Electrodeposition on a Resistive Patterned Wafer

Introduction

This example models a cupplater reactor, where copper is electrodeposited on a patterned silicon wafer. It is also demonstrated how to make the deposited layer more uniform by the use of a current thief.

The deposition reaction occurs on a seed layer on an otherwise insulating wafer, with the effect that all current going into the metal layer is transported tangentially along the surface. As the deposition process progresses, and more metal is added to the surface, the tangential current conductivity of the layer increases.

To cope with the very different geometric scales of the metal layer (tens of micrometers) and the electrolyte chamber (millimeters), which would otherwise pose problems in regards to mesh quality and/or problem size, the current conduction in the wafer metal layer is modeled using the Electrode, Shell interface, which uses a boundary formulation for the metal current conduction.

The model qualitatively reproduces the results of Purcar and others (Ref. 1).

Model Definition

The geometry is shown in Figure 1 and consists of one electrolyte domain. The top boundary is the anode. The bottom circular area represents the wafer surface, on top of which a metal seed layer has been deposited, followed by the application of a photoresist mask.

In the cell, the metal deposits on the patterned surface, which acts as cathode. The effect of the ring current thief is investigated by letting the surface be inactive as electrode in a first study, and then comparing the results to when letting also the current thief act as cathode. The area between the current thief and pattern is covered by a photoresist, and is inactive to the deposition reaction. A small edge segment of the current thief ring is used as current collector. The area outside the ring is insulating and does not conduct current in this model.

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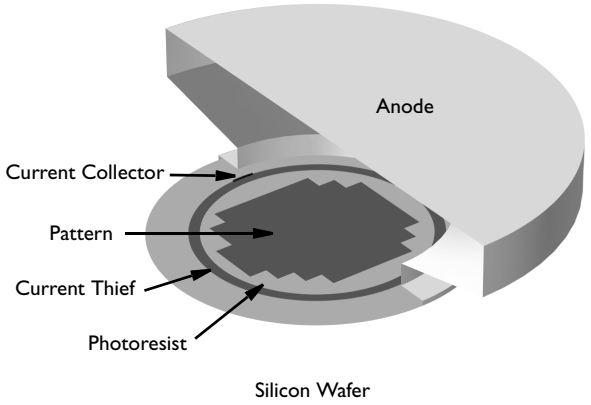

Figure 1: Model geometry.

The model is set up using two different interfaces: an Electrodeposition, Secondary interface, which solves for the electrolyte potential, ϕ_s , and the deposited concentration, c_{dep}, on the patterned wafer, and an Electrode, Shell interface, which solves for the electric potential on the metal layer on the wafer, $\phi_{s,wafer}$.

ELECTRODEPOSITION, SECONDARY

The single domain is modeled as an Electrolyte domain. A constant conductivity of 20 S/m is used for the electrolyte.

The anode is assumed to a have a negligible polarization and an Electrolyte Current boundary condition, with a condition for the total current of 0.4 A, is used for the top boundary.

An External Depositing Electrode boundary condition is used for the active cathode boundaries, with an electric potential for this electrode set to the electric potential of the Electrode, Shell interface. The kinetics are described by Butler-Volmer kinetics, and the thickness of the deposited layer is based on the molar mass and density of copper.

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All other boundaries are isolated.

ELECTRODE SHELL

An Electrode boundary is used for the inactive parts of the surface, where only current conduction occurs. A constant conductivity value, $5.6 \cdot 10^7$ S/m, is used for all parts of the surface. On the inactive parts, the metal layer thickness is equal to the seed layer thickness, 0.1 µm.

For the active parts of the wafer surface, the cathode, a Depositing Electrode boundary node is used. Here, the metal layer thickness is set to the seed layer thickness plus the electrode thickness change (due to the cathode depositing reaction), which is coupled to the External Depositing Electrode node in the Electrodeposition, Secondary interface.

The electrode reactions also give rise to a current source on the cathode boundaries, these are also coupled to the External Depositing Electrode node in the Electrodeposition, Secondary interface.

The current collector edge is grounded, whereas all other edges are isolated.

STUDIES

The problem is solved using a Time-dependent with Initialization, Fixed Geometry study type, simulating the deposition process for 600 s.

By using a study type for a fixed geometry, the change in geometry, which is expected to be in the range of micrometers, is not included in the variables that are solved for by the solver.

Two studies are performed. In the first, Study 1, only the pattern is used as active electrode on the wafer. In Study 2 both the ring current thief and the wafer pattern is used as cathodes.

Discussion

Figure 2 shows the electrolyte potential at the end of the Study 1, without the current thief. The potential in the outer parts of the patterned area is almost 40 mV higher than in the central parts.

