Boat Reactor for Low Pressure Chemical Vapor Deposition

Introduction

Chemical vapor deposition (CVD) is an important step in the process of manufacturing microchips. A common application is the deposition of silicon on wafers at low pressure. Low-pressure reactors are used to get a high diffusivity of the gaseous species, which results in a uniform deposition thickness, because the process becomes limited by the deposition kinetics (Ref. 1 and Ref. 2).

In this example you model the momentum and mass transport equations coupled to the reaction kinetics for the deposition process. You treat a low-pressure boat reactor, where the goal of the simulation is to describe the rate of deposition as a function of the fluid mechanics and kinetics in the system.

The gas, in this case silane (SiH$_4$), enters the reactor from the left and reacts on the wafers to form hydrogen and silicon. The remaining mixture leaves the reactor through the outlet on the right. The deposition of silicon on the surface of the wafers depends on the local concentration of silane, which is determined by the operating conditions for the reactor.

You can find more details about this example in Elements of Chemical Reaction Engineering by H. Scott Fogler (Ref. 1).
**Model Definition**

First assume that the density of the gas is constant throughout the reactor. This implies that the reacting gas is either diluted in a carrier gas or that the conversion in the reactor is small. Moreover, only account for the mass transport of the reactant gas, in this case silane, and assume constant temperature in the reactor.

In the wafer bundle you can neglect convection transport, so that the reacting gas can only be transported through diffusion. To save time and computational memory, also simplify the geometrical description of the wafer bundle by modeling it as an anisotropic medium. To this end, because silane cannot diffuse through the physical wafers, assume that the axial diffusivity in the wafer bundle is zero. Furthermore, correct the diffusivity in the radial direction according to the degree of packing in the bundle. Finally, neglect the influence of the support boat on the transport process that holds the wafer bundle in place. The structure of the boat reactor means that you can reduce the 3D geometry to a 2D axisymmetric model. The modeling domain is shown in Figure 2.

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**Figure 2**: The model geometry showing the domain and boundary labels.

The chemical reaction you account for in this example is given below:
The rate of this reaction depends on the partial pressure of silane and the temperature in the reactor.

The assumptions mentioned above in combination with the chemical reaction for the deposition process make it possible to define an equation system. The momentum equations and the continuity equations for laminar flow in cylindrical coordinates read:

\[
\frac{\partial}{\partial r} \left( -\eta r \frac{\partial u}{\partial r} \right) + \frac{\partial}{\partial z} \left( -\eta r \frac{\partial u}{\partial z} \right) + \rho r \left( u \frac{\partial u}{\partial r} + v \frac{\partial u}{\partial z} \right) + r \frac{\partial p}{\partial r} = 0 \quad \text{in } \Omega_{ff}
\]

\[
\frac{\partial}{\partial r} \left( -\eta r \frac{\partial v}{\partial r} \right) + \frac{\partial}{\partial z} \left( -\eta r \frac{\partial v}{\partial z} \right) + \rho r \left( u \frac{\partial v}{\partial r} + v \frac{\partial v}{\partial z} \right) + r \frac{\partial p}{\partial z} = 0 \quad \text{in } \Omega_{ff}
\]

\[
r \left( \frac{\partial u}{\partial r} + \frac{\partial u}{\partial z} \right) + v = 0 \quad \text{in } \Omega_{ff}
\]

Here \( \eta \) (kg/(m·s)) denotes the viscosity; \( \rho \) (kg/m\(^3\)) is the density of the gas; \( u \) and \( v \) (m/s) refer to the velocity vector’s \( r \)- and \( z \)-components, respectively; and \( p \) (Pa) is the pressure.

The mass transport in the free-fluid domain is given by the following equation, expressed in cylindrical coordinates:

\[
\frac{\partial}{\partial r} \left( -D \frac{\partial c}{\partial r} \right) + \frac{\partial}{\partial z} \left( -D \frac{\partial c}{\partial z} \right) + r u \frac{\partial c}{\partial r} + r v \frac{\partial c}{\partial z} = 0 \quad \text{in } \Omega_{ff}
\]

Here \( D \) denotes the diffusivity (m\(^2\)/s) and \( c \) is the concentration of silane (mol/m\(^3\)).

You obtain the corresponding mass transport equation for the wafer bundle domain by neglecting transport by convection and adding a reaction-rate term for the dissociation of silane:

\[
\frac{\partial}{\partial r} \left( -D_{\text{eff},rr} \frac{\partial c}{\partial r} \right) = -rkS_a c \quad \text{in } \Omega_{wb}
\]

Because you neglect diffusion in the axial direction, the effective diffusivity tensor, \( D_{\text{eff}} \), only has an \( rr \)-component. In the equation above, \( k \) (m/s) denotes the rate constant for the reaction, and \( S_a \) (m\(^2\)/m\(^3\)) refers to the specific surface area.

You solve the system of equations defined above by using the proper boundary conditions. For laminar flow, no-slip conditions apply at the reactor-wall surface and between the free channel and the wafer bundle:
\[(u, v) = (0, 0) \quad \text{at } \partial \Omega \text{_{wall}}, \partial \Omega \text{_{iw}}, \text{ff}, \text{ and } \partial \Omega \text{_{wb}}, \text{ff} \] \hspace{1cm} (5)

At the symmetry axis, the radial velocity component vanishes:

\[u = 0 \quad \text{at } \partial \Omega \text{_{sym}} \] \hspace{1cm} (6)

The last three conditions for the momentum equations and continuity equation are

\[
\begin{align*}
  u &= 0 & \text{at } \partial \Omega \text{_{in}} \\
  v &= v_0 & \text{at } \partial \Omega \text{_{in}} \\
  p &= p_0 & \text{at } \partial \Omega \text{_{out}} \\
  \eta (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \mathbf{n} &= 0 & \text{at } \partial \Omega \text{_{out}}
\end{align*}
\] \hspace{1cm} (7)

For the mass transport Equation 3 and Equation 4, the boundary conditions are

\[
\begin{pmatrix}
-D_{i,rr} \frac{\partial c}{\partial r}, & -D_{i,zz} \frac{\partial c}{\partial z}
\end{pmatrix} \cdot \mathbf{n} = 0 \quad \text{at } \partial \Omega \text{_{wall}}, \partial \Omega \text{_{sym}}, \text{ and } \partial \Omega \text{_{iw}} \] \hspace{1cm} (8)

where \(D_i\) represents the diffusivity in \(\Omega\)_{ff} or \(\Omega\)_{wb} depending on to which boundary segment you apply the equation. This equation implies that there is no flux perpendicular to these boundaries. At the inlet, the composition of the gas is known, which yields:

\[c = c_0 \quad \text{at } \partial \Omega \text{_{in}} \] \hspace{1cm} (9)

At the outlet, assume that the transport of species takes place mainly by convection and neglect the concentration gradients perpendicular to this boundary:

\[
\begin{pmatrix}
-D \frac{\partial c}{\partial r}, & -D \frac{\partial c}{\partial z}
\end{pmatrix} \cdot \mathbf{n} = 0 \quad \text{at } 0 \partial \Omega \text{_{out}}
\] \hspace{1cm} (10)

It remains to discuss the material parameters appearing in Equation 4: \(D_{\text{eff}}, r, r\), \(S_a\), and \(k\). First, calculate the specific surface area (that is, the area per unit volume) of the wafer bundle, \(S_a\), by assuming a certain pitch between the wafers; see Figure 3.
Furthermore, to estimate the effective diffusivity in the radial direction inside the wafer bundle, multiply the diffusivity in the free-fluid domain by the ratio of the contact area between the free gas and the wafer bundle to the total lateral surface area of the wafer-bundle domain:

\[ D_{\text{eff,rr}} = \left(1 - \frac{d_w}{d_{cc}}\right)D \text{ in } \Omega_{\text{wb}} \]  

The rate constant, \( k \) (m/s), is a function of the partial pressure of silane. At 600 °C and a total system pressure of 25 Pa, Ref. 2 provides the value \( k = 8.06 \cdot 10^{-3} \text{ m/s} \).

A crucial characteristic of the reactor’s performance is the silicon deposition rate, \( \Delta_{\text{Si}} \), which expresses the growth rate of the silicon layer on the wafers. The amount of silicon deposited on the wafers, expressed in mass per unit area per unit time, is the product of the rate constant, \( k \), the silane concentration, \( c \), and the molar mass of silicon, \( M_{\text{Si}} \) (kg/mol). Dividing the so obtained quantity by the density of silicon, \( \rho_{\text{Si}} \) (kg/m³), gives the deposition rate:

\[ \Delta_{\text{Si}} = \frac{k c M_{\text{Si}}}{\rho_{\text{Si}}} \text{ (nm/min)} \]  

In this model, you study the radial and axial distribution of \( \Delta_{\text{Si}} \) inside the wafer bundle.

**Results**

Figure 4 shows the concentration distribution in the boat reactor, indicating that the conversion is quite small.
Figure 4: Concentration distribution in the reactor. Figure 5 shows the flow distribution in the reactor.

Figure 5: Flow distribution in the reactor. The surface color and the arrows both represent the velocity.
The plots in Figure 6 display the deposition rate for the inlet velocities 1 m/s (top panel) and 2 m/s (bottom panel).

Figure 6: The deposition rate in the wafer bundle for the inlet velocities 1 m/s (top) and 2 m/s (bottom).
In both cases, the highest deposition rate is obtained near the reactor inlet and close to the free-fluid channel. The difference in deposition rate between the center and periphery of the wafers is approximately 0.1 nm/min (or roughly 2.5%), and that along the length of the reactor approximately 0.5 nm/min (roughly 12.5%). Thus, as desired, the variations in the deposition rate inside the reactor are rather small.

Moreover, comparing the plots it is evident that the deposition rate changes only marginally when the gas inlet velocity is doubled, showing that convection does not have a major influence on reactors of this type.

References


Model Library path: Chemical_Reaction_Engineering_Module/Surface_Reactions_and_Deposition_Processes/boat_reactor

Modeling Instructions

**MODEL WIZARD**

1. Go to the Model Wizard window.

2. Click the 2D axisymmetric button.

3. Click Next.


5. Click Add Selected.

6. In the Add physics tree, select Chemical Species Transport>Transport of Diluted Species (chds).

7. Click Add Selected.

8. Click Next.

**GLOBAL DEFINITIONS**

**Parameters**

1. In the **Model Builder** window, right-click **Global Definitions** and choose **Parameters**.
2. Go to the **Settings** window for Parameters.
3. Locate the **Parameters** section. In the **Parameters** table, enter the following settings:

<table>
<thead>
<tr>
<th>NAME</th>
<th>EXPRESSION</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>R_a</td>
<td>40[mm]</td>
<td>Wafer radius</td>
</tr>
<tr>
<td>d_cc</td>
<td>2.5[mm]</td>
<td>Wafer spacing</td>
</tr>
<tr>
<td>d_w</td>
<td>0.5[mm]</td>
<td>Wafer thickness</td>
</tr>
<tr>
<td>S_a</td>
<td>2*(R_a^2+R_a<em>d_w)/(R_a^2</em>d_cc)</td>
<td>Specific surface area</td>
</tr>
<tr>
<td>p_tot</td>
<td>25[Pa]</td>
<td>Total system pressure</td>
</tr>
<tr>
<td>D_amb</td>
<td>5e-5[m^2/s]</td>
<td>SiH4 diffusivity in air at 1 atm</td>
</tr>
<tr>
<td>D</td>
<td>D_amb*1[atm]/p_tot</td>
<td>Pressure-corrected diffusivity</td>
</tr>
<tr>
<td>D_eff</td>
<td>D*(1-d_w/d_cc)</td>
<td>Effective diffusivity in wafer bundle</td>
</tr>
<tr>
<td>k</td>
<td>8.06[mm/s]</td>
<td>Rate constant</td>
</tr>
<tr>
<td>M_N2</td>
<td>28[g/mol]</td>
<td>Molar mass, N2</td>
</tr>
<tr>
<td>M_Si</td>
<td>28[g/mol]</td>
<td>Molar mass, Si</td>
</tr>
<tr>
<td>M_SiH4</td>
<td>32[g/mol]</td>
<td>Molar mass, SiH4</td>
</tr>
<tr>
<td>T_r</td>
<td>873[K]</td>
<td>Reactor temperature</td>
</tr>
<tr>
<td>rho</td>
<td>p_tot*(0.2<em>M_SiH4+0.8</em>M_N2)/(R_const*T_r)</td>
<td>Gas density</td>
</tr>
<tr>
<td>eta</td>
<td>3.1e-5[Pa*s]</td>
<td>Dynamic viscosity</td>
</tr>
<tr>
<td>c0</td>
<td>0.2<em>p_tot/(R_const</em>T_r)</td>
<td>Inlet concentration, SiH4</td>
</tr>
<tr>
<td>v0</td>
<td>1[m/s]</td>
<td>Inlet axial flow velocity</td>
</tr>
<tr>
<td>rho_Si</td>
<td>2e3[kg/m^3]</td>
<td>Silicon density</td>
</tr>
<tr>
<td>Re</td>
<td>R_a<em>v0</em>rho/eta</td>
<td>Reynolds number</td>
</tr>
</tbody>
</table>
DEFINITIONS

Variables 1
1 In the Model Builder window, right-click Model 1>Definitions and choose Variables.
2 Go to the Settings window for Variables.
3 Locate the Variables section. In the Variables table, enter the following settings:

<table>
<thead>
<tr>
<th>NAME</th>
<th>EXPRESSION</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>Delta_Si</td>
<td>c<em>k</em>M_Si/rho_Si</td>
<td>Silicon deposition rate</td>
</tr>
</tbody>
</table>

GEOMETRY 1
1 In the Model Builder window, click Model 1>Geometry 1.
2 Go to the Settings window for Geometry.
3 Locate the Units section. From the Length unit list, select mm.

Bézier Polygon 1
1 Right-click Model 1>Geometry 1 and choose Bézier Polygon.
2 Go to the Settings window for Bézier Polygon.
3 Locate the Polygon Segments section. Click the Add Linear button.
4 Find the Control points subsection. In row 2, set r to 60.
5 Click the Add Linear button.
6 In row 2, set z to 140.
7 Click the Add Quadratic button.
8 In row 2, set z to 180.
9 In row 3, set r to 20.
10 In row 3, set z to 180.
11 Click the Add Linear button.
12 In row 2, set r to 0.
13 Click the Add Linear button.
14 Click the Close Curve button.
15 Click the Build Selected button.

Rectangle 1
1 In the Model Builder window, right-click Geometry 1 and choose Rectangle.
2 Go to the Settings window for Rectangle.
3 Locate the **Size** section. In the **Width** edit field, type R_a.
4 In the **Height** edit field, type 5.
5 Locate the **Position** section. In the **z** edit field, type 35.
6 Click the **Build Selected** button.

**Rectangle 2**
1 In the **Model Builder** window, right-click **Geometry 1** and choose **Rectangle**.
2 Go to the **Settings** window for Rectangle.
3 Locate the **Size** section. In the **Width** edit field, type R_a.
4 In the **Height** edit field, type 100.
5 Locate the **Position** section. In the **z** edit field, type R_a.
6 Click the **Build Selected** button.

**Rectangle 3**
1 In the **Model Builder** window, right-click **Geometry 1** and choose **Rectangle**.
2 Go to the **Settings** window for Rectangle.
3 Locate the **Size** section. In the **Width** edit field, type R_a.
4 In the **Height** edit field, type 5.
5 Locate the **Position** section. In the **z** edit field, type 140.
6 Click the **Build Selected** button.

**Point 1**
1 In the **Model Builder** window, right-click **Geometry 1** and choose **Point**.
2 Go to the **Settings** window for Point.
3 Locate the **Point** section. In the **r** edit field, type 20.
4 Click the **Build Selected** button.

**Compose 1**
1 In the **Model Builder** window, right-click **Geometry 1** and choose **Boolean Operations>Compose**.
2 Select the objects b1, r1, r2, and r3 only.
3 Go to the **Settings** window for Compose.
4 Locate the **Compose** section. In the **Set formula** edit field, type b1+r2-r1-r3.
5 Click the **Build Selected** button.
**Form Union**

In the Model Builder window, right-click **Form Union** and choose **Build Selected**.

**DEFINITIONS**

**Explicit 1**

1. In the Model Builder window, right-click **Model 1>Definitions** and choose **Selections>Explicit**.
2. Right-click **Explicit 1** and choose **Rename**.
3. Go to the **Rename Explicit** dialog box and type *wafers* in the **New name** edit field.
4. Click **OK**.
5. Select Domain 2 only.

**Explicit 2**

1. In the Model Builder window, right-click **Definitions** and choose **Explicit**.
2. Right-click **Explicit 2** and choose **Rename**.
3. Go to the **Rename Explicit** dialog box and type *reactor* in the **New name** edit field.
4. Click **OK**.
5. Select Domain 1 only.

**LAMINAR FLOW**

1. In the Model Builder window, click **Model 1>Laminar Flow**.
2. Go to the **Settings** window for Laminar Flow.
3. Locate the **Domain Selection** section. From the **Selection** list, select *reactor*.

**Fluid Properties 1**

1. In the Model Builder window, expand the Laminar Flow node, then click **Fluid Properties 1**.
2. Go to the **Settings** window for Fluid Properties.
3. Locate the Fluid Properties section. From the \( \rho \) list, select *User defined*. In the associated edit field, type \( \text{rho} \).
4. From the \( \mu \) list, select *User defined*. In the associated edit field, type \( \text{eta} \).

**Inlet 1**

1. In the Model Builder window, right-click Laminar Flow and choose **Inlet**.
2. Select Boundary 2 only.
3. Go to the **Settings** window for Inlet.
4 Locate the **Velocity** section. In the $U_0$ edit field, type $v_0$.

**Outlet 1**
1 In the **Model Builder** window, right-click **Laminar Flow** and choose **Outlet**.
2 Select Boundary 9 only.

**TRANSPORT OF DILUTED SPECIES**

**Convection and Diffusion 1**
1 In the **Model Builder** window, expand the **Model 1>Transport of Diluted Species** node, then click **Convection and Diffusion 1**.
2 Go to the **Settings** window for Convection and Diffusion.
3 Locate the **Diffusion** section. In the $D_i$ edit field, type $D$.
4 Locate the **Model Inputs** section. From the $u$ list, select **Velocity field (spf/fp1)**.

**Convection and Diffusion 2**
1 In the **Model Builder** window, right-click **Transport of Diluted Species** and choose **Convection, Diffusion, and Migration**.
2 Go to the **Settings** window for Convection and Diffusion.
3 Locate the **Domain Selection** section. From the **Selection** list, select **wafers**.
4 Locate the **Diffusion** section. From the list below the **Diffusion coefficient** edit field, select **Diagonal**.
5 In the $D_i$ table, enter the following settings:

<table>
<thead>
<tr>
<th>$D_{eff}$</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

**Reactions 1**
1 In the **Model Builder** window, right-click **Transport of Diluted Species** and choose **Reactions**.
2 Go to the **Settings** window for Reactions.
3 Locate the **Domain Selection** section. From the **Selection** list, select **wafers**.
4 Locate the **Reactions** section. In the $R_c$ edit field, type $-(k*S_a)*c$.

**Inflow 1**
1 In the **Model Builder** window, right-click **Transport of Diluted Species** and choose **Inflow**.
2 Select Boundary 2 only.
3 Go to the **Settings** window for Inflow.
4 Locate the **Concentration** section. In the $c_0$ edit field, type $c_0$.

**Outflow 1**
1 In the **Model Builder** window, right-click **Transport of Diluted Species** and choose **Outflow**.
2 Select Boundary 9 only.

**Mesh 1**
1 In the **Model Builder** window, click **Model 1>Mesh 1**.
2 Go to the **Settings** window for Mesh.
3 Locate the **Mesh Settings** section. From the **Element size** list, select **Extra fine**.
4 Click the **Build All** button.

**Study 1**

*Step 1: Stationary*
1 In the **Model Builder** window, click **Study 1>Step 1: Stationary**.
2 Go to the **Settings** window for Stationary.
3 Click to expand the **Extension** section.
4 Select the **Continuation** check box.
5 Under **Continuation parameter**, click **Add**.
6 Go to the **Add** dialog box.
7 In the **Continuation parameter** list, select v0 (**Inlet axial flow velocity**).
8 Click the **OK** button.
9 Go to the **Settings** window for Stationary.
10 Locate the **Extension** section. In the **Parameter values** edit field, type 1 1.5 2.
11 In the **Model Builder** window, right-click **Study 1** and choose **Compute**.

**Results**

*Velocity (spf)*
1 In the **Model Builder** window, click **Results>Velocity (spf)**.
2 Go to the **Settings** window for 2D Plot Group.
3 Locate the **Data** section. From the **Parameter value (v0)** list, select 1.
4 In the **Model Builder** window, click **Surface 1**.
5 Go to the Settings window for Surface.
6 In the upper-right corner of the Expression section, click Replace Expression.
7 From the menu, choose Concentration (c).
8 Click the Plot button.
9 Click the Zoom Extents button on the Graphics toolbar.
10 In the upper-right corner of the Expression section, click Replace Expression.
11 From the menu, choose Laminar Flow>Velocity magnitude (spf.U).
12 In the Model Builder window, right-click Velocity (spf) and choose Arrow Surface.
13 Go to the Settings window for Arrow Surface.
14 Locate the Arrow Positioning section. Find the z grid points subsection. In the Points edit field, type 25.
15 Locate the Coloring and Style section. In the Scale factor edit field, type 1.
16 Click the Plot button.
17 Click the Zoom Extents button on the Graphics toolbar.

Data Sets
1 In the Model Builder window, right-click Results>Data Sets and choose Solution.
2 Go to the Settings window for Solution.
3 Locate the Solution section. From the Solution list, select Solver 1.
4 Right-click Solution 2 and choose Add Selection.
5 Go to the Settings window for Selection.
6 Locate the Geometric Entity Selection section. From the Geometric entity level list, select Domain.
7 Select Domain 2 only.

2D Plot Group 6
1 In the Model Builder window, right-click Results and choose 2D Plot Group.
2 Right-click Results>2D Plot Group 6 and choose Surface.
3 Go to the Settings window for Surface.
4 Locate the Data section. From the Data set list, select Solution 2.
5 From the Parameter value (v0) list, select 1.
6 In the upper-right corner of the Expression section, click Replace Expression.
7 From the menu, choose Definitions>Silicon deposition rate (Delta_Si).
8 Click the **Plot** button.

9 Click the **Zoom In** button on the Graphics toolbar.

10 Locate the **Data** section. From the **Parameter value (v0)** list, select **2**.

11 Click the **Plot** button.