follows (Chua *et al.*, 2005):

$$\begin{aligned} x_s(t+\Delta t) \ = \ & (I_s + \Delta t \cdot \Lambda_s) x_s(t) + \\ & \Delta t \cdot \lambda f_s(x_s,0) + \Delta t \cdot \xi_s(t) \end{aligned} \tag{15}$$

where I_s is a $2m \times 2m$ identity matrix. To study the dynamics of P_s, we approximate the dirac function, $\delta(\cdot)$ involved in the covariances of ξ_s by $\frac{1}{\Delta t}$, assume that $\xi_s(t)$ is independent of $x_s(t)$, and neglect the terms with Δt^2. The following equation for P_s can be obtained:

$$\begin{aligned} P_s(t+\Delta t) \ = \ & P_s(t) + \Delta t \cdot \{\Lambda_s P_s(t) + P_s(t)\Lambda_s^T + \\ & \lambda \left\langle x_s(t) f_s(x_s,0)^T + f_s(x_s,0) x_s(t)^T \right\rangle \\ & + R_s\} \end{aligned} \tag{16}$$

where R_s is the intensity of ξ_s and $R_s \delta(t-t') = \langle \xi_s(t) \xi_s^T(t) \rangle$. In this work, $R_s = \sigma^2 I_{2m \times 2m}$.

By setting $\Delta t \to 0$, we have the following system of deterministic ODEs for the state covariance of the system of Eq.14:

$$\begin{aligned} \frac{dP_s(t)}{dt} \ = \ & \Lambda_s P_s(t) + P_s(t)\Lambda_s^T + R_s + \\ & \lambda \left\langle x_s(t) f_s(x_s,0)^T + f_s(x_s,0) x_s(t)^T \right\rangle \end{aligned} \tag{17}$$

Eq.17 is a finite-dimensional nonlinear deterministic ODE system. Note that the linear part of this equation is the Lyapunov equation used in covariance controller design for linear systems (Hotz and Skelton, 1987).

4.3 *Parameter identification*

The four parameters of the stochastic PDE process model of Eq.5 can be identified from Eq.17. Specifically, the parameters ν and κ are included in the matrix Λ_s of Eq.17 and the parameter λ is associated to the nonlinear term of Eq.17. To this end, we need to obtain P_s and $\left\langle x_s(t) f_s(t)^T + f_s(t) x_s(t)^T \right\rangle$, which are both functions of x_s, to perform the parameter identification. The data of $x_s = [\alpha_1(t) \cdots \alpha_m(t) \ \beta_1(t) \cdots \beta_m(t)]^T$ can be obtained from kinetic Monte-Carlo simulation of the same sputtering process. The kinetic Monte-Carlo simulation algorithm and the method to compute $\alpha_n(t)$ and $\beta_n(t)$ (for $n = 1, 2, \cdots, m$) from surface snapshots for the sputtering process can be found in (Lou and Christofides, 2005; Lou and Christofides, 2006) and are omitted here for brevity.

Once x_s is obtained from the kinetic Monte-Carlo simulation, $f_s(x_s,0)$ = $[f_{1\alpha}(x_s,0) \cdots f_{m\alpha}(x_s,0)$ $f_{1\beta}(x_s,0)$ $\cdots$ $f_{m\beta}(x_s,0)]^T$ can be computed as follows:

$$\begin{aligned} f_{n\alpha}(x_s,0) \ = \ & \frac{1}{2} \int_{-\pi}^{\pi} \phi_n(x) \cdot \\ & \left(\sum_{j=1}^{m} \alpha_j(t) \frac{d\phi_j}{dx}(x) + \sum_{j=0}^{m} \beta_j(t) \frac{d\psi_j}{dx}(x) \right)^2 dx \end{aligned} \tag{18}$$

$$f_{n\beta}(x_s,0) = \frac{1}{2}\int_{-\pi}^{\pi} \psi_n(x)\cdot \left(\sum_{j=1}^{m}\alpha_j(t)\frac{d\phi_j}{dx}(x)+\sum_{j=0}^{m}\beta_j(t)\frac{d\psi_j}{dx}(x)\right)^2 dx$$

$$;n = 1,2,\cdots,m.$$

To compute the expected values for $x_s(t)\cdot x_s(t)^T$ and $x_s(t)f_s(x_s,0)^T + f_s(x_s,0)x_s(t)$, multiple kinetic Monte-Carlo simulation runs for the same sputtering process should be performed and the profiles of $x_s(t)\cdot x_s(t)^T$ and $x_s(t)f_s(x_s,0)^T + f_s(x_s,0)x_s(t)$ should be averaged to obtain the expected values. The expected value of $x_s(t)\cdot x_s(t)^T$ is $P_s(t)$. The time derivative of $P_s(t)$ can be computed by using values of P_s at t and $t+\Delta t$ as follows:

$$\frac{dP_s(t)}{dt} = \frac{P_s(t+\Delta t)-P_s(t)}{\Delta t} \tag{19}$$

where Δt is a small time interval.

