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Chemical Engineering Science 60 (2005) 1603–1617

Chemical Engineering Science

www.elsevier.com/locate/ces

Dynamics and control of thin film surface microstructure in a complex deposition process

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Received 5 January 2004; received in revised form 8 October 2004

Abstract

In this work, a complex deposition process, which includes two types of macromolecules whose growth behaviors are very different, is investigated. This deposition process is influenced by both short- and long-range interactions. The study of this process is motivated by recent experimental results on the growth of high-κ dielectric thin films using plasma-enhanced chemical vapor deposition. A multi-component kinetic Monte-Carlo (kMC) model is developed for the deposition. Both single- and multi-component cases are simulated and the dependence of the surface microstructure of the thin film, such as island size and surface roughness, on substrate temperature and gas phase composition is studied. The surface morphology is found to be strongly influenced by these two factors and growth regimes governed by short- and long-range interactions are observed. Furthermore, two kMC model-based feedback control schemes which use the substrate temperature to control the final surface roughness of the thin film are proposed. The closed-loop simulation results demonstrate that robust deposition with controlled thin film surface roughness can be achieved under a kMC estimator-based proportional integral (PI) feedback controller in the short-range interaction dominated growth regime, while a kMC model-predictive controller is needed to control the surface roughness in the long-range interaction dominated growth regime.

Keywords: Thin film deposition; Feedback control; Complex dynamics; Kinetic Monte-Carlo simulation; Model-predictive control; Long-range interaction; Short-range interaction

1. Introduction

The industrial demands for advanced materials having desirable properties, have driven the development of thin film technology. Today, thin films are used in a wide range of applications, e.g., microelectronic devices, optics, micro-electro-mechanical systems (MEMS) and biomedical products. Various deposition methods, such as physical vapor deposition (PVD) and chemical vapor deposition (CVD), have been developed and widely used to prepare thin films. However, the dependence of the thin film properties, such as spatial uniformity, composition and microstructure, on the deposition conditions, is a severe constraint on reproducing the performance of the thin film. Therefore, in order to meet the stringent requirements on the quality of thin films, real-time feedback control of thin film deposition becomes increasingly important.

Significant research efforts have been made on the feedback control of thin film deposition processes with emphasis on control of film spatial uniformity in rapid thermal processing (RTP) (Baker and Christofides, 1999; Theodoropoulou et al., 1999; Christofides, 2001) and plasma-enhanced chemical vapor deposition (PECVD) (Armaou and Christofides, 1999). In addition to achieving spatially uniform deposition of thin films, one would like to regulate film properties such as microstructure (Lou and Christofides, 2003a, 2005a,b,c) and composition (Ni et al., 2004) that characterize film quality. While deposition uniformity control can be accomplished on the basis of continuum

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0009-2509/$ - see front matter © 2004 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ces.2004.11.005

type distributed models, precise control of film properties requires models that predict how the film state (microscopic scale) is affected by changes in the controllable process parameters (macroscopic scale). This need has motivated extensive research on the development of fundamental mathematical models describing thin film growth.

Kinetic Monte-Carlo (kMC) simulation provides a framework for modelling the effect of macroscopic process variables on the thin film microstructure and has been widely used to simulate CVD processes (see Battaile and Srolovitz (2002) for a review of kMC simulation of CVD). However, the majority of these works have focused on studying the growth kinetics or interface structure while only a few works (Vlachos, 1997; Reese et al., 2001) have addressed the computational efficiency which strongly affects the use of such kMC models within real-time feedback control systems. Recently, a methodology for feedback control of thin film growth using kMC models was developed by Lou and Christofides (2003a,b). The methodology leads to the design of (a) real-time roughness estimators by using multiple small lattice kMC 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 kMC process model (Lou and Christofides, 2005a). Other approaches have also been developed to: (a) identify linear deterministic models from outputs of kMC simulators and perform controller design by using linear control theory (Siettos et al., 2003; Armaou et al., 2004), (b) construct reduced-order approximations of the master equation (Gallivan and Murray, 2004), and (c) construct stochastic partial differential equation models using kMC simulations (Ni and Christofides, 2005a,b).

However, among these computationally attractive models, most of them consider only single component systems, and long-range interactions have not been modelled explicitly. In reality, most CVD processes are heterogeneous deposition processes where more than one species participate in the film growth. Moreover, direct long-range interactions (Einstein, 1996) and substrate-mediated long-range interactions (Merrick et al., 2003) are very important in many of these processes. For example, in the PECVD ZrO_2 process, there is a large number of different species present in the gas phase during the deposition, and many of them participate in the thin film growth, particularly, zirconium hydroxide and hydrocarbon species (see Cho et al. (2002) for detailed experimental results). Moreover, recent experimental results (Cho et al., 2003) have shown that, when zirconium hydroxides are the dominant species in the gas phase, the deposited ZrO_2 thin film has a very smooth surface with a roughness value less than half ZrO_2 monolayer, which suggests that the zirconium hydroxide species tend to uniformly cover the substrate surface. On the other hand, when hydrocarbons dominate the gas phase, the deposited ZrO_2 thin film has a very rough surface characterized by big islands, which suggests that the aggregation of the hydrocarbon species on the substrate surface, as a result of long-range interactions, is quite significant. It is quite obvious that a single component kMC model considering only short-range interactions is inadequate to describe the thin film growth in this process. Therefore, a computationally efficient kMC model of heterogeneous deposition processes in which long-range interactions are accounted for is needed.

In this work, a complex deposition process, which includes two types of macromolecules whose growth behaviors are very different, is investigated. This deposition process is influenced by both short- and long-range interactions. The study of this process is motivated by recent experimental results on the growth of high-κ dielectric thin films using plasma-enhanced chemical vapor deposition (PECVD). A multi-component kMC model is developed for the deposition. Both single- and multi-component cases are simulated and the dependence of the surface microstructure of the thin film, such as island size and surface roughness, on substrate temperature and gas phase composition are studied. The surface morphology is found to be strongly influenced by these two factors and growth regimes governed by short- and long-range interactions are observed. Furthermore, two kMC model-based feedback control schemes which use the substrate temperature to control the final surface roughness of the thin film are proposed. The closed-loop simulation results demonstrate that robust deposition with controlled thin film surface roughness can be achieved under a kMC estimator-based proportional integral (PI) feedback controller in the short-range interaction dominated growth regime, while a kMC model-predictive controller is needed to control the surface roughness in the long-range interaction dominated growth regime.

2. Surface microstructure model for thin film growth

Deposition processes such as PECVD, often involve large numbers of participating species with heterogeneous growth behaviors. Here, we study a heterogeneous deposition process in which two types of macromolecules of very different growth behavior, type A and type B, are present. Type A macromolecule is significantly affected by long-range attractions and tends to aggregate with other A macromolecules into clusters, i.e., it favors Volmer-Weber (VW) growth mode (Gilmer et al., 1998). Hydrocarbon molecules generated from the decomposition of metal-organic (MO) precursors in a PECVD process are good examples of such type. Type B macromolecule favors surface sites of local minimum height, which usually results in Frank-van der Merwe (FM) type of film growth (Gilmer et al., 1998). Metal oxides or hydroxides originated from the MO precursors may behave similar to macromolecules of type B as discussed in the introduction.