Influence of Gas Composition on Wafer Temperature in a W CVD Reactor: Experimental Measurements, Model Development, and Parameter Identification

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Overview

- **Research motivation:** significant mismatch between single available temperature measurement and true wafer temperature;

- **Experimental observations** of strong influence of gas composition on wafer temperature;

- **Gas phase simulations** and assessing the applicability of global eigenfunction expansion methods and other OO-MWR;

- **Process recipe development** using a validated dynamic process model; parameter ID issues.
Tungsten CVD

Reactor chamber details

ULVAC cluster tool
ULVAC W CVD Operating and Control Structure

- Look-up table: static and not always activated
Data Acquisition and Experiment Setup

- Signals captured synchronously
- Hardware and software integration

**Challenges:**
- Signals are of different types and different ranges
- Noise reduction of TC signal

**Offset wafer to assess gas/susceptor thermal conduction effects**
Experimental Results at 0.5 Torr

- **Constant lamp power**
  - Temp change due to gas composition change
    - System TC is outside reactor chamber
    - Look-up table is inactive in I/O mode
- **Temp increased as N$_2$ increased** $\kappa_{H_2} \approx 6 \kappa_{N_2}$ at 0.5 Torr
- **TC5 had the largest temp change** Both sides of wafer contact gas mixture
Gas Flow and Heat Transfer Model

Assumptions

- Fully-developed, laminar gas flow
- Transport and gas thermodynamic properties in bulk gas phase are constant
- No buoyancy or wafer rotation induced flow ($Gr = 1.99; Ra = 1.35$)
- Heat generated by viscous dissipation and gas and surface reactions are negligible

$(Chang \ & Adomaitis, \ 1999 \ Int. \ J. \ Heat \ & \ Fluid \ Flow)$

\[
0 = \frac{\partial v_x}{\partial x} \quad \text{Gas velocity, temperature}
\]

\[
\beta_v = \frac{\partial^2 v_x}{\partial y^2} + \alpha_v \frac{\partial^2 v_x}{\partial z^2}
\]

\[
\nu_x \frac{\partial T_g}{\partial x} = \left[ \delta_{gt} \frac{\partial^2}{\partial x^2} + \beta_{gt} \frac{\partial^2}{\partial y^2} + \gamma_{gt} \frac{\partial^2}{\partial z^2} \right] T_g = LT_g
\]

\[
T_g = 0 \quad \text{at } x = 0
\]

\[
\frac{\partial T_g}{\partial x} = 0 \quad \text{at } x = 1
\]

\[
T_g = 0 \quad \text{at } y = 0, 1
\]

\[
T_g = \begin{cases} 
C_t(T_{sh}^*) & \text{at } z = 1, \ (x, y) \in \Omega_{sh} , \\
0 & \text{at } z = 1, \ (x, y) \notin \Omega_{sh}
\end{cases}
\]

\[
T_g = \begin{cases} 
C_b(T_w^*) & \text{at } z = 0, \ (x, y) \in \Omega_w , \\
0 & \text{at } z = 0, \ (x, y) \notin \Omega_w
\end{cases}
\]
W CVD Simulation  Chang, Adomaitis, Kidder, and Rubloff, 2000 Annual AIChE Meeting

Wafer/Susceptor Thermal Dynamics Model

\[
\Delta_w \rho_w \frac{d}{dt} C_{pw} T_w = \alpha_w(T_w) Q_{lp}(u) u(t) + F_{e, top} F_{A, top} \sigma \left( T_{sh}^4 - T_w^4 \right) \\
+ h_{wf}(T_w)(T_f - T_w) + F_{e, bot} F_{A, bot} \sigma \left( T_f^4 - T_w^4 \right) + k_g(x_{H2}) \left. \frac{\partial T_g}{\partial z} \right|_{z=0}
\]

\[
\Delta_s \rho_s \frac{d}{dt} C_{ps} T_{sh} = \alpha_{sh}(T_{sh}) Q_{lp}(u) u(t) + F_{e, sh-w} F_{A, sh-w} \sigma \left( T_w^4 - T_{sh}^4 \right) \\
+ F_{e, sh-f} F_{A, sh-f} \sigma \left( T_f^4 - T_{sh}^4 \right) + h_{sh}(T_c - T_{sh})
\]

\[
h_{wf}(T_w) = h_{wf,0} + \alpha_0(T_w - T_w, N_2) \quad (TC1-3)
\]

\[
h_{wf}(T_w) = \frac{k_g}{(\Delta z_{wf} + 2 \beta_{wf})} \lambda \quad (TC5)
\]

\[
Q_{lp}(u) = Q_{lp,0} + \gamma_0(u - u_0)
\]

Estimated parameters: \( Q_{lp,0}, \beta_{wf}, h_{wf,0}, \alpha_0 \) (steady state/Gauss-Newton)

\( \gamma_0, \Delta_w, \Delta_s \) (colloc int/G-N, physical arguments)

