FEEDBACK CONTROL OF GROWTH RATE AND SURFACE ROUGHNESS IN THIN FILM GROWTH

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INTRODUCTION

- **Surface roughness is an important property of thin films.**
    - ◇ **Abruptness of semiconductor interfaces to the electronic properties of devices (e.g., $GaAs$ thin films).**
    - ◇ **Importance of surface roughness of thin films of high-κ materials to the effective capacities of the gate dielectrics (e.g., ZrO_2 thin films).**
- **Feedback control of thin film growth.**
    - ◇ **Increasingly stringent requirements on the thin film quality.**
    - ◇ **Improvement of productivity.**
- **Multiscale distributed models for thin film growth.**
    - ◇ **Coupled PDE models for gas phase dynamics and kinetic Monte-Carlo models for surface microstructure.**
- **Measurements of surface roughness of thin films in atomic resolution.**
    - ◇ **Scanning tunneling microscopy or atomic force microscopy.**

MOCVD $GaAs$ FILMS / EXPERIMENTAL RESULTS

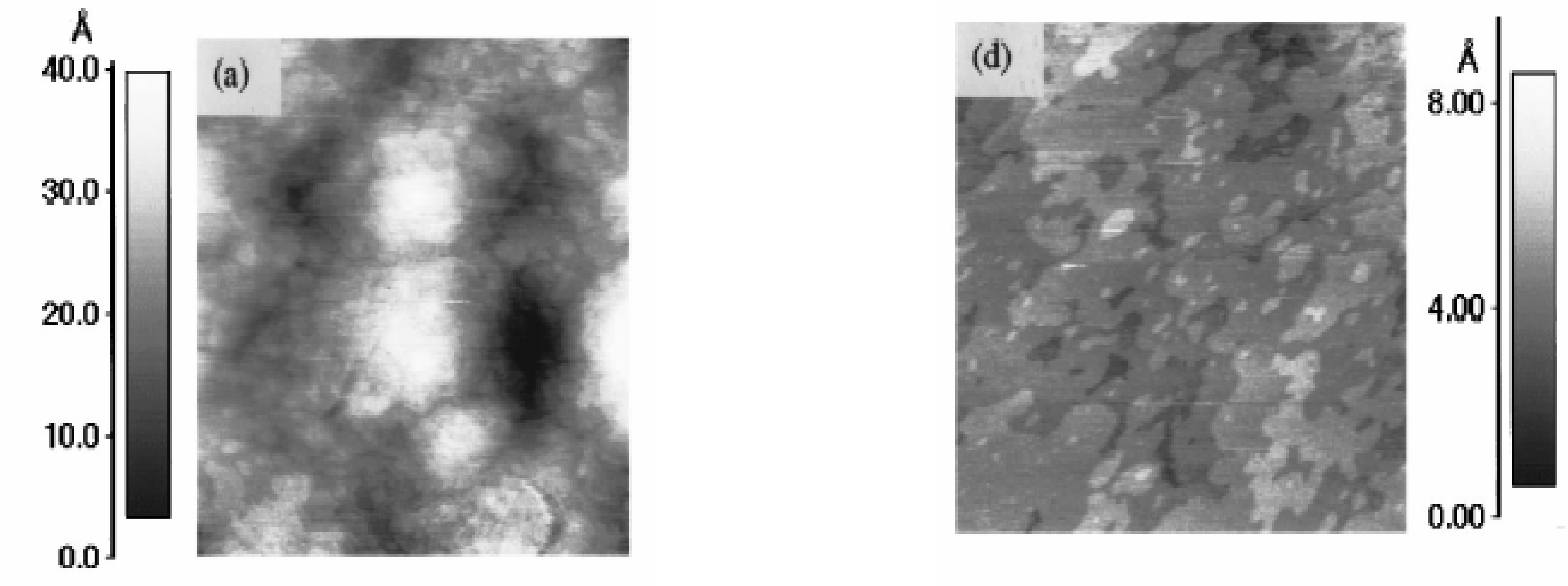
(Law, et. al., *J. Appl. Phys.*, 2000)

- **Surface roughness can be controlled by manipulating the substrate temperature.**

Scanning tunneling micrographs ($2 \times 2\mu m^2$) of $GaAs$ surface after MOCVD growth at difference substrate temperatures.

Left: Surface configuration at T=825K (roughness=2.9$\mathring{A}$).

Right: Surface configuration at T=900K (roughness=1.3$\mathring{A}$).



PREVIOUS WORK ON MODELING AND CONTROL OF THIN FILM MICROSTRUCTURE

- **Rigorous derivation of kinetic Monte-Carlo algorithms (Gillespie,** *J. Comput. Phys.*, **1976) and their applications to** *GaAs* **thin film growth by molecular beam epitaxy (MBE) (Shitara, et. al.,** *Phys. Rev. B*, **1992).**

- **Multiscale integration hybrid algorithms (Vlachos,** *AIChE J.*, **1997).**

- **Control of microscopic models using coarse timesteppers (Siettos et. al.,** *AIChE J.*, **2003).**

- **Feedback control of thin film growth using kinetic Monte-Carlo models (Lou & Christofides,** *Chem. Eng. Sci.*, **2003).**

- **Model reduction for thin film growth directly based on the master equation (Gallivan & Murray,** *Proc. ACC*, **2003).**

PRESENT WORK

(Lou and Christofides, *AIChE J., 2003; Comp. & Chem. Eng., 2004*)

- **Feedback control of surface roughness of $GaAs$ thin films.**
  - ◇ **MOCVD of $GaAs$ thin films in a horizontal-flow reactor.**
  - ◇ **Kinetic Monte-Carlo model for the surface roughness.**
  - ◇ **Real-time roughness estimator based on a kMC simulator using multiple small-lattice models.**
  - ◇ **Estimator/controller structure.**
- **Multivariable feedback control of thin film growth.**
  - ◇ **Thin film growth in a stagnation point geometry.**
  - ◇ **Multiscale distributed model.**
  - ◇ **Feedback control design using state estimator and input/output interaction compensation.**

PROCESS DESCRIPTION

(Law, et. al., *J. Appl. Phys.*, 2000)

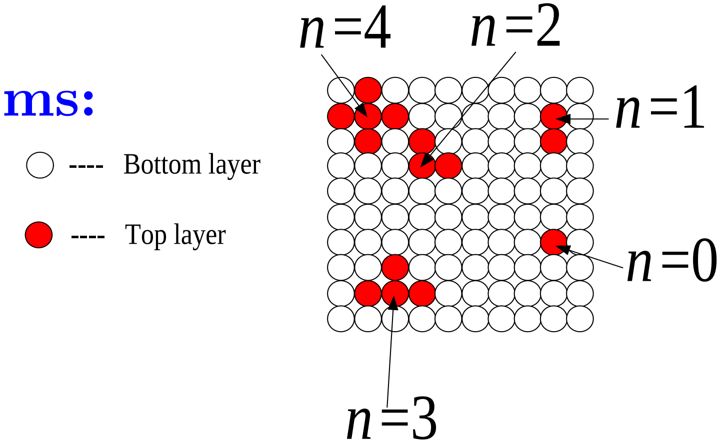
- **A MOCVD of $GaAs$ thin film growth process.**
- **Horizontal-flow reactor.**
- **Triisobutylgallium ($TIBGa$) and tertiarybutylarsine ($TBAs$) as precursors and H_2 as carrier gas.**
- **Growth rate:** $0.5\mu m/hr$**.**
- As**-rich environment (P_{As} / P_{Ga} ~100).**
  - ◇ As **reaction and migration kinetics are not rate-limiting steps.**
- **Very fast decomposition of the MO precursors on the surface and desorption of butyl groups.**
  - ◇ **Substrate temperature:** $825K \sim 900K$**.**
  - ◇ **Surface reactions are not rate-limiting steps.**
- **Adsorption and migration of** Ga **atoms as rate-limiting steps.**

SURFACE MICROSTRUCTURE MODEL

- **Surface micro-processes are assumed to be Poisson processes.**
- **Both the master equation and the Monte-Carlo algorithm can be derived using the same assumption (Gillespie, *J. Comput. Phys.*, 1976).**
- **Kinetic Monte-Carlo model for rate-limiting steps.**
  - ◇ **Effects of non-rate-limiting steps can be incorporated into the model by adjusting model parameters.**
- **Rates of adsorption and migration of *Ga* atoms:**

$$w_a = F \text{ (for a fixed growth rate)}$$

$$w_m(n) = \nu_0 exp(-\frac{E_s + nE}{kT})$$



SURFACE MICROSTRUCTURE MODEL

- **The life time of every MC event:**

$$\boxed{\tau = \frac{-\ln \xi}{W_{tot}}; \quad W_{tot} = N^2 w_a + \sum_{i=0}^{4} M_i \nu_0 \exp(-\frac{E_s + iE_n}{k_B T})}$$

ξ: **a random number in the $(0,1)$ interval.**

M_i: **number of surface atoms that have i side-neighbors on the surface.**

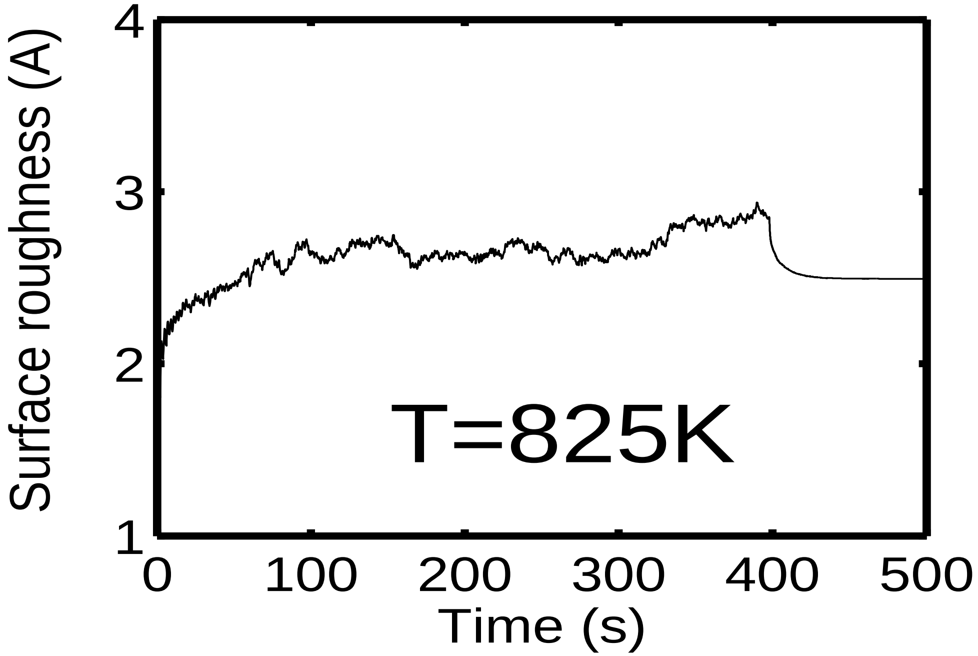
- **Surface roughness and surface micro-processes.**
  - ◇ **Adsorption events make the surface rough.**
  - ◇ **Migration events make the surface smooth.**
  - ◇ **High temperature reduces surface roughness by increasing the rate of migration.**

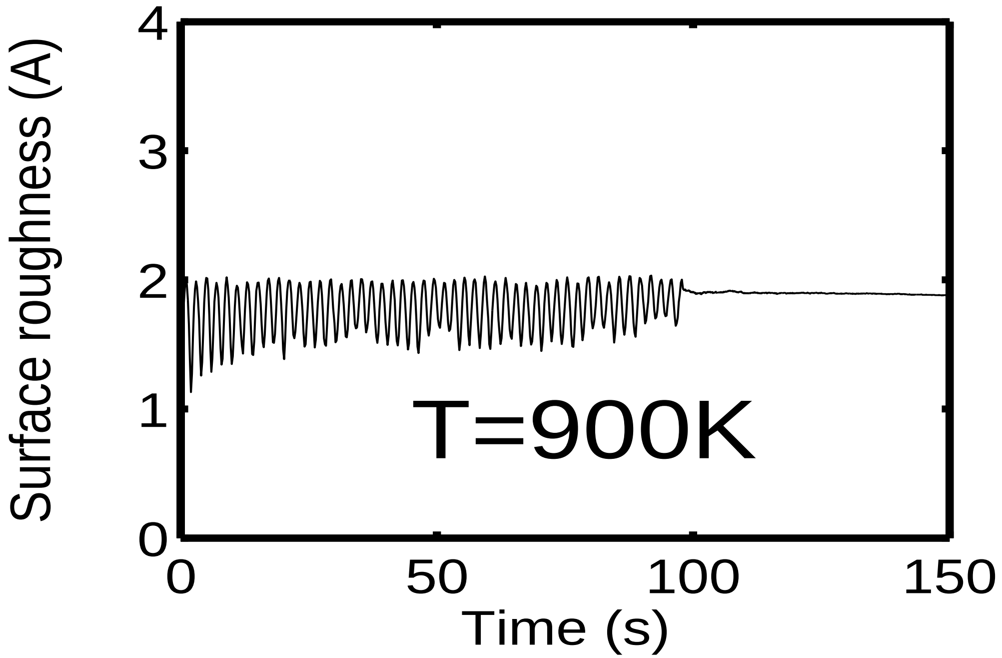
KINETIC MONTE-CARLO SIMULATION RESULTS

- **Fitting model parameters based on experimental results in (Law, et. al.** *J. Appl. Phys.*, **2000).**

$$\boxed{\nu_0 = 5.8 \times 10^{13} s^{-1} \quad E_s = 1.82eV \quad E_n = 0.27eV}$$

- **Cooling down the deposited thin films to the room temperature at** $2K/s$.
- **Surface roughness from Monte-Carlo simulations:** $r_{825K} = 2.5\mathring{A}$, $r_{900K} = 1.6\mathring{A} \sim 2.0\mathring{A}$ **(Experimental results:** $r_{825K} = 2.8\mathring{A}$, $r_{900K} = 1.3\mathring{A}$**).**





REAL-TIME ROUGHNESS ESTIMATOR USING KMC SIMULATOR BASED ON MULTIPLE SMALL-LATTICES

- **Methodology developed in a previous work (Lou & Christofides, *Chem. Eng. Sci.*, 2003).**
- **Kinetic Monte-Carlo simulator based on multiple small-lattice models.**
  - ◇ **Solution time comparable to the real-time evolution of the process.**
  - ◇ **Fluctuation reduction by averaging outputs from multiple small-lattice kMC models.**
- **Adaptive filter for noise reduction.**
- **Measurement error compensator to reduce the error between the roughness estimates and the roughness measurements.**

ADAPTIVE FILTER

- **A second-order adaptive filter.**

$$\begin{aligned} \frac{d\hat{y}_r}{d\tau} &= y_1 \\ \frac{dy_1}{d\tau} &= \frac{K}{\tau_I}(y_r - \hat{y}_r) - \frac{1}{\tau_I}y_1 \end{aligned}$$

- **The adaptive tuning law for the filter gain.**

$$K(\tau) = K_0 \frac{|\int_{\tau-\Delta\tau}^{\tau} y_r(t)dt - \int_{\tau-2\Delta\tau}^{\tau-\Delta\tau} y_r(t)dt|}{\Delta\tau^2} + K_s$$

$$\tau_I(\tau) = \frac{0.5}{K(\tau)}$$

K_s: **Steady state gain for the adaptive filter.**

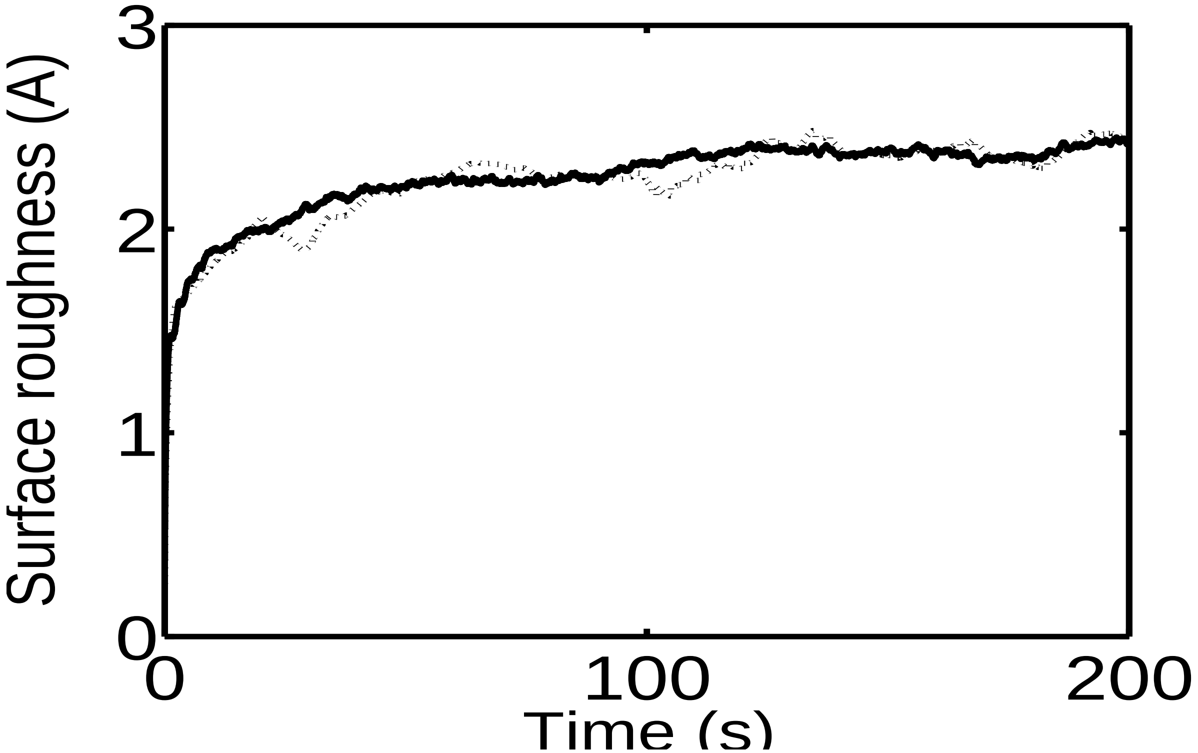
$\Delta\tau$: **Time interval between two updates of** K.

THE MEASUREMENT ERROR COMPENSATOR

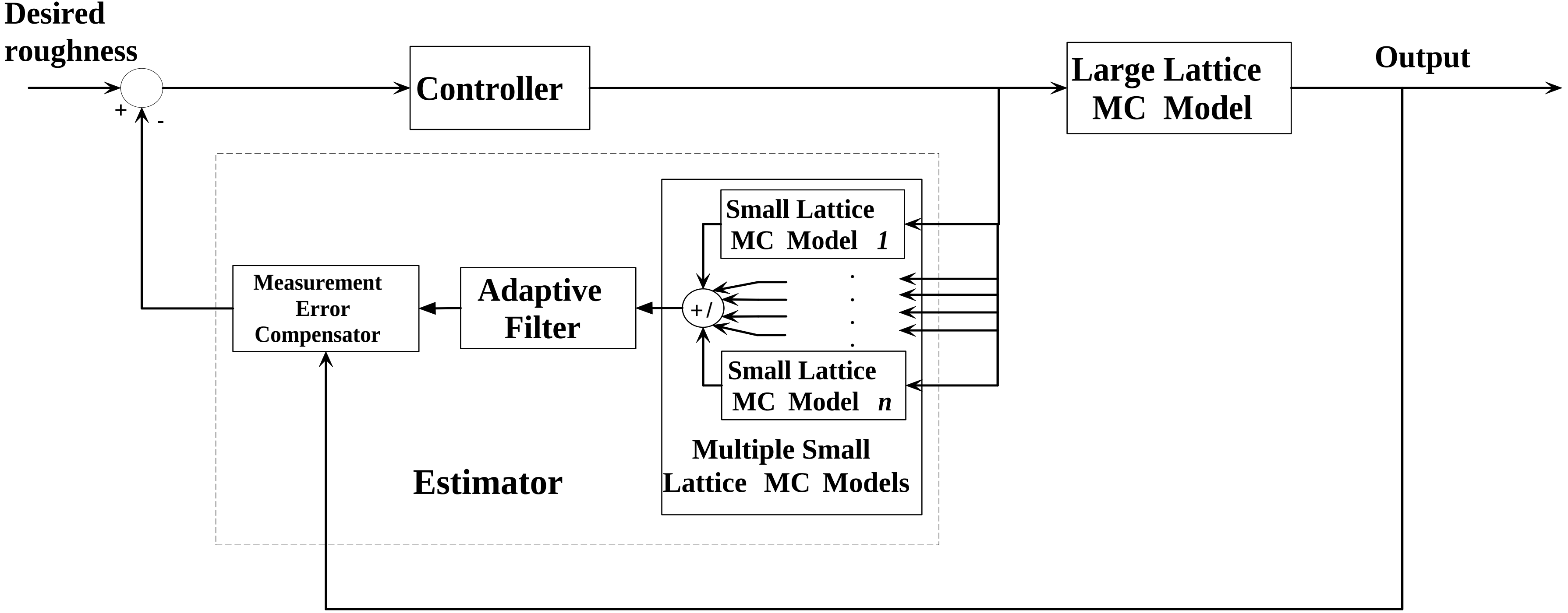
- **A first-order measurement error compensator.**

$$\begin{aligned} \frac{de}{d\tau} &= K_e(y_h(\tau_{m_i}) - \hat{y}(\tau_{m_i})); \quad \tau_{m_i} < \tau \leq \tau_{m_{i+1}}; \qquad i = 1, 2, \cdots \\ \hat{y} &= \hat{y}_r + e \end{aligned}$$

- **Comparison of roughness profiles from the roughness estimator using a KMC simulator based on six 30×30 lattices (dashed line) and that based on a 150×150 lattice (solid line).**



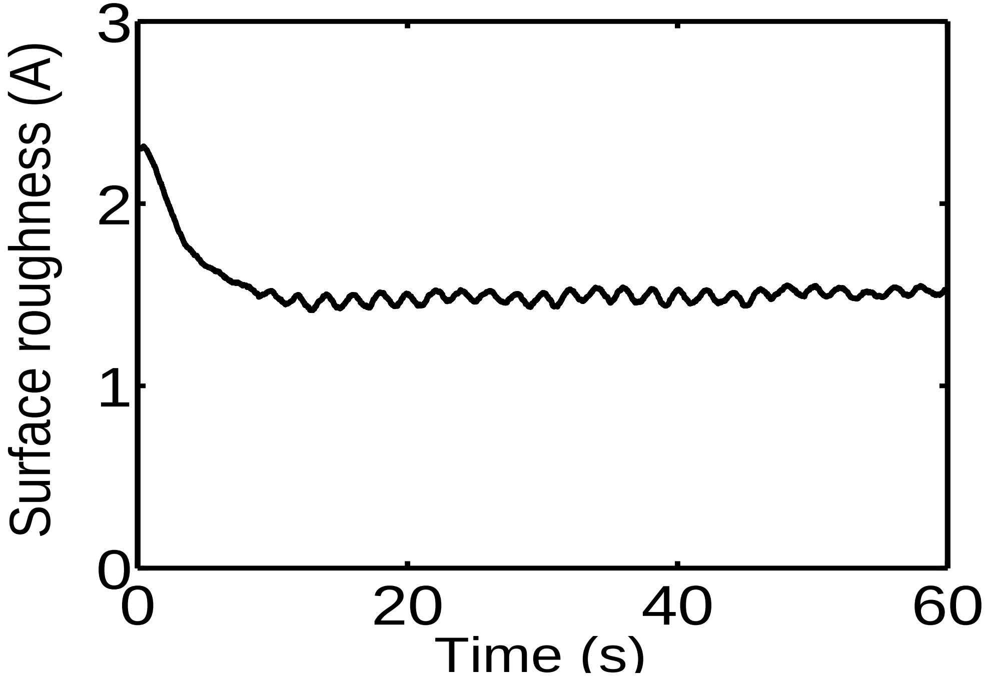
FEEDBACK CONTROL OF SURFACE ROUGHNESS OF $GaAs$ THIN FILMS

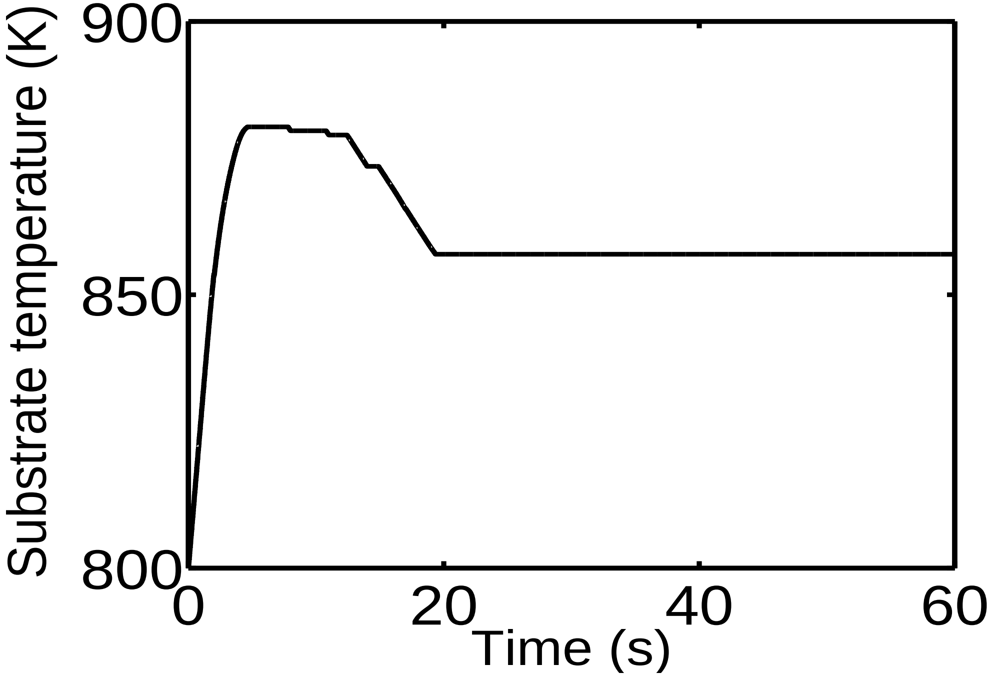


- The estimator/controller structure.
- Available on-line roughness measurement techniques could be used to provide roughness measurement data.
- Control objective: Stabilization of the surface roughness value to a desired level with a certain tolerance ϵ.