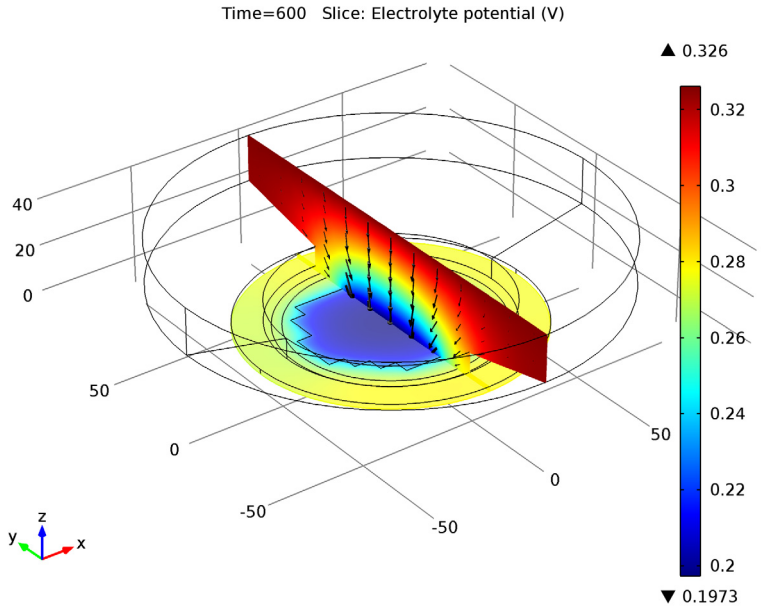

Figure 2: Electrolyte currents and potential at the end of the simulation without a current thief.

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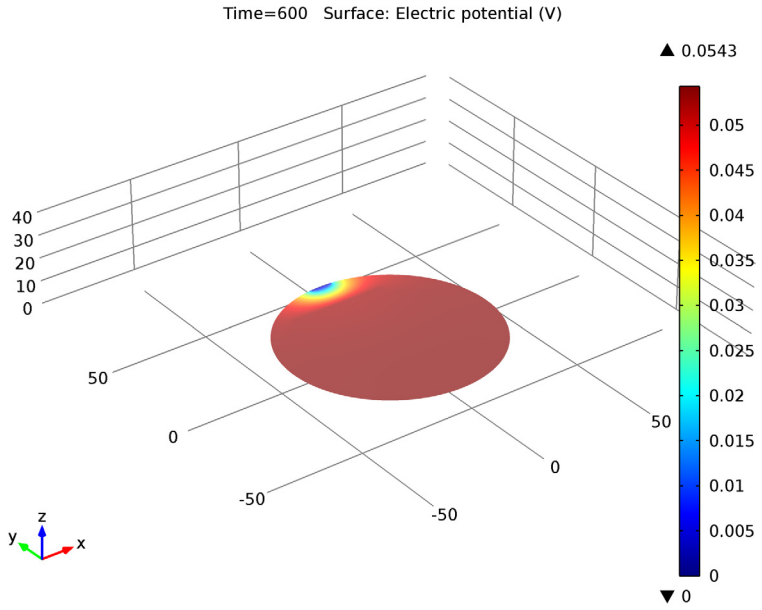

Figure 3: Electric potential in the copper layer at the end of the simulation without a current thief.

Figure 3 shows the potential in the metal on the wafer at the end of the Study 1. Close to the current collector there is a significant potential drop. The potential is however fairly uniform for the active part of the wafer.

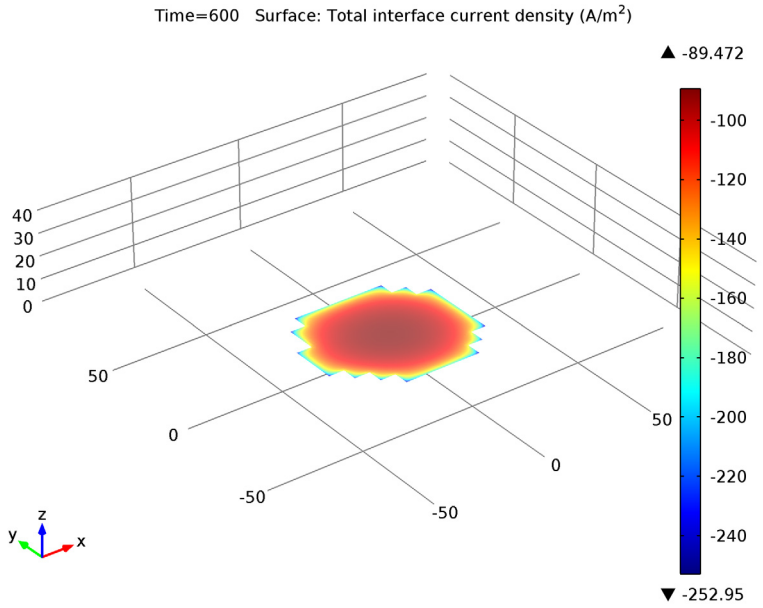

Figure 4: Electrode reaction current density at the end of the simulation without a current thief.