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Gas Phase Model Solution

Global (eigenfunction) expansion

\[ T_g = T_\Omega + T_{\partial \Omega, t} + T_{\partial \Omega, b} \]
\[ = \sum_{l,m,n=1}^{L,M,N} b_{lmn} \phi_l(x) \psi_m(y) \zeta_n(z) + \sum_{l,m=1}^{L,M} a_{lm} \phi_l(x) \psi_m(y) z + \sum_{l,m=1}^{L,M} d_{lm} \phi_l(x) \psi_m(y) (1 - z) \]

\[ L \phi \psi \zeta = \lambda \phi \psi \zeta \]

\[ \mathcal{R} = \mathcal{L} T_\Omega + \mathcal{L} (T_{\partial \Omega, t} + T_{\partial \Omega, b}) - v_x \frac{\partial T_g}{\partial x} \]
\[ b_{i,j,k} = - \left( \mathcal{L} (T_{\partial \Omega, b}) - v_x \frac{\partial T_g}{\partial x}, \phi_i \psi_j \zeta_k \right) / \lambda_{i,j,k} \]
\[ \langle f, g \rangle = \int_0^1 \int_0^1 \int_0^1 f g \, dx \, dy \, dz \]

- Projection operations carried out by quadrature
- Object-oriented version of MWRtools (www.ench.umd.edu/software/MWRtools)
  - Trial function objects for 3D temperature field
  - SD objects to represent modeling equations/solution; collocation time integrator
  - PARAM objects to facilitate Gauss-Newton procedure

\[ v_x \] by Galerkin’s method

Iterative solution procedure

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W CVD Simulation  
Chang, Adomaitis, Kidder, and Rubloff, 2000 Annual AIChE Meeting

Model Solution / Parameter Identification Procedure

Simulation Approach

\[
[rhs, J, drdp] = ulvac\_fun(t,s,p)
\]

- unpack state \( s \) and parameter \( p \) objects
- evaluate diff-eq “rhs”, Jacobian, and derivatives w.r.t parameters to be identified; define in terms of SD objects

Main script

- Set initial state \( s \) and parameter \( p \) objects
- \( s = \text{newtraph}(s,p) \)
- \( S = \text{odaepc}(s,p) \)
- \( p = \text{gnstep}(s,p) \)

MWRtools: www.ench/umd.edu/software/MWRtools

Parameter Estimation Sequence

1) Using TC5 data estimate \( Q_{lp,0} \) and \( \beta_{wf} \); steady-state model and data
2) Identify \( h_{wf,0} \) and \( \alpha_0 \) with TC1-3 measurements; steady-state model/data
3) Identify \( \gamma_0, \Delta_w, \Delta_s \) with TC1-3 measurements; transient model/data
Representative Gauss-Newton Iterations

Identify $h_{wf,0}$ and $\alpha_0$ with TC1-3 measurements:

Results: $h_{wf,0}=3.0 \text{ W/m}^2/\text{K}$  $\alpha_0=-0.03 \text{ W/m}^2/\text{K}$  $Q_{lp,0}=30.3 \text{ kW/m}^2$  $\beta_{wf}=17.8$

Physically reasonable values: Chang et. al. (2001), JVST B, to appear

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Mean model prediction error is less than 3 K for each data set.

Significant model nonlinearities.
Experimental Results at 0.5 Torr (cont.):

- Temp differences were less than 5 K at corresponding s.s. points repeat gas composition change in reverse order
- TC5 responded to the initial ramping faster than other TCs
- Insignificant temp changes for N₂ 100 → 60 sccm and H₂ 40 → 100 sccm

*Gas convective heat transfer modeling term relatively unimportant in the low pressure condition of the ULVAC system*


**Heat Flux Across Wafer Top/Gas Boundary**

- The difference of energy flux $\Delta q < 7 \text{ W/(m}^2\text{K)}$ is small compared to heat transfer rate $q$ itself; convective heat transfer is negligible compared to gas conduction.

- Relative insensitivity of the wafer temp to gas velocity field justifies omission of combined side inlet and showerhead inlet streams in flow simulation.

$N_2 = 100 \text{ sccm and 0.5 Torr}$

$\Delta q = q_{N_2=100} - q_{N_2=60}$
1) Three different temperature setpoints
2) Collocation-based time integration

$\gamma_0 = 12 \text{ kW/m}^2$

$\Delta_w = 0.8 \text{ mm (cf. 0.5 mm wafer)}$

$\Delta_s = 0.65 \text{ cm (cf. 2 cm showerhead)}$
Model validation

- Re-check dynamic model validity with final set of parameter values;
- $T_{sh}(0)$ depends on time since previous reactor operating cycle.
**W CVD Simulation**  
*Chang, Adomaitis, Kidder, and Rubloff, 2000 Annual AIChE Meeting*

### Deposition Process Recipe

**H₂ flushing** | **Cold wafer background** | **Heating** | **Hot wafer deposition** | **Cool down**
--- | --- | --- | --- | ---
H₂ | 40sccm | 40scm | 40scm | 40scm | 200scm
WF₆ | 0scm | 10scm | 0scm | 10scm | 0scm
Pressure | 0.5Torr | 0.5Torr | 0.5Torr | 0.5Torr | 0.5Torr

**Temperature:**

**Process Prep.**

**Dep.**

**Quadrupole Mass Spectrometer data by Dr. Yiheng Xu**
Conclusions and Current Work

- **Simulator validation**: excellent agreement between model predictions and measured wafer temperature;

- **Extrapolation** of wafer temperature predictions to true process operating gas composition;

- **Current simulation research** to investigate wafer temperature nonuniformity, gas phase reduced-basis discretization methods; validation of blanket W deposition model;

- **Extension** of simulation methods to CVD reactor design and other semiconductor manufacturing processes.