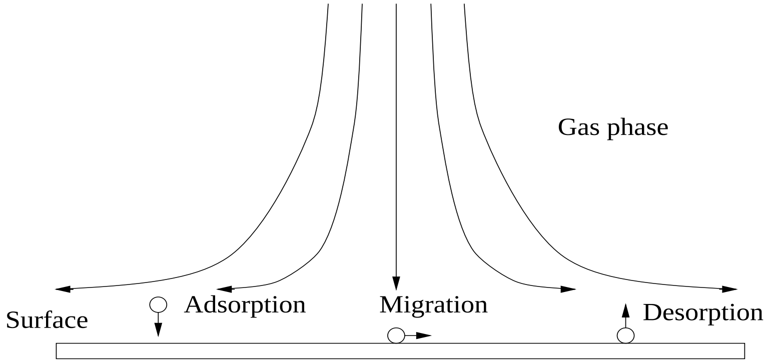
SIMULATION RESULTS

- **Initial growth at $T = 800K$.**
- **Real-time measurement of surface roughness is available every $3.0s$ (Curtis, et. al., *Rev. Sci. Instrum.*, 1997).**
- **The desired roughness is $1.5\AA$ with a tolerance $\epsilon = 0.1\AA$.**
- **Range of the substrate temperature: $750K \leq T \leq 950K$.**





MULTISCALE MODELING OF THIN FILM GROWTH



- **Problems due to the large disparity of time and length scales of phenomena occurring in gas phase and surface:**
  - ◇ **The assumption of continuum is not valid on the surface.**
  - ◇ **Computationally impossible to model the whole system from a molecular point of view.**
- **Solution to bridge the macroscopic and microscopic scales:**
  - ◇ **Model the continuous gas phase by PDEs.**
  - ◇ **Model the configuration of the surface by Monte-Carlo techniques.**
  - ◇ **Incorporate the results of MC simulation to PDEs via boundary conditions.**

GAS PHASE MODEL

- **Conservation of momentum, energy and mass in a stagnation flow geometry (Sharma, et. al.** *Combust. Sci. Technol., 1969***):**

$$\frac{\partial}{\partial\tau}\left(\frac{\partial f}{\partial\eta}\right)=\frac{\partial^3 f}{\partial\eta^3}+f\frac{\partial^2 f}{\partial\eta^2}+\frac{1}{2}\left[\frac{\rho_b}{\rho}-\left(\frac{\partial f}{\partial\eta}\right)^2\right]$$
$$\frac{\partial T}{\partial\tau}=\frac{1}{P_r}\frac{\partial^2 T}{\partial\eta^2}+f\frac{\partial T}{\partial\eta}$$
$$\frac{\partial y_i}{\partial\tau}=\frac{1}{Sc_j}\frac{\partial^2 y_i}{\partial\eta^2}+f\frac{\partial y_i}{\partial\eta}$$

- **Boundary conditions:**

For $(\eta\rightarrow\infty)$:

$$T=T_{bulk},\frac{\partial f}{\partial\eta}=1,$$
$$y_j=y_{jb},j=1,\ldots,N_g$$

For $(\eta\rightarrow 0)$:

$$T=T_{surface},f=0,\ \frac{\partial f}{\partial\eta}=0$$
$$\frac{\partial y_i}{\partial\eta}=\frac{Sc_{growing}(R_a-R_d)}{\sqrt{2a\mu_b\rho_b}}$$

SURFACE MICROSTRUCTURE MODEL

- **Rates of adsorption, desorption and migration:**

$$r_a = \frac{s_0 P}{\sqrt{2\pi mkT} C_{tot}}$$

$$r_d(n) = \nu_0 \exp(-\frac{E_s + nE}{kT})$$

$$r_m(n) = \nu_0 A \exp(-\frac{E_s + nE}{kT})$$

- **The life time of every MC event is determined by a random number and the total rate:**

$$\Delta t = \frac{-\ln \xi}{r_{tot}}$$

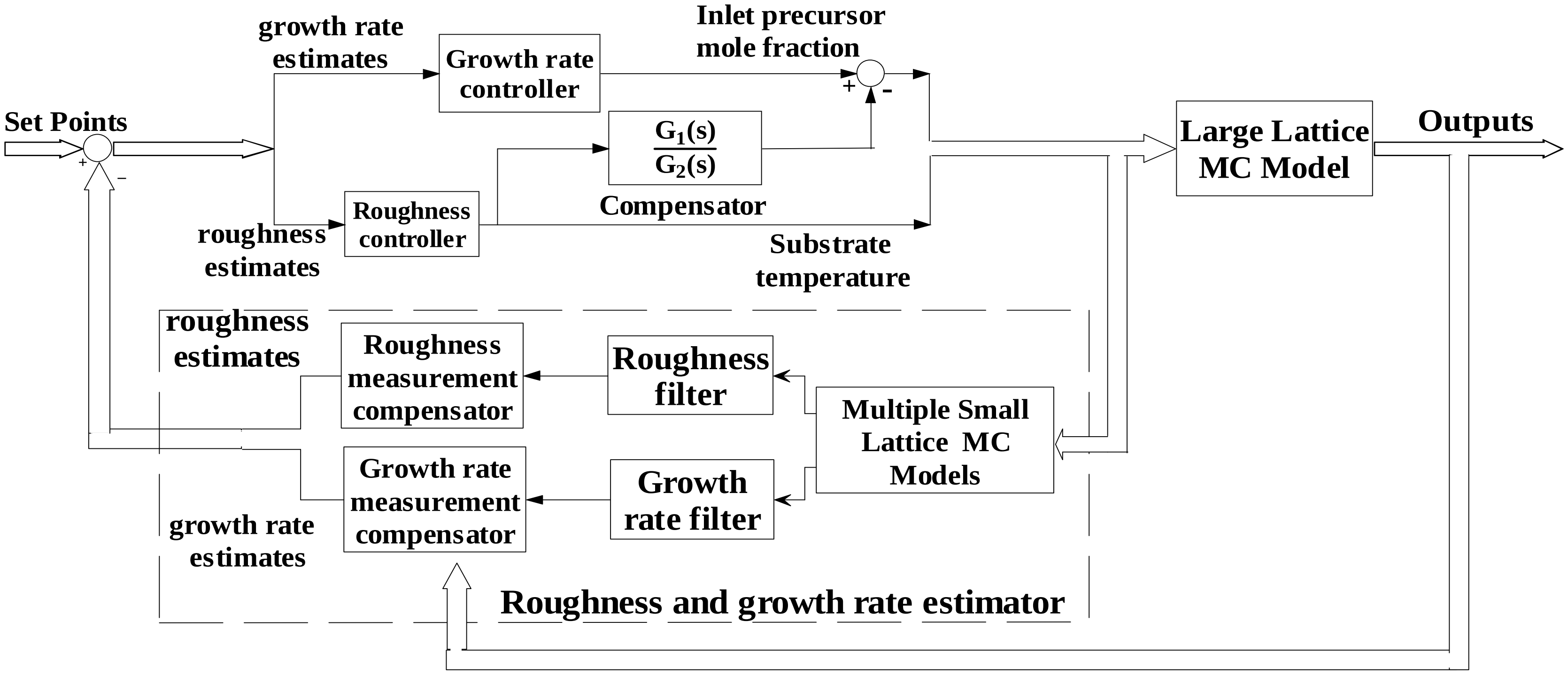
$$r_{tot} = r_a \times N_T + \nu_0 (1 + A) \sum_{m=0}^{4} N_m \exp(-\frac{E_s + mE}{kT})$$

MULTIVARIABLE FEEDBACK CONTROL

(Lou & Christofides, *AIChE J., 2003*)

- **Multiple control objectives to be achieved simultaneously.**
- **Problem formulation: control growth rate and surface roughness simultaneously by manipulating inlet precursor concentration and substrate temperature.**
- **Growth rate and roughness estimator involving a kinetic MC simulator based on multiple small-lattice models, adaptive filters and measurement error compensators.**
- **Identification of input/output interactions.**
- **Multivariable control system with input/output interaction compensation.**

MULTIVARIABLE FEEDBACK CONTROL SYSTEM WITH INTERACTION COMPENSATION

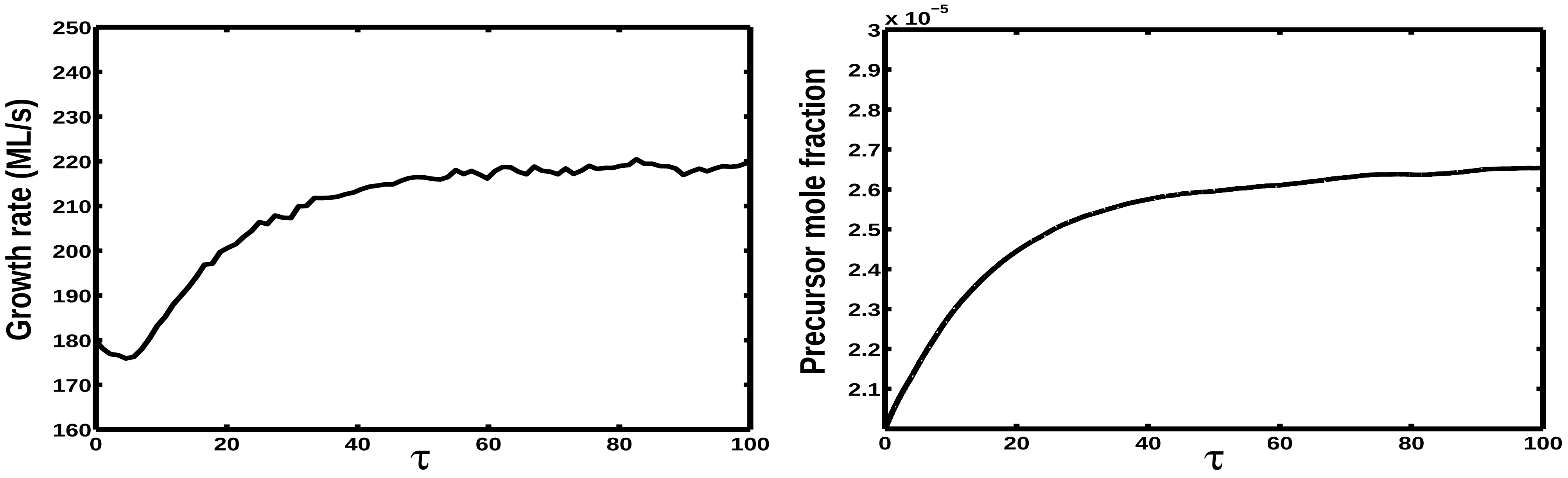


- Compensation for the influence of temperature to growth rate only.
- Compensation is computed from the transfer function between substrate temperature and the growth rate (G_1) and that between inlet precursor mole fraction and the growth rate (G_2).
- Identification of G_1 and G_2 from step tests.