Figure 4 shows the electrode currents at the end of the Study 1. The reaction currents are significantly higher in the outer parts of the patterned area, especially in the corners. This is mainly an effect of the large differences in electrolyte potential seen in Figure 2.

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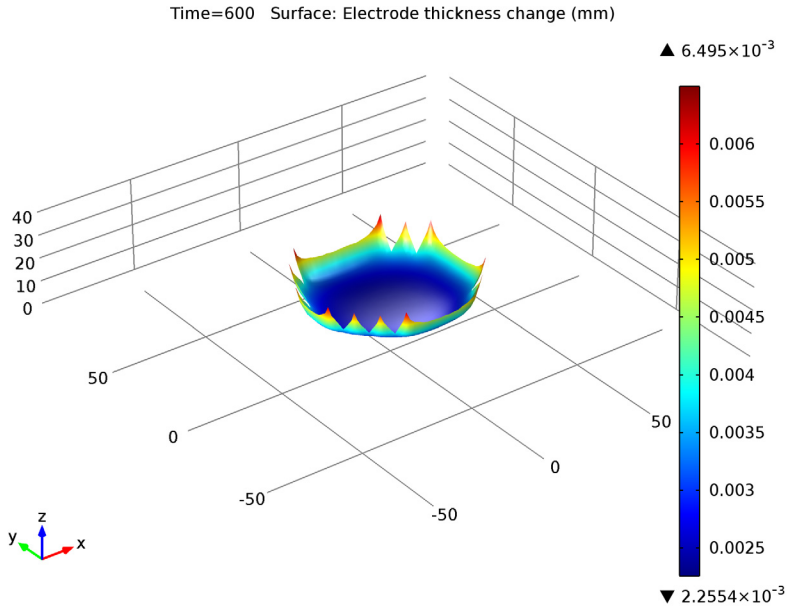

Figure 5: Deposited thickness at the end of the simulation without a current thief. The surface is deformed in the z-direction according to the layer thickness.

Figure 5 shows the resulting electrode thickness change at the end of Study 1. As a result of the higher electrode currents seen in Figure 4, the deposited thickness is non-uniform with higher thickness towards the outer rim of the pattern.

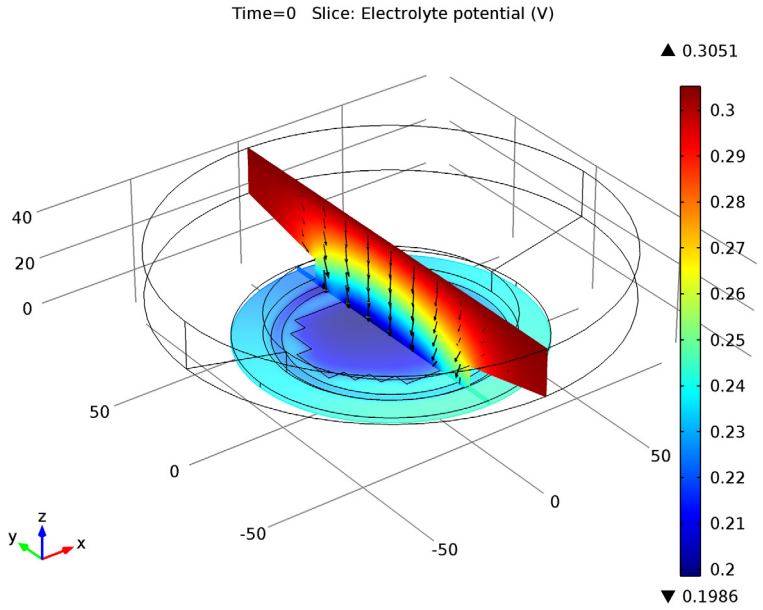

Figure 6: Electrolyte currents and potential at the end of the simulation with a current thief.

Figure 6 shows the electrolyte potential at the end of Study 2. Compared to Figure 2 the potential distribution is more uniform on the patterned surface.

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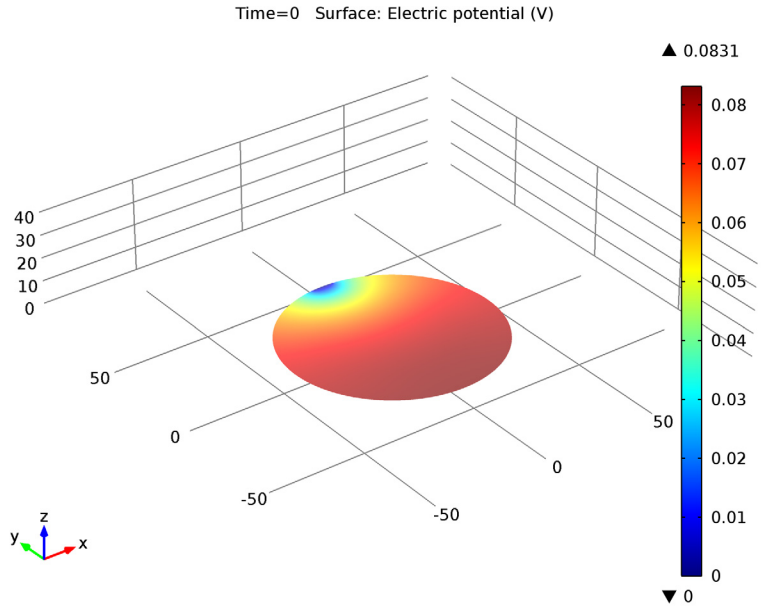

Figure 7: Electric potential in the copper layer at the end of the simulation with a current thief.

Figure 7 shows the electric potential distribution at the end of Study 2 when using a current thief. The deposit build-up results in less steeper potential gradients close to the current collector. The potential over the patterned area is still fairly uniform.

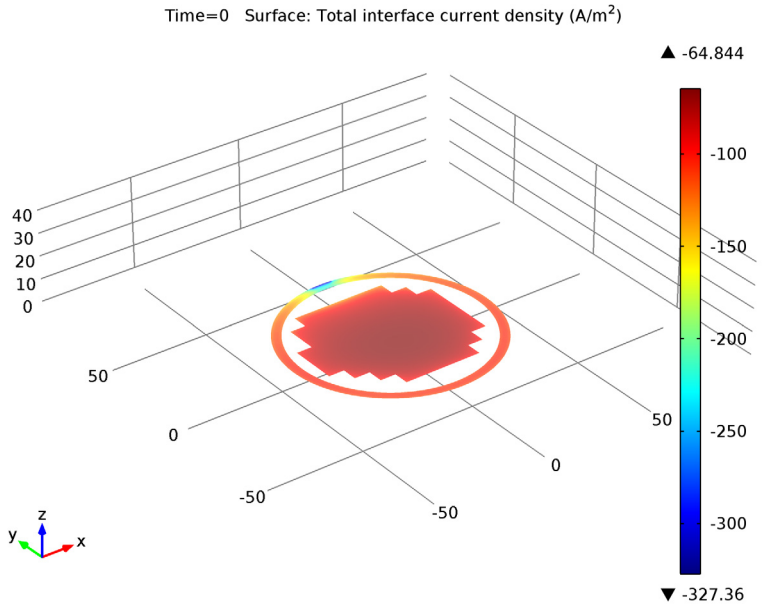

Figure 8: Electrode reaction current density at the end of the simulation with a current thief.

Figure 8 shows the electrode current distribution at the end of Study 2. Compared Figure 4 to the electrode currents are more uniform on the patterned wafer. It can also be seen that the electrode currents densities are higher on the current thief than on the pattern, with a maximum at the current collector.

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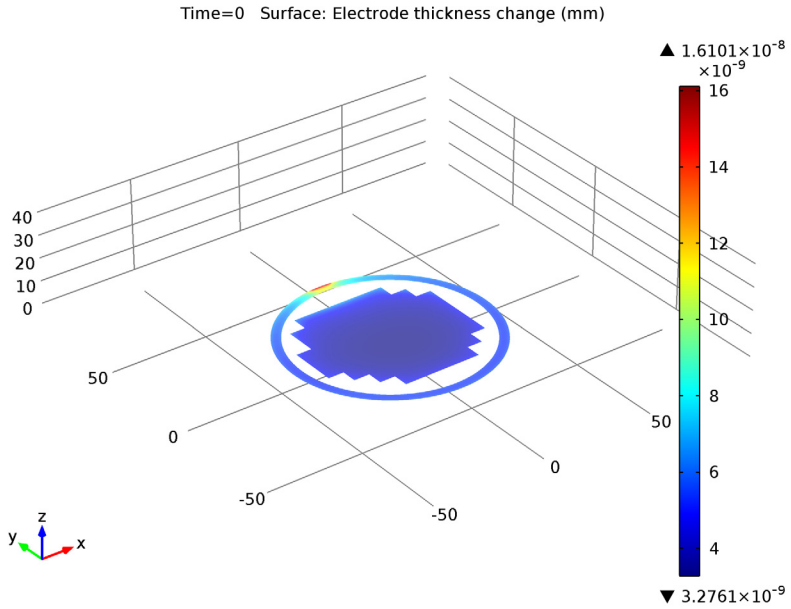

Figure 9: Deposited thickness at the end of the simulation without a current thief.

