Created in COMSOL Multiphysics 5.6

Chemical Etching

Introduction

This example illustrates the principle of wet chemical etching. Wet chemical etching is particularly important for microelectronics industry for patterning of integrated circuit, MEMS devices, optoelectronic and pressure sensors. Wet etching processes use solution based ("wet") etchants, where the substrate to be etched is immersed in a controlled flow of etchant. Wet etching process is selective isotropic, fast (usually reaction rate limited) and reproducible. Due to its reproducibility the technique is often used for micropatterning of substrates.

A wet etching process involves chemical reaction that consume the original reactant and produce new reactant. The wet etch process can be described by three basic steps:

- Transport of the liquid etchant to the structure that is to be removed.
- The reaction between the liquid etchant and the material being etched away. A reduction-oxidation (redox) reaction usually occurs. This reaction entails the oxidation of the material followed by dissolution.
- Transport of the by products in the reaction from the reacted surface.

The purpose of this tutorial is to examine how the copper substrate material is depleted and how the cavity shape evolves during the wet etching process. The rate of the etching reaction depends on the local concentration of a reactant, which is transported to the surface by coupled convection-diffusion. The laminar flow profile of the etchant fluid changes due to the shape evolution of the etched cavity.

Model Definition

The simplified 2D model geometry consists of a masked copper substrate with an exposed surface which is to be wet etched. The geometry is shown in Figure 1. The top rectangular domain has fluid flowing over the exposed copper substrate as marked in the x-direction. The fluid reacts only with the unmasked copper as the etching proceeds.

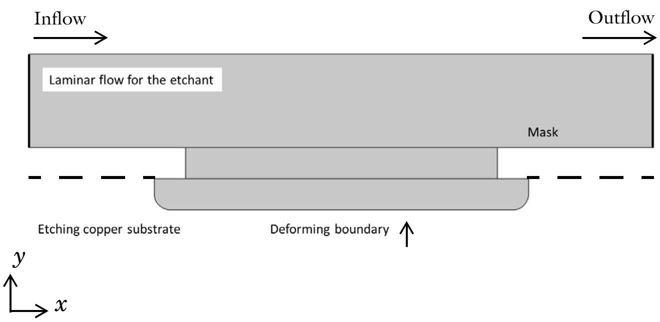

Figure 1: Schematic diagram of the chemical etching under a laminar flow of the etchant.

TRANSPORT OF CHEMICAL SPECIES

Equation 1 describes mass flux of the etching species as given by diffusion and convection

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = \nabla \cdot (D \nabla c) \tag{1}$$

where D (SI unit: m^2/s) denotes the diffusion coefficient and c (SI unit: mol/m^3) is the concentration. The modeled species has a diffusion coefficient of $1 \cdot 10^{-9}$ m^2/s. At the inlet and top boundary of the flow, concentration is equal to the bulk concentration the etchant solution. At the etching surface (moving boundary) the flux condition is considered as in Equation 2:

$$D \nabla c \cdot \mathbf{n} = -kc \tag{2}$$

where k (SI unit: m/s) is the etching rate constant for linear kinetics of the etching species and $\mathbf{n}$ is the normal vector. k is assumed to be independent of the position on the surface. A No Flux condition is used for all other boundaries except the moving boundary.

LAMINAR FLOW

At the cavity, the flow field can be calculated by Equation 3:

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] + \mathbf{F} \tag{3}$$

where ρ is the fluid density (SI unit: kg/m^3), p is the pressure (SI unit: Pa), μ is the dynamic viscosity (SI unit: Pa·s), $\mathbf{F}$ is the volume force vector (indicated as the boundary stress in the modeling instructions), and $\mathbf{u}$ is the fluid velocity (SI unit: m/s). Along with continuity Equation 4

$$\rho\nabla\cdot\mathbf{u} = 0 \tag{4}$$

Along the moving wall, a no slip condition is applied.

DEFORMED GEOMETRY

The movement of the boundary is defined by an interfacial condition on the boundary,

$$\upsilon = \frac{DM}{\rho} \tag{5}$$

where υ is velocity of the moving mesh in the normal direction, D, M, and ρ are the diffusion coefficient (SI unit: m^2/s), molar mass (SI unit: mol/m^3), and density (SI unit: kg/m^3) of the etching species, respectively.

Results and Discussion

Figure 2 shows the concentration of etchant species $CuCl_2$ at t = 10000 s for an initial cavity radius of 0.5 mm. The etch profile is asymmetric owing to the fluid flow in the x-direction. The etch rate is higher around the area where laminar flow first encounters the boundary layer in fluid direction. Concentration becomes uniform deeper into the cavity as laminar flow can no longer transport reactant to the boundary layer owing to larger aspect ratio. (See also the velocity profile in Figure 3.)

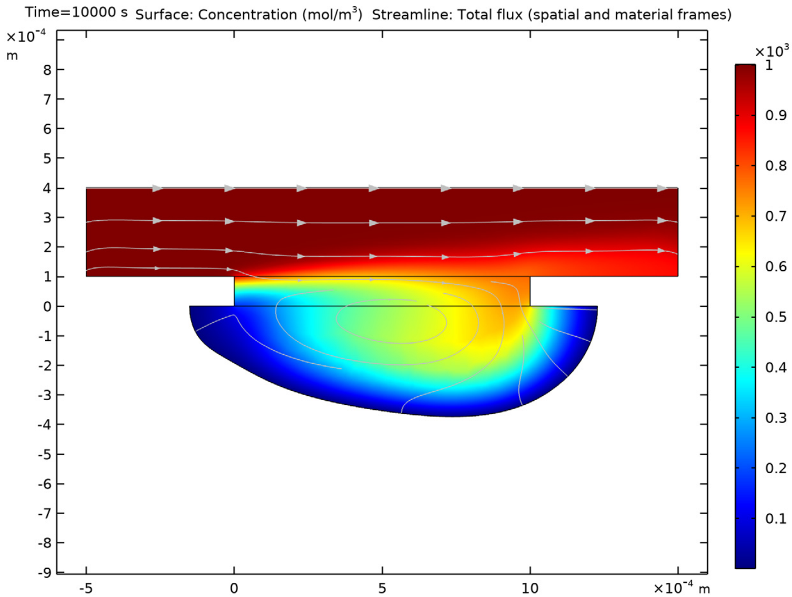

Figure 2: Concentration profile of $CuCl_2$ etchant at $t = 10000$ s over unmasked copper cavity.

[Figure 3](#) shows the velocity profile for etchant flow at t = 10000 s. The velocity is zero close to the moving boundary. The fluid flow eventually becomes weak deeper as the aspect ratio of cavity increases with time.

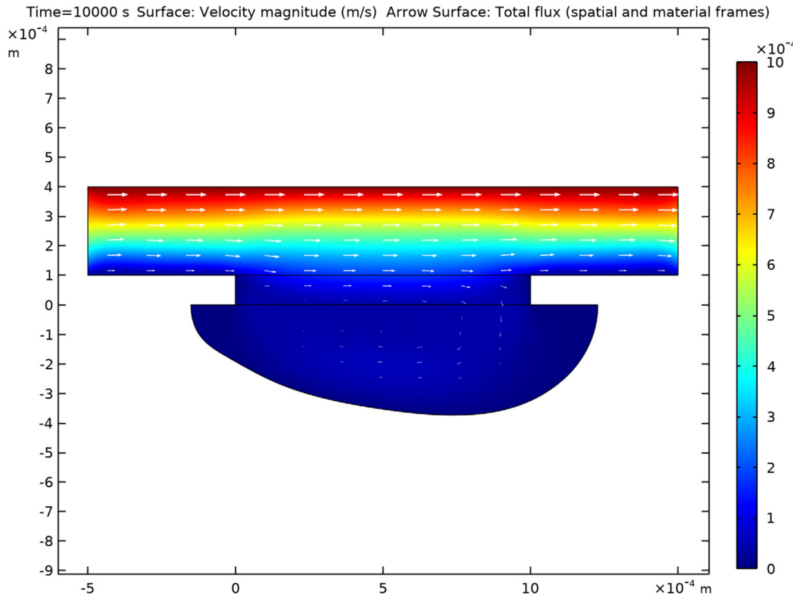

Figure 3: Arrow surface plot depicting velocity profile of $CuCl_2$ etchant after t=10000 s over the deformed geometry of copper cavity.

