



Lecture: Modeling and Control of Deposition Processes

Jürgen Geiser

March 12, 2008

Humboldt Univer-sität zu Berlin
Institut für Mathematik

Unter den Linden 6, D-10099 Berlin, Deutschland

Outline of the talk

Modeling and Control of Deposition Processes

- 0) Introduction and Models
- 1) Recent Publications and Works to the Modeling and Control of Deposition Processes
- 2) Mathematical Background
- 3) Simulatable Models
- 4) Control Methods
- 5) Future Works

Introduction

Modelling and Optimization of deposition projects can be done in different model regimes :

- 1 Reaction-diffusion equations, see [Gobbert1996] (macro-model);
- 2 Boltzmann-Lattice equations, see [Senega/Brinkmann2006] (micro-model).
- 3 Clausius-Clapyperon equations, see [Ohring2002] (Thin-Film evaporation process, CVD-method, Micro-modell)
- 4 Level-set method for the surface (Sputter Deposition, PVD-method, Micro-modell)

Models of the Deposition Process

- Macro-Scale Models : Simulation of the Gas-Transport through the chamber
- Micro-Scale Models :
 - CVD-Method : Simulation of the Vaporisation (solid-vapor) process
 - PVD-Method (Sputtering): Simulation of the ion-interaction (plasma simulation)
 - PVD-Method (Sputter Deposition) : Simulation of the Topology of the surface (e.g. Level set method)

Macro-Scale Model : (Small Knudsen Numbers, Far Field Model)

For this model we can assume a continuum flow, and the fluid equations can be treated with a Navier-Stokes or especially with a reaction-diffusion equation.

$$\frac{\partial}{\partial t} \mathbf{c} + \nabla \cdot \mathbf{F} - R_g = 0, \text{ in } \Omega \times [0, T] \quad (1)$$

$$\mathbf{F} = \mathbf{v}\mathbf{c} - D\nabla\mathbf{c},$$

$$c(x, t) = c_0(x), \text{ on } \Omega, \quad (2)$$

$$c(x, t) = c_1(x, t), \text{ on } \partial\Omega \times [0, T], \quad (3)$$

where c is the molar concentration and F the flux of the species. v is the velocity, D is the diffusivity matrix and R_g is the reaction term.

Micro-Scale Model : Simulation of the Vaporisation (CVD-method)

The vaporisation can be modeled with a heat conduction equation :

$$\rho(T)C(T)\partial_t T - \nabla k(T)\nabla T = Q(x, t), \text{ in } \Omega \times [0, T] \quad (4)$$

$$T(x, t) = T_0(x), \text{ on } \Omega, \quad (5)$$

$$T(x, t) = T_1(x, t), \text{ on } \partial\Omega \times [0, T], \quad (6)$$

where T is the temperatur distribution, ρ the mass density, k the thermal conductivity, C the specitif heat. The source term Q represents the laser energy.

The flow of material can be modeled by the Hertz-Knudsen equation and we can derive the ablation rate :

$$v(T) = (1 - \beta) \sqrt{m / (2\pi k_b T)} p / p_0 \exp(l_v / k_b (\frac{1}{T_B} - \frac{1}{T})), \quad (7)$$

where T_B is the boiling temperature, k_b the Boltzmann constant, β the back flux coefficient and l_v the latent heat of the vaporisation of the material.

Micro-Scale Model : Ion Interaction (Large Knudsen Numbers, Near Field Model)

The model assumes that the heavy particles can be described with a dynamical fluid model, where the elastic collisions define the dynamics and few inelastic collisions are, among other reasons, responsible for the chemical reactions.

Model for Large Knudsen Numbers (Near Field Model)

The Boltzmann equation for heavy particles (ions and neutral elements) is now given as

$$\frac{\partial}{\partial t} n_s + \frac{\partial}{\partial \mathbf{r}} \cdot (n_s \mathbf{u} + n_s \mathbf{c}_s) = Q_n^{(s)}, \quad (8)$$

$$\frac{\partial}{\partial t} \rho \mathbf{u} + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho \mathbf{u} \mathbf{u} + n T \underline{\underline{I}} - \underline{\underline{\tau}}^*) = \sum_{s=1}^N q_s n_s \langle \mathbf{E} \rangle, \quad (9)$$

$$\frac{\partial}{\partial t} \mathcal{E}_{\text{tot}}^* + \frac{\partial}{\partial \mathbf{r}} \cdot (\mathcal{E}_{\text{tot}}^* \mathbf{u} + \mathbf{q}^* + n T \mathbf{u} - \underline{\underline{\tau}}^* \cdot \mathbf{u}) = \sum_{s=1}^N q_s n_s (\mathbf{u} + \mathbf{c}_s) \cdot \langle \mathbf{E} \rangle - Q_{\mathcal{E}, \text{inel}}^{(e)}, \quad (10)$$

Model for Large Knudsen Numbers (Near Field Model)

where ρ denotes the mass density, \mathbf{u} is the velocity, and T the temperature of the ions. $\mathcal{E}_{\text{tot}}^*$ is the total energy of the heavy particles.

Model for Large Knudsen Numbers (Near Field Model)

Further the production terms are $Q_n^{(s)} = \sum_r a_{\text{sign}} k_{\alpha,r} n_\alpha n_r$ with the rate coefficients $k_{\alpha,r}$.

We have drift diffusion for heavy particles in the following fluxes. The dissipative fluxes of the impulse and energy balance are linear combinations of gene-realized forces,

$$\mathbf{q}^* = \lambda_E \langle \mathbf{E} \rangle - \lambda \frac{\partial}{\partial \mathbf{r}} T - \sum_{s=1}^N \sum_{\alpha=1}^N \lambda_n^{(\alpha,s)} \frac{1}{n_s} \frac{\partial}{\partial \mathbf{r}} n_\alpha,$$

$$\underline{\underline{\tau}}^* = -\eta \left(\frac{\partial}{\partial \mathbf{r}} \mathbf{u} + \left(\frac{\partial}{\partial \mathbf{r}} \mathbf{u} \right)^\top - \frac{2}{3} \left(\frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{u} \right) \underline{\underline{I}} \right),$$

$$\mathcal{E}_{\text{tot}}^* = \sum_{s=1}^N 1/2 \rho_s c_s^2 + 1/2 \rho u^2 + 3/2 n T.$$

Model for Large Knudsen Numbers (Near Field Model)

Diffusion of the species are underlying to the given plasma and described by the following equations

$$\frac{\partial}{\partial t} n_s + \frac{\partial}{\partial \mathbf{r}} \cdot (n_s \mathbf{u} + n_s \mathbf{c}_s) = Q_n^{(s)},$$

$$\mathbf{c}_s = \mu_s \langle \mathbf{E} \rangle - d_T^{(s)} \frac{\partial}{\partial \mathbf{r}} T - \sum_{\alpha=1}^N D_n^{(\alpha,s)} \frac{1}{n_s} \frac{\partial}{\partial \mathbf{r}} n_\alpha.$$

The density of the species are dynamical values and the species transport and mass transport are underlying to the following constraint conditions:

$$\sum_s m_s n_s = \rho,$$

$$\sum_s n_s m_s \mathbf{c}_s = 0.$$

Model for Large Knudsen Numbers (Near Field Model)

Field Model

The plasma transport equations are maxwell equations and are coupled with a field. They are given as

$$\frac{1}{\mu_0} \nabla \times \mathbf{B}_{\text{dyn}} = -en_e \mathbf{u}_e + \tilde{\mathbf{j}}_{\text{ext}}, \quad (11)$$

$$\nabla \cdot \mathbf{B}_{\text{dyn}} = 0, \quad (12)$$

$$\nabla \times \mathbf{E} = -\frac{\partial}{\partial t} \mathbf{B}_{\text{dyn}}, \quad (13)$$

where \mathbf{B} is the magnetic field and \mathbf{E} is the electric field.

Micro-Scale Model : Sputter Deposition

1.) Level Set Method

Tracking a moving boundary

Simulated with a Hamilton-Jacobian Method :

$$\partial_t \phi = v |\nabla \phi|, \quad (14)$$

where ϕ is the surface.

2.) MD (Molecular Dynamics)

Here atoms and molecules are interacting for a period of time, under known laws of physics, giving a view of the motion of the atoms. One can use numerical methods to solve the equations. We can simulate the Newton's equation for an example a system of N particles with coordinates x and velocities v :

$$F(X) = -\nabla U(X) = M\dot{V}(t), \quad (15)$$

$$V(t) = \dot{X}(t), \quad (16)$$

where U is the potential energy function.

Often the Verlet algorithm is used for such a simulation.

Literature to the models

Literature:

M.K. Gobbert and C.A. Ringhofer.

An asymptotic analysis for a model of chemical vapor deposition on a microstructured surface.

SIAM Journal on Applied Mathematics, 58, 737–752, 1998.

S. Krumdieck.

Kinetic model of low pressure film deposition from single precursor vapor in a well-mixed, cold-wall reactor

Acta Materialia, 49, 4, 583-588, 2001.

M. Ohring.

Materials Science of Thin Films.

Academic Press, San Diego, New York, Boston, London,
Second edition, 2002.

National Projects

BMBF-Project: (Funding period: Mai 1995 - April 1998.)
Parallel algorithms for the simulation and optimization of
chemical vapour deposition processes

Aim : Development of precise mathematical models to
represent coupled 3D flow, heat and mass calculations of
compressible gases, complex homogeneous and
heterogeneous chemical reactions, rotation of the susceptor,
deposition on reactor walls and heat transport in the gas as well
as efficient numerical methods for three-dimensional process
simulation of the above parameters.

Prof. Dr. Arndt Bode , Prof. Dr. Hans Michael Gerndt,
TU-Munich, Department of Computer Sciences.

International Projects

International Projects :

Prof. Michel Ortiz, California Institute of Technology, USA,
Project: ArMax : A lightweight, Hierarchical , MAX Phase Armor
(NRL)

Study of armor, based on Max-phase materials :
Computational simulations of the ArMAX armor system
(constitutive laws, stress as a function strain, strain rate and
temperature)

Simulation of the MAX-Phase material : microstructural
examination to characterize the mechanism of deformation
(Simulation of the application of a MAX-phase material)

Mathematical Background

The models are discussed in different partial differential equations, e.g. heat transfer, mass transfer, diffusion-processes, etc.

Based on the underlying domains, boundary conditions, etc. often analytical solutions are not possible to derive.

We have to use numerical methods, e.g. finite element, finite volume methods to discretise the model-equations and to apply special solver for the equation system, e.g. multi-grid methods, direct solvers, etc.

Mathematical Background

To analyse the discretisation methods, one have to study the weak-solutions of the equations and to derive the error-estimates.

Theoretical tools are Sobolev-spaces, Semi-group theory, Galerkin-approach etc.

Optimal Control with PID-Control

In this section we discuss a forward control, or P-Control (proportional control), see [Munoz et al 2003]. A first idea to control linearly the error of the solved PDE.

Optimal Control with PID-Control

Optimal Control based on Error Estimate

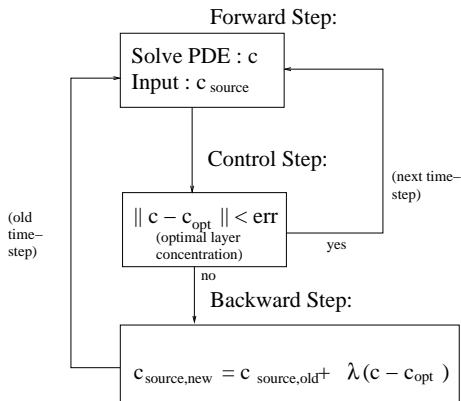


Figure: P-controller for the solution u .

Optimal Control with PID-Control

Our control problem is given with the control of the error to the optimal concentration of the layer and correct the source-flux.

$$\partial_t \mathbf{c} + \mathbf{v} \nabla \mathbf{c} - \nabla D \nabla \mathbf{c} = \mathbf{c}_{source}, \text{ in } \Omega \times [0, T] \quad (17)$$

$$\mathbf{c}(x, t) = \mathbf{c}_0(x), \text{ on } \Omega, \quad (18)$$

$$\mathbf{c}(x, t) = \mathbf{c}_1(x, t), \text{ on } \partial\Omega \times [0, T], \quad (19)$$

where $\mathbf{c}_{source}(x, t)$ is a discontinuous or continuous source flow of the concentration \mathbf{c} .

Optimal Control with PID-Control

We assume an optimal concentration at the layer :
 $c_{opt}(x, t)$ where the layer is given as $x \in \Omega_{layer}$
and our constraints are given as :

$$C_{source,min} \leq C_{source} \leq C_{source,max}$$

Remark

Taken into account the hysteresis of the deposition process, we apply a linear increase of the optimal control with respect to time, see Figure 2.

Optimal Control with PID-Control

Linear optimal constraint

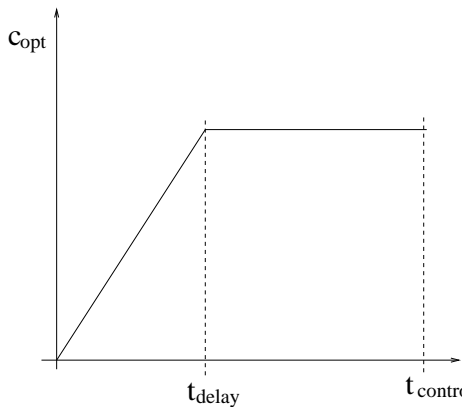


Figure: Linear constraint c_{opt} for the deposition process

Transport-Reaction Models

In the first experiment, we take the moving distance steps equal 5, and in the second experiment we take the moving distance step equal to 10.

In Figure 3 we present the first experiment of the single source.

Transport-Reaction Models

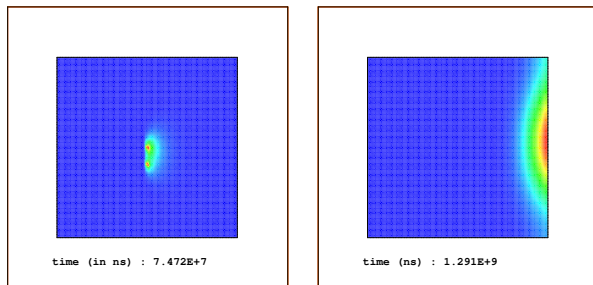


Figure: Source is moving in y direction with step 5 .

Transport-Reaction Models

In Figure 4 we present the deposition rates of the first experiment of the single source.

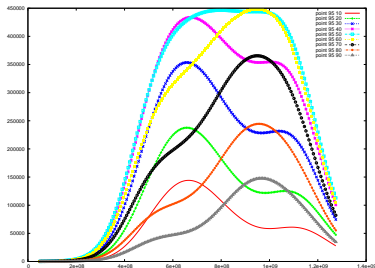


Figure: Source is moving in y direction with step 5 .

FutureWorks

Outview

- 1) Simulation of a CVD process with respect to the kinetics of the reactive gas.
- 2) Optimal Control of the Deposition layer.
- 3) Decomposition the deposition process, e.g. kinetic and flux processes