Figure 9 shows the deposited layer thickness at the end of Study 2. Compared to Figure 5 the deposited thickness is more uniform, all though the deposited thickness still is significantly higher in the corners of the pattern than in the central parts.

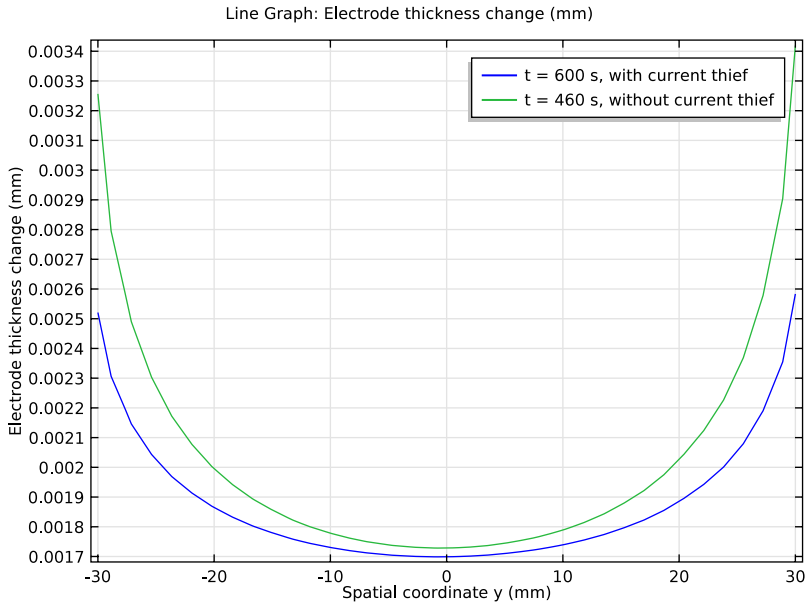

Figure 10: Comparison of deposited thicknesses, with current thief at t = 600 s, without current thief at t = 460 s.

Finally, the deposit uniformity effect of using a current thief is shown in Figure 10, where the deposit profile along the *y*-axis is compared for the two studies. The current thief results in a more uniform deposit, but also results in a longer deposition time due to the lower electrode current on the wafer pattern.

Reference

1. M. Purcar, B. Van den Bossche , L. Bortels, J. Deconninck, and G. Nelissen, "Three-Dimensional Current Density Distribution Simulations for a Resistive Patterned Wafer," *J. Electrochem.Soc.*, vol. 151, no. 9, pp. D78–D86, 2004.

Model Library path: `Electrodeposition_Module/Tutorial_Models/resistive_wafer`

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Modeling Instructions

MODEL WIZARD

1 Go to the **Model Wizard** window.

2 Click **Next**.

3 In the **Add physics** tree, select **Electrochemistry>Electrode, Shell (els)**.

4 Click **Add Selected**.

5 Find the **Dependent variables** subsection. In the **Electric potential** edit field, type `phis_wafer`.

6 In the **Add physics** tree, select **Electrochemistry>Electrodeposition, Deformed Geometry>Electrodeposition, Secondary (edsec)**.

7 Click **Add Selected**.

8 Click **Next**.

9 Find the **Studies** subsection. In the tree, select **Preset Studies for Selected Physics>Time Dependent with Initialization, Fixed Geometry**.

10 Click **Finish**.

GEOMETRY 1

This model utilizes a pre-made geometry file for which the length unit is millimeters.

1 In the **Model Builder** window, under **Model 1** click **Geometry 1**.

2 In the **Geometry** settings window, locate the **Units** section.

3 From the **Length unit** list, choose **mm**.

Import 1

1 Right-click **Model 1>Geometry 1** and choose **Import**.

2 In the **Import** settings window, locate the **Import** section.

3 Click the **Browse** button.

4 Browse to the model's Model Library folder and double-click the file `resistive_wafer.mphbin`.

5 Click the **Import** button.

GLOBAL DEFINITIONS

Load the parameter values for this model from a text file.

Parameters

1 In the **Model Builder** window, right-click **Global Definitions** and choose **Parameters**.

2 In the **Parameters** settings window, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Model Library folder and double-click the file `resistive_wafer_parameters.txt`.