SIMULATION RESULTS

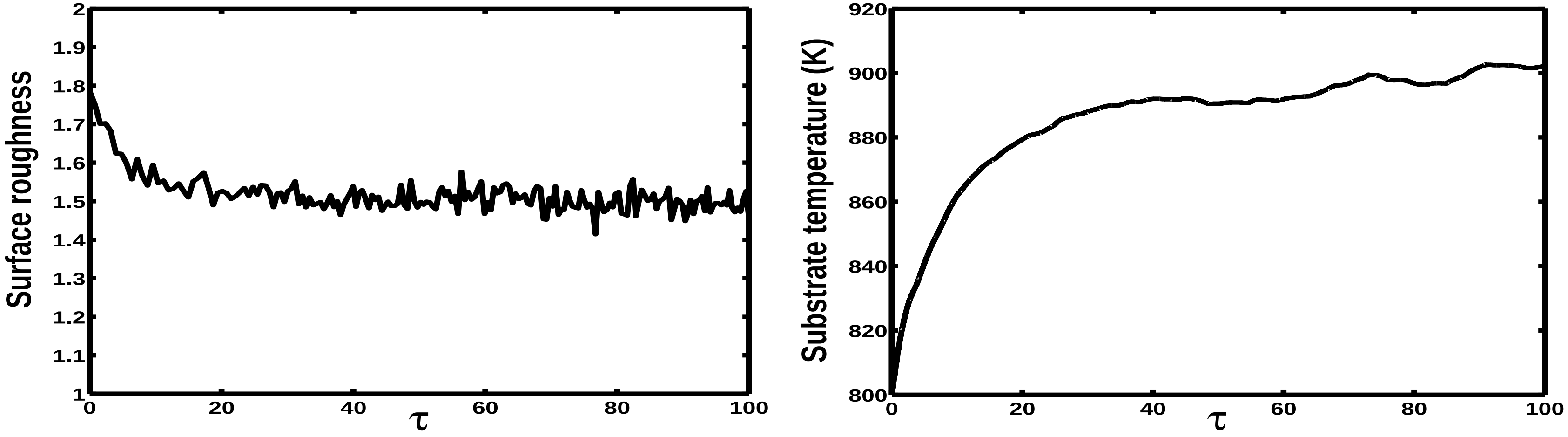
- **Initial growth conditions:** $T = 800K$**, and** $y = 2.0 \times 10^{-5}$**.**
- **Initial roughness:** 1.8 **and initial growth rate:** $180ML/s$**.**
- **The desired roughness:** 1.5 **and desired growth rate:** $220ML/s$**.**

The growth rate (left plot) and inlet precursor mole fraction (right plot) under multivariable feedback control.

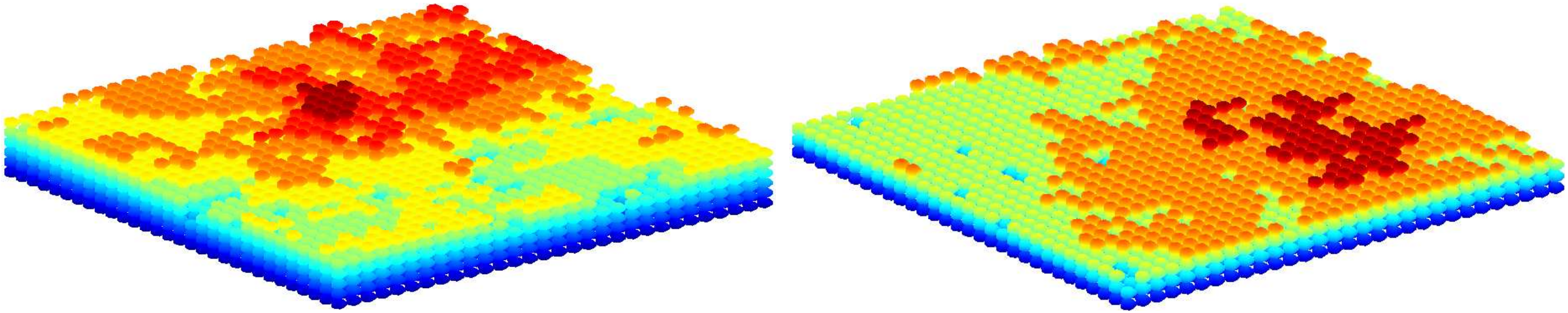


SIMULATION RESULTS

- **The surface roughness (left plot) and substrate temperature (right plot) under multivariable feedback control.**



- **Surface micro-configuration at the beginning of the closed-loop simulation run (left plot) and that at the end of the simulation run (right plot).**



SUMMARY

- **Feedback control of thin film growth.**
- **MOCVD $GaAs$ thin films in a horizontal-flow reactor.**
- **Kinetic Monte-Carlo models for surface roughness.**
  - ◇ **Fitting model parameters using experimental data.**
- **Estimator/controller.**
  - ◇ **Real-time estimator based on kMC models.**
- **Multiscale distributed model for thin film growth in a stagnation point geometry.**
- **Multivariable feedback control of thin film growth with state estimator and input/output interaction compensation.**

ACKNOWLEDGMENT

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