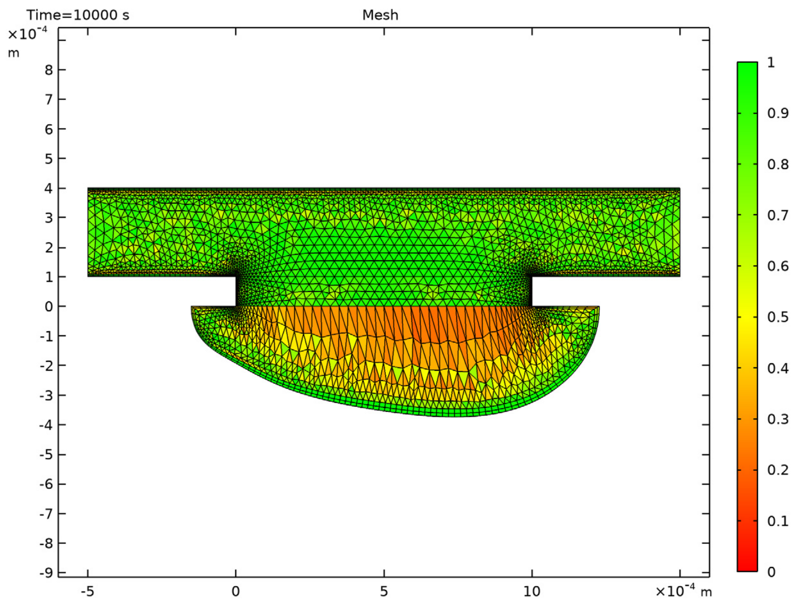

Figure 4: Mesh deformation after t=10000 s over the etching unmasked copper cavity.

Figure 4 shows mesh deformation for deforming geometry at t = 10000 s.

Reference

1. D.J. Economou and others, "Effect of transport and reaction on the shape evolution of cavities during wet chemical etching", *J. Electrochem. Soc.*, vol. 136, no. 7, pp. 1997–2004, 1989.

Application Library path: `COMSOL_Multiphysics/Chemical_Engineering/chemical_etching`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D**.

Add the required physics.

2 In the **Select Physics** tree, select **Chemical Species Transport>Transport of Diluted Species (tds)**.

3 Click **Add**.

4 In the **Concentration** text field, type `cCuCl2`.

5 In the **Select Physics** tree, select **Mathematics>Deformed Mesh>Deformed Geometry (dg)**.

6 Click **Add**.

7 In the **Select Physics** tree, select **Fluid Flow>Single-Phase Flow>Laminar Flow (spf)**.

8 Click **Add**.

9 Click **Study**.

10 In the **Select Study** tree, select **General Studies>Stationary**.

11 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Definitions** node, then click **Global Definitions>Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `chemical_etching_parameters.txt`.

Next, define the variable `v_surface` corresponding to the velocity of the moving boundary.

DEFINITIONS

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, locate the **Variables** section.

3 In the table, enter the following settings:

Name	Expression	Unit	Description
v_surface	-r_surface*M_Cu/rho_Cu	m/s	Surface normal velocity
r_surface	-kf*cCuCl2	mol/(m^2·s)	

GEOMETRY 1

Rectangle 1 (r1)

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Geometry 1** node.

2 Right-click **Geometry 1** and choose **Rectangle**.

3 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

4 In the **Width** text field, type `d_mask`.

5 In the **Height** text field, type `h_mask`.

Rectangle 2 (r2)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `h_boundary_layer`.

4 In the **Height** text field, type `h_seed_cavity`.

5 Locate the **Position** section. In the **x** text field, type `-h_seed_cavity`.

6 In the **y** text field, type `-h_seed_cavity`.

Fillet 1 (fil1)

1 In the **Geometry** toolbar, click **Fillet**.

2 Click the **Zoom Extents** button in the **Graphics** toolbar.

3 On the object **r2**, select Points 1 and 2 only.

4 In the **Settings** window for **Fillet**, locate the **Radius** section.

5 In the **Radius** text field, type `h_seed_cavity/2`.

Rectangle 3 (r3)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `d_mask*2`.

4 In the **Height** text field, type `3*h_mask`.

5 Locate the **Position** section. In the **x** text field, type `-d_mask/2`.

6 In the **y** text field, type `h_mask`.

7 Click **Build All Objects**.

DEFINITIONS

Moving Boundary

1 In the **Definitions** toolbar, click **Explicit**.

2 In the **Settings** window for **Explicit**, type `Moving Boundary` in the **Label** text field.

3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundaries 4, 6, 13, 15, and 16 only.

ADD MATERIAL

1 In the **Home** toolbar, click **Add Material** to open the **Add Material** window.

2 Go to the **Add Material** window.

3 In the tree, select **Built-in>Water, liquid**.

4 Click **Add to Component** in the window toolbar.

5 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

TRANSPORT OF DILUTED SPECIES (TDS)

Transport Properties 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Transport of Diluted Species (tds)>Transport Properties 1** node, then click **Transport Properties 1**.

2 In the **Settings** window for **Transport Properties**, locate the **Convection** section.

3 From the **u** list, choose **Velocity field (spf)**.

4 Locate the **Diffusion** section. In the D_{cCuCl2} text field, type `D`.

Concentration 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Transport of Diluted Species (tds)>No Flux 1** node.

2 Right-click **Transport of Diluted Species (tds)** and choose **Concentration**.

3 Select Boundaries 1 and 3 only.

4 In the **Settings** window for **Concentration**, locate the **Concentration** section.

5 Select the **Species cCuCl2** check box.

6 In the $c_{0,\mathrm{cCuCl2}}$ text field, type `cCuCl2_bulk`.

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundary 14 only.

Flux 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Flux**.

2 In the **Settings** window for **Flux**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Moving Boundary**.

4 Locate the **Inward Flux** section. Select the **Species cCuCl2** check box.

5 In the $J_{0,\mathrm{cCuCl2}}$ text field, type `r_surface`.

DEFORMED GEOMETRY (DG)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Deformed Geometry (dg)**.

2 In the **Settings** window for **Deformed Geometry**, locate the **Frame Settings** section.

3 From the **Geometry shape function** list, choose **1**.

4 Locate the **Free Deformation Settings** section. From the **Mesh smoothing type** list, choose **Hyperelastic**.

Free Deformation 1

1 In the **Physics** toolbar, click **Domains** and choose **Free Deformation**.

2 Select Domain 2 only.

Zero Normal Mesh Displacement 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Zero Normal Mesh Displacement**.

2 Select Boundaries 5 and 11 only.

Prescribed Normal Mesh Velocity 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Prescribed Normal Mesh Velocity**.

2 In the **Settings** window for **Prescribed Normal Mesh Velocity**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Moving Boundary**.

4 Locate the **Normal Mesh Velocity** section. In the v_n text field, type `v_surface`.

LAMINAR FLOW (SPF)

In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.

Wall 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Wall**.

2 Select Boundary 3 only.

3 In the **Settings** window for **Wall**, click to expand the **Wall Movement** section.

4 From the **Translational velocity** list, choose **Manual**.

5 Specify the $\mathbf{u}_{tr}$ vector as

`1[mm/s]`	x
0	y

Boundary Stress 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Boundary Stress**.

2 Select Boundaries 1 and 14 only.

STUDY 1

Step 1: Stationary

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check box for **Deformed Geometry (dg)**.

Time Dependent

1 In the **Study** toolbar, click **Study Steps** and choose **Time Dependent> Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `range(0,500,10000)`.

4 In the **Study** toolbar, click **Compute**.

RESULTS

Concentration (tds)

1 Click the **Zoom Extents** button in the **Graphics** toolbar.

2 In the **Concentration (tds)** toolbar, click **Plot**.

Arrow Surface 1

1 In the **Model Builder** window, right-click **Velocity (spf)** and choose **Arrow Surface**.

2 In the **Settings** window for **Arrow Surface**, locate the **Coloring and Style** section.

3 From the **Arrow length** list, choose **Logarithmic**.

4. From the **Color** list, choose **White**.
5. In the **Velocity (spf)** toolbar, click **Plot**.

Pressure (spf)

1. Click the **Zoom Extents** button in the **Graphics** toolbar.
2. In the **Model Builder** window, click **Pressure (spf)**.
3. In the **Pressure (spf)** toolbar, click **Plot**.

Mesh

1. In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.
2. Right-click **2D Plot Group 4** and choose **Rename**.
3. In the **Rename 2D Plot Group** dialog box, type `Mesh` in the **New label** text field.
4. Click **OK**.

Mesh 1

1. Right-click **Mesh** and choose **Mesh**.
2. In the **Mesh** toolbar, click **Plot**.

Animation 1

1. In the **Results** toolbar, click **Animation** and choose **Player**.
2. In the **Settings** window for **Animation**, click **Show Frame**.
3. Locate the **Frames** section. From the **Frame selection** list, choose **All**.
4. In the **Frame number** text field, type `101`.
5. Right-click **Animation 1** and choose **Play**.