DEFINITIONS

Make selections of the geometry to be used later on when setting up the physics.

Explicit 1

1 In the **Model Builder** window, under **Model 1** right-click **Definitions** and choose **Selections>Explicit**.

2 In the **Explicit** settings window, locate the **Input Entities** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundaries 12–14 only.

5 Right-click **Model 1>Definitions>Explicit 1** and choose **Rename**.

6 Go to the **Rename Explicit** dialog box and type `Wafer surface` in the **New name** edit field.

7 Click **OK**.

Explicit 2

1 Right-click **Definitions** and choose **Selections>Explicit**.

2 In the **Explicit** settings window, locate the **Input Entities** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 14 only.

In the first study, use the patterned part of the wafer surface as the cathode. Later, you will add the outer ring as current thief.

5 Right-click **Model 1>Definitions>Explicit 2** and choose **Rename**.

6 Go to the **Rename Explicit** dialog box and type `Cathode` in the **New name** edit field.

7 Click **OK**.

Explicit 3

1 Right-click **Definitions** and choose **Selections>Explicit**.

2 In the **Explicit** settings window, locate the **Input Entities** section.

3 From the **Geometric entity level** list, choose **Boundary**.

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4 Select Boundary 5 only.

5 Right-click **Model 1>Definitions>Explicit 3** and choose **Rename**.

6 Go to the **Rename Explicit** dialog box and type `Anode` in the **New name** edit field.

7 Click **OK**.

ELECTRODEPOSITION, SECONDARY

Electrolyte 1

Now start setting up the physics, beginning with the current distribution in the electrolyte.

1 In the **Electrolyte** settings window, locate the **Electrolyte** section.

2 From the σ_l list, choose **User defined**. In the associated edit field, type `sigma`.

Electrolyte Current 1

In this model you do not model the anode reactions explicitly. Use a total current condition instead.

1 In the **Model Builder** window, right-click **Electrodeposition, Secondary** and choose **Electrolyte>Electrolyte Current**.

2 In the **Electrolyte Current** settings window, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Anode**.

4 Locate the **Electrolyte Current** section. In the $I_{l,total}$ edit field, type `I_cell`.

External Depositing Electrode 1

Use the External Depositing Electrode to model the wafer electrode reaction and the deposit growth.

1 Right-click **Electrodeposition, Secondary** and choose **External Depositing Electrode**.

2 In the **External Depositing Electrode** settings window, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Cathode**.

The electric potential of the External Depositing Electrode is equal to phis_wafer, which is the potential solved for by the Electrode, Shell interface (which you set up shortly).

4 Locate the **Boundary Condition** section. In the $\phi_{s,ext}$ edit field, type `phis_wafer`.

Surface Properties 1

1 In the **Model Builder** window, expand the **External Depositing Electrode 1** node, then click **Surface Properties 1**.

2 In the **Surface Properties** settings window, locate the **Deposited Species** section.

3 In the M_{cdep} edit field, type `M`.

4 In the ρ_{cdep} edit field, type `rho`.

Electrode Reaction 1

1 In the **Model Builder** window, under **Model 1>Electrodeposition, Secondary>External Depositing Electrode 1** click **Electrode Reaction 1**.

2 In the **Electrode Reaction** settings window, locate the **Model Inputs** section.

3 In the T edit field, type `T`.

4 Locate the **Equilibrium Potential** section. In the $E_{\text{eq},ref}$ edit field, type `Eeq_cathode`.

5 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Butler-Volmer**.

6 In the i_0 edit field, type `i0_cathode`.

7 In the α_a edit field, type `alpha_a`.

8 In the α_c edit field, type `alpha_c`.

9 Locate the **Stoichiometric Coefficients** section. In the n_m edit field, type `2`.

10 In the ν_{cdep} edit field, type `1`.

Initial Values 1

1 In the **Model Builder** window, under **Model 1>Electrodeposition, Secondary** click **Initial Values 1**.

2 In the **Initial Values** settings window, locate the **Initial Values** section.

3 In the *phil* edit field, type `-Eeq_cathode`.

ELECTRODE, SHELL

Now set up the Electrode, Shell interface, which models the electric currents in the thin copper layer on the wafer.

1 In the **Model Builder** window, under **Model 1** click **Electrode, Shell**.

2 In the **Electrode, Shell** settings window, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Wafer surface**.

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Depositing Electrode 1

1 Right-click **Model 1>Electrode, Shell** and choose **Depositing Electrode**.

The Depositing Electrode is coupled to the Electrodeposition, Secondary interface via the thickness of the electrode and the electrode currents.

2 In the **Depositing Electrode** settings window, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Cathode**.

4 Locate the **Depositing Electrode** section. In the s_0 edit field, type `s_init`.

5 From the Δs list, choose **Total electrode thickness change (edsec/ede1/sp1)**.

6 From the σ list, choose **User defined**. In the associated edit field, type `w`.

7 Locate the **Electrode Current Density** section. From the i_n list, choose **Local current density (edsec/ede1/er1)**.

Electrode 1

1 In the **Model Builder** window, under **Model 1>Electrode, Shell** click **Electrode 1**.

2 In the **Electrode** settings window, locate the **Electrode** section.

3 In the s edit field, type `s_init`.

4 From the σ list, choose **User defined**. In the associated edit field, type `w`.

Ground 1

1 In the **Model Builder** window, right-click **Electrode, Shell** and choose **Ground**.

2 Select Edge 34 only.

MESH 1

Edit the default mesh to make the mesh finer in the domain and on the wafer surface.

Size

1 In the **Model Builder** window, under **Model 1** right-click **Mesh 1** and choose **Edit Physics-Induced Sequence**.

2 In the **Model Builder** window, under **Model 1>Mesh 1** click **Size**.

3 In the **Size** settings window, locate the **Element Size** section.

4 From the **Predefined** list, choose **Finer**.

Size 1

1 In the **Model Builder** window, under **Model 1>Mesh 1** right-click **Free Tetrahedral 1** and choose **Size**.

2 In the **Size** settings window, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 From the **Selection** list, choose **Wafer surface**.

5 Locate the **Element Size** section. Click the **Custom** button.

6 Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.

7 In the associated edit field, type `2[mm]`.

8 In the **Model Builder** window, right-click **Mesh 1** and choose **Build All**.

STUDY 1

The problem is now ready for solving. Modify the default solver sequence to use fully coupled solvers.

Solver 1

1 In the **Model Builder** window, right-click **Study 1** and choose **Show Default Solver**.

2 Expand the **Solver 1** node.

3 In the **Model Builder** window, expand the **Study 1>Solver Configurations>Solver 1>Stationary Solver 1** node.

4 Right-click **Study 1>Solver Configurations>Solver 1>Stationary Solver 1** and choose **Fully Coupled**.

5 In the **Model Builder** window, expand the **Study 1>Solver Configurations>Solver 1>Time-Dependent Solver 1** node.

Step 2: Time Dependent, Fixed Geometry

1 Right-click **Study 1>Solver Configurations>Solver 1>Time-Dependent Solver 1** and choose **Fully Coupled**.

2 In the **Model Builder** window, under **Study 1** click **Step 2: Time Dependent, Fixed Geometry**.

3 In the **Time Dependent, Fixed Geometry** settings window, locate the **Study Settings** section.

4 In the **Times** edit field, type `range(0,20,600)`.

5 In the **Model Builder** window, click **Study 1**.

6 In the **Study** settings window, locate the **Study Settings** section.

7 Clear the **Generate default plots** check box.

8 Click the **Compute** button.

RESULTS

Reproduce Figure 2 through Figure 5 by following the instructions below.

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3D Plot Group 1

1 In the **Model Builder** window, right-click **Results** and choose **3D Plot Group**.

2 Right-click **3D Plot Group 1** and choose **Slice**.

3 In the **Slice** settings window, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Electrodeposition, Secondary>Electrolyte potential (phil)**.

4 Locate the **Plane Data** section. In the **Planes** edit field, type 1.

5 Click the **Plot** button.

6 In the **Model Builder** window, right-click **3D Plot Group 1** and choose **Arrow Volume**.

7 In the **Arrow Volume** settings window, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Electrodeposition, Secondary>Electrolyte current density vector (Spatial) (edsec.Ilx,...,edsec.Ilz)**.

8 Click to expand the **Title** section. From the **Title type** list, choose **None**.

9 Locate the **Arrow Positioning** section. Find the **x grid points** subsection. In the **Points** edit field, type 1.

10 Find the **y grid points** subsection. In the **Points** edit field, type 13.

11 Locate the **Coloring and Style** section. From the **Color** list, choose **Black**.

12 Right-click **3D Plot Group 1** and choose **Slice**.

13 In the **Slice** settings window, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Electrolyte potential (phil)**.

14 Click to expand the **Title** section. From the **Title type** list, choose **None**.

15 Locate the **Plane Data** section. From the **Plane** list, choose **xy-planes**.

16 From the **Entry method** list, choose **Coordinates**.

17 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Slice 1**.

18 Click the **Plot** button.

19 Click the **Zoom Extents** button on the Graphics toolbar.

Data Sets

1 In the **Model Builder** window, expand the **Results>Data Sets** node.

2 Right-click **Solution 1** and choose **Duplicate**.

3 Right-click **Results>Data Sets>Solution 3** and choose **Add Selection**.

4 In the **Selection** settings window, locate the **Geometric Entity Selection** section.

5 From the **Geometric entity level** list, choose **Boundary**.

6 From the **Selection** list, choose **Wafer surface**.

3D Plot Group 2

1 In the **Model Builder** window, right-click **Results** and choose **3D Plot Group**.

2 In the **3D Plot Group** settings window, locate the **Plot Settings** section.

3 Clear the **Plot data set edges** check box.

4 Right-click **Results>3D Plot Group 2** and choose **Surface**.

5 Right-click **Results>3D Plot Group 2>Surface 1** and choose **Plot**.

6 Click the **Zoom Extents** button on the Graphics toolbar.

3D Plot Group 3

1 Right-click **3D Plot Group 2** and choose **Duplicate**.

2 In the **Model Builder** window, expand the **3D Plot Group 3** node, then click **Surface 1**.

3 In the **Surface** settings window, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Electrodeposition, Secondary>Electrode kinetics>Total interface current density (edsec.itot)**.

4 Click the **Plot** button.

5 Click the **Zoom Extents** button on the Graphics toolbar.

3D Plot Group 4

1 In the **Model Builder** window, right-click **3D Plot Group 3** and choose **Duplicate**.

2 In the **Model Builder** window, expand the **3D Plot Group 4** node, then click **Surface 1**.

3 In the **Surface** settings window, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Electrode, Shell>Material properties>Electrode thickness change (els.deltas)**.

4 Click the **Plot** button.

5 Right-click **Results>3D Plot Group 4>Surface 1** and choose **Deformation**.

6 In the **Deformation** settings window, locate the **Expression** section.

7 In the **z component** edit field, type `els.deltas`.

8 Locate the **Scale** section. Select the **Scale factor** check box.

9 In the associated edit field, type `5000`.

10 Click the **Plot** button.

11 Click the **Zoom Extents** button on the Graphics toolbar.

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STUDY 1

Solver 1

Now modify the problem to use the ring on the wafer as current thief. First store the current solution to be able to compare the results later.

1 In the **Model Builder** window, under **Study 1>Solver Configurations** right-click **Solver 1** and choose **Solution>Copy**.

DEFINITIONS

Cathode

1 In the **Model Builder** window, under **Model 1>Definitions** click **Cathode**.

2 Select Boundaries 12 and 14 only.

STUDY 1

In the **Model Builder** window, right-click **Study 1** and choose **Compute**.

RESULTS

Data Sets

The following creates a plot for comparing the deposited thicknesses between the two studies.

1 In the **Model Builder** window, under **Results** right-click **Data Sets** and choose **Cut Line 3D**.

2 In the **Cut Line 3D** settings window, locate the **Line Data** section.

3 In row **Point 1**, set **y** to `-30`.

4 In row **Point 2**, set **y** to `30`.

5 Select the **Snap to closest boundary** check box.

6 Right-click **Results>Data Sets>Cut Line 3D 1** and choose **Duplicate**.

7 In the **Cut Line 3D** settings window, locate the **Data** section.

8 From the **Data set** list, choose **Solution 4**.

1D Plot Group 5

1 In the **Model Builder** window, right-click **Results** and choose **1D Plot Group**.

2 In the **1D Plot Group** settings window, locate the **Data** section.

3 From the **Data set** list, choose **Cut Line 3D 1**.

4 Right-click **Results>1D Plot Group 5** and choose **Line Graph**.

5 In the **Line Graph** settings window, locate the **Data** section.

6 From the **Data set** list, choose **Cut Line 3D 1**.

7 From the **Time selection** list, choose **From list**.

8 In the **Times** list, select **600**.

9 Locate the **y-Axis Data** section. In the **Expression** edit field, type `els.deltas`.

10 Click to expand the **Legends** section. Select the **Show legends** check box.

11 From the **Legends** list, choose **Manual**.

12 In the table, enter the following settings:

Legends
`t = 600 s, with current thief`

13 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

14 In the **Expression** edit field, type `y`.

15 Click the **Plot** button.

16 Right-click **Results>1D Plot Group 5>Line Graph 1** and choose **Duplicate**.

17 In the **Line Graph** settings window, locate the **Data** section.

18 From the **Data set** list, choose **Cut Line 3D 2**.

19 In the **Times** list, select **460**.

20 Click to expand the **Title** section. From the **Title type** list, choose **None**.

21 Locate the **Legends** section. In the table, enter the following settings:

Legends
`t = 460 s, without current thief`

22 Click the **Plot** button.

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