Using the values of $dP_s(t)/dt$, $P_s(t)$ and $\langle x_s(t)f_s(x_s,0)^T + f_s(x_s,0)x_s(t)^T\rangle$ in Eq.17 obtained through kMC simulation runs at a set of discrete time instants ($t = t_1,t_2,\cdots,t_k$), Eq.17 becomes a system of linear algebraic equations for the four model parameters. When the number of equations is larger than the number of parameters to be identified, the least-squares method can be used to determine the model parameters.

To simplify the development, we propose to formulate the system of algebraic equation for least-squares fitting of the model parameters by using only the diagonal elements of the system of Eq.17. The system of ODEs that corresponding to the diagonal elements of Eq.17 is as follows:

$$\begin{aligned}\frac{d\langle\alpha_n^2(t)\rangle}{dt} &= 2(\nu n^2-\kappa n^4)\cdot \langle\alpha_n^2(t)\rangle + 2\lambda\cdot\langle\alpha_n(t)\cdot f_{n\alpha}(t)\rangle+\sigma^2\\ \frac{d\langle\beta_n^2(t)\rangle}{dt} &= 2(\nu n^2-\kappa n^4)\cdot \langle\beta_n^2(t)\rangle + 2\lambda\cdot\langle\beta_n(t)\cdot f_{n\beta}(t)\rangle+\sigma^2\\ & n=1,\ldots,m\end{aligned} \tag{20}$$

where $f_{n\alpha}$ and $f_{n\beta}$ are defined in Eq.18 for $n = 1,2,\cdots,m$. Note thta values of the $\langle\alpha_n^2(t)\rangle$, $\langle\alpha_n^2(t)\rangle$, $\alpha_n(t)\cdot f_{n\alpha}(t)$, and $\beta_n(t)\cdot f_{n\beta}(t)$ at $t = t_1, t_2, \cdots, t_k$ are obtained through kMC simulations of the sputtering process. The system of Eq.20 is, therefore, a linear system with respect to ν, κ, λ and σ^2. It is straightforward to reformulate Eq.20 in the form of the following linear system to identify ν, κ, λ and σ^2 using least-squares method:

$$b = A\theta \tag{21}$$

where $\theta = [\nu\ \kappa\ \lambda\ \sigma^2]^T$ and the expressions for matrix A and b are omitted for brevity. The least-squares fitting of the model parameters can be obtained as follows:

$$\hat{\theta} = (A^TA)^{-1}A^T\cdot b \tag{22}$$

5. SIMULATION RESULTS

In this section, we present an application of the method of system identification to the nonlinear stochastic KSE model of a sputtering process. We consider the sputtering process that occurs on a lattice containing 200 sites. Therefore, $a = 0.0314$. The sputtering yield function, $Y(\phi_i)$ is a nonlinear function of ϕ_i, which takes the form of Eq.1. y_0, y_1 and y_2 are chosen such that $Y(0) = 0.5, Y(\pi/2) = 0$ and $Y(1) = 1$ (Cuerno *et al.*, 1995).

We first compute the profiles of the state covariance and the expected values for $\alpha_n\cdot f_{n\alpha}$ and $\beta_n\cdot f_{n\beta}$ from kMC simulations of the sputtering processes. $\alpha_n\cdot f_{n\alpha}$ and $\beta_n\cdot f_{n\beta}$ are computed by using Eq.18 with $m = 10$ for n = 1, 2, $\cdots$, 10. The expected profiles are the averages of profiles obtained from 10000 independent kMC simulation runs. The covariance profiles of α_1, α_3, α_5, α_7, and α_9 are shown in Fig.2 (top) and the profiles for the expected values of $\alpha_1 f_{1\alpha}$, $\alpha_3 f_{3\alpha}$, $\alpha_5 f_{5\alpha}$,$\alpha_7 f_{7\alpha}$, and $\alpha_9 f_{9\alpha}$ are shown in Fig.2 (bottom). Similar profiles are observed for the covariance of β_n and $\beta_n f_{n\beta}$, and are omitted here for brevity.

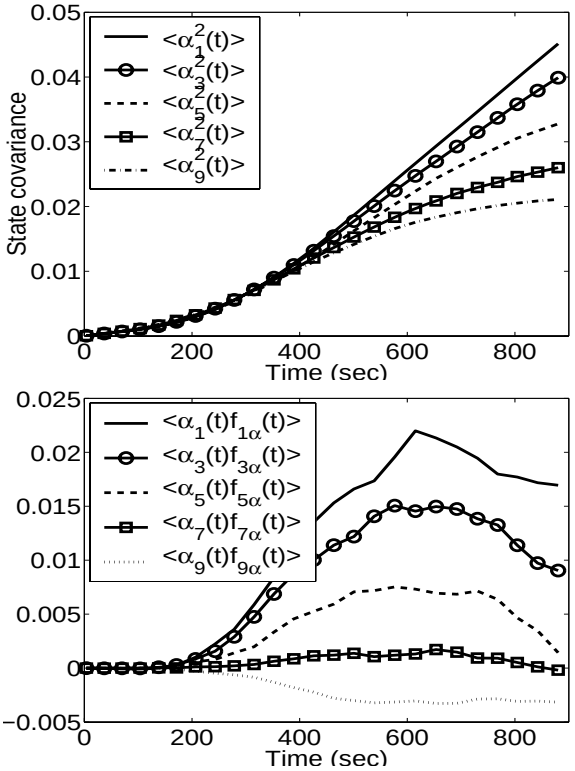

Fig. 2. Profiles of the state covariance $\langle\alpha_n^2(t)\rangle$ (top) and the expected value for $\alpha_n\cdot f_{n\alpha}(t)$ (bottom) for n=1, 3, 5, 7, and 9.

Since we use $m = 10$, the first $2m = 20$ modes are used for the system identification. Specifically, $d\langle\alpha_n^2(t)\rangle/dt$, $d\langle\beta_n^2(t)\rangle/dt$, $\langle\alpha_n^2(t)\rangle$, $\langle\beta_n^2(t)\rangle$, $\langle\alpha_n(t)\cdot$

$f_{n\alpha}(t)\rangle$, and $\langle \beta_n(t) \cdot f_{n\beta}(t)\rangle$ are evaluated at the first 150 discrete time instants available in the data obtained from kMC simulations. Therefore, in the least-squares fitting formulations of Eqs.21 and 22, A is a 3000×4 matrix, b is a 3000×1 vector and $\theta = [\nu\ \kappa\ \lambda\ \sigma^2]^T$. The values of the four parameters obtained from least-squares fitting are $\nu = 2.76 \times 10^{-5}$, $\kappa = 1.54 \times 10^{-7}$, $\lambda = 3.06 \times 10^{-3}$, and $\sigma^2 = 1.78 \times 10^{-5}$.

To validate the model identification method, we compute the expected surface roughness from the stochastic KSE model of Eq.5 using the identified parameters and compare it to that from the kMC simulations. The surface roughness, r, is computed as $r(t) = \sqrt{\frac{1}{2\pi}\int_{-\pi}^{\pi}[h(x,t) - \bar{h}(t)]^2 dx}$, where $\bar{h}(t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} h(x,t)dx$ is the average surface height. The expected surface roughness, $\langle r \rangle = \frac{1}{n}\sum_{i=1}^{n} r_i$, is computed from the stochastic KSE and the kMC simulation by averaging surface roughness profiles obtained from 100 and 10000 independent runs, respectively. The simulation result is shown in Fig.3 (top). It is clear that the identified model parameters result in consistent expected surface roughness profile from the stochastic KSE model of Eq.5 and that from the kMC simulator for the sputtering process. However, there is still observable difference between the two profiles. This might be caused by the error introduced into the identification process by the noise contained in the data generated by the kMC simulator. Filtering techniques may be useful to reduce noise from kMC simulators (Lou and Christofides, 2003) and improve the fidelity of the identified parameters, which is an interesting topic for future research. In this work, we decide to compensate this error by increasing the value of σ^2 by 40%, from 1.78×10^{-5} to 2.49×10^{-5}. The comparison of the two profiles after this compensation is shown in Fig.3 (bottom). It is clear that the two profiles are close, which demonstrates the effectiveness of the proposed system identification method.

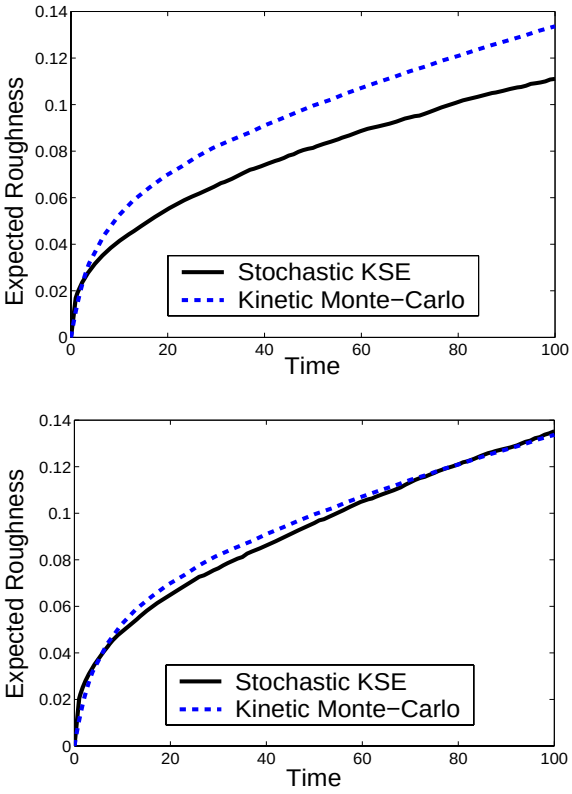

Fig. 3. Comparison of the open-loop profile of the expected surface roughness of the sputtering process from the kMC simulator and that from the solution of the stochastic KSE using the identified parameters (top) and that after compensation of the value of σ^2 (bottom).

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