

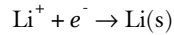


# Lithium Plating with Deformation

## *Introduction*

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In a lithium metal battery, lithium metal is deposited during charging on the negative electrode according to



Due to mass transport and ohmic effects in the electrolyte, small initial protrusions on the metal surface will be subjected to accelerated growth during charging, which in worst cases may lead to the formation of dendrites, and in turn result in internal short circuits and thermal runaway scenarios.

This example explores the method of reverse pulse charging for mitigating the formation of dendrites.

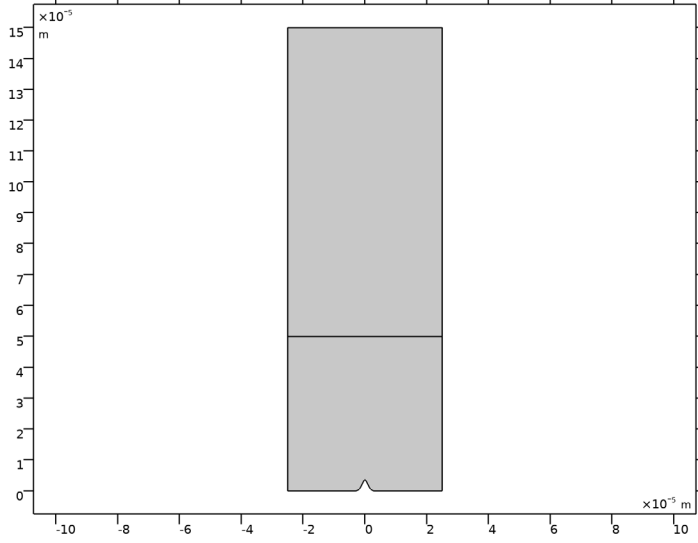
The model uses the Lithium-Ion Battery, Deformed Geometry model wizard entry that adds a Lithium-Ion Battery interface along with Deformed Geometry formulation. Additionally, an Events interface is used to set up the forward and reverse current duty cycles.

## *Model Definition*

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[Figure 1](#) shows the model geometry of the lithium-ion battery that consists of two domains (positive porous electrode and separator). The negative lithium metal electrode surface is located at  $y = 0$  mm, with a small protrusion with a height of 40 mm, centered

around  $x = 0$ . The materials considered are NMC 622 and LiPF6 3:7 EC:EMC for the positive electrode and electrolyte, respectively.



*Figure 1: Model geometry.*

In the first part of the tutorial, a forward current plating model is set up to simulate how a small protrusion of lithium grows during the plating process. A constant electrode current density of 1 C is applied on the top boundary of the positive porous electrode, and the resulting growth velocity along the negative lithium electrode surface is used as a boundary condition for the deformed geometry (ALE) time-dependent simulation.

In the second part of the tutorial, a forward and reverse current duty cycle is set up to examine how the protrusion of lithium is attenuated depending on the length of the reverse pulse. The current density for the reverse pulse  $i_{\text{rev}}$  on the top boundary of the positive porous electrode is set to -15 C. Denoting the forward duty cycle (the relative time spent in forward mode) as  $t_{\text{fwd}}$  (dimensionless), the forward pulse current density  $i_{\text{fwd}}$  can be calculated as

$$i_{\text{fwd}} = \frac{(i_{\text{avg}} - (1 - t_{\text{fwd}})i_{\text{rev}})}{t_{\text{fwd}}} \quad (1)$$

The total simulated plating time is 0.75 h. The cycle time for a single forward and reverse duty cycle is 180 s. The Events interface is used to set up an Event Sequence consisting of the forward and reverse current duty cycles. The applied electrode current density on the top boundary of the positive porous electrode is appropriately calculated based on the

forward and reverse states and respective current densities. A parametric sweep is set up in the second part of the tutorial to simulate different lengths of the forward plating duty cycle  $t_{\text{fwd}}$  and examine the lithium electrode surface evolution during the forward and reverse current duty cycle.

This model uses linear elements for all the dependent variables in the Lithium-Ion Battery interface for faster computation times.

### Results and Discussion

Figure 2 shows the lithium electrode surface profile evolution during the forward plating cycle. The initial protrusion grows in size and will result in an uneven surface.

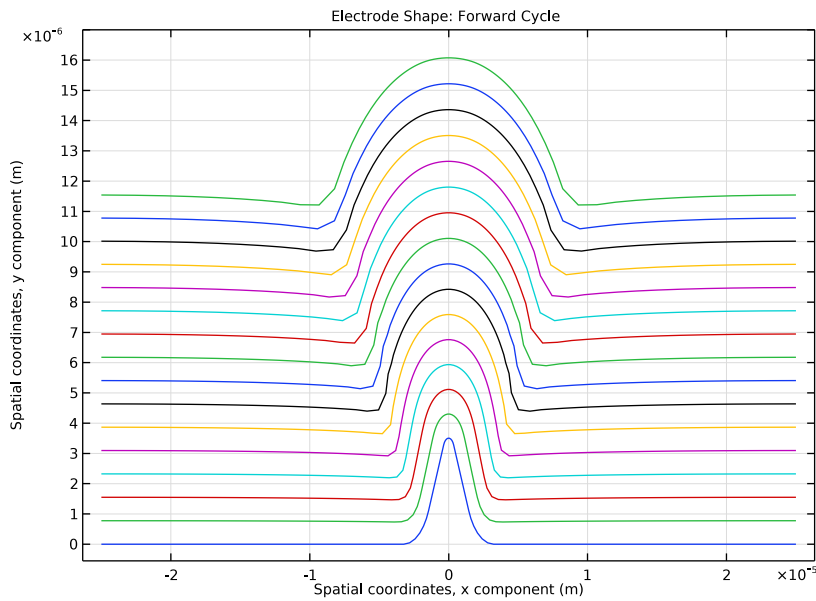


Figure 2: Electrode shape evolution for forward current duty cycle ( $t_{\text{fwd}} = 1$ ).

Figure 3 shows the lithium electrode surface profile evolution during the forward and reverse current duty cycle, for  $t_{\text{fwd}} = 0.85$ . The initial protrusion is now attenuated as the plating proceeds.

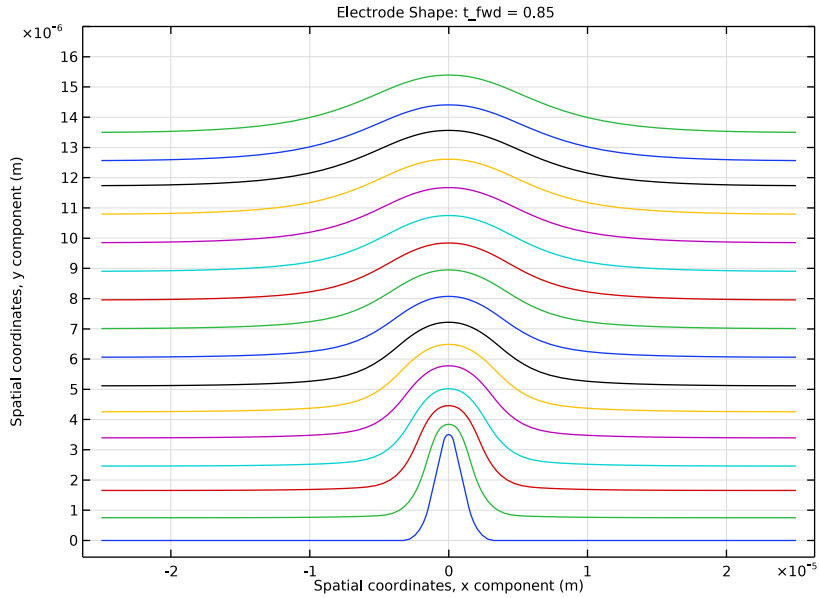


Figure 3: Electrode shape evolution for forward and reverse current duty cycle ( $t_{\text{fwd}} = 0.85$ ).

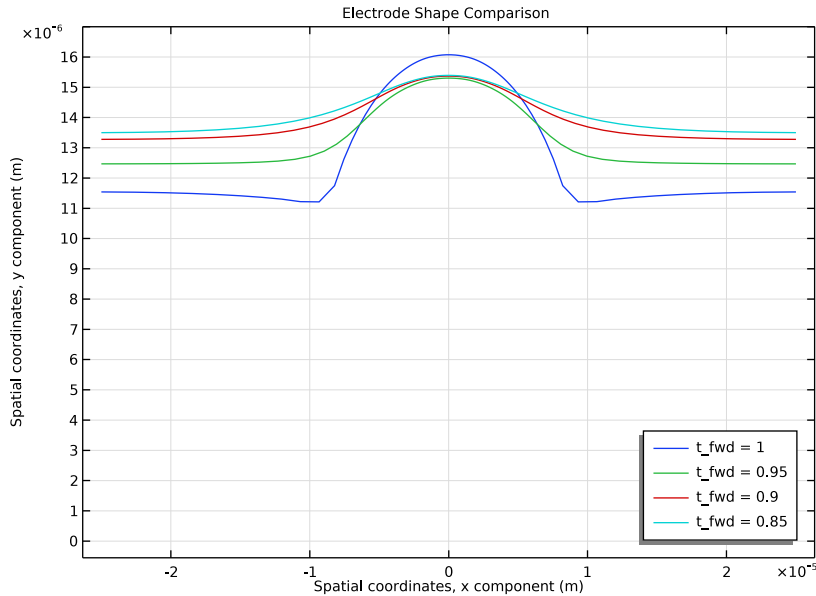


Figure 4: Comparison of final electrode surface profiles for different values of  $t_{\text{fwd}}$ .

Finally, Figure 4 shows a comparison of the lithium electrode surface profiles at the last time step for different values of the forward plating duty cycle  $t_{\text{fwd}}$ .

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**Application Library path:** Battery\_Design\_Module/Batteries,\_Lithium-Ion/  
li\_plating\_with\_deformation

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### *Modeling Instructions*

This tutorial consists of two parts. In the first part you will set up a forward current plating model to simulate how a small protrusion of lithium grows during the plating process.




In the second part you will set up a forward and reverse current duty cycle, and examine how the protrusion of lithium is attenuated depending on the length of the reverse pulse.

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

## NEW

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


## MODEL WIZARD

- 1 In the **Model Wizard** window, click  **2D**.
- 2 In the **Select Physics** tree, select **Electrochemistry>Batteries>Lithium-Ion Battery, Deformed Geometry**.
- 3 Click **Add**.
- 4 Click  **Study**.
- 5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Time Dependent with Initialization**.
- 6 Click  **Done**.

## GLOBAL DEFINITIONS

### *Parameters 1*


Load the model parameters from a text file.

- 1 In the **Model Builder** window, under **Global Definitions** click **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 `li_plating_with_deformation_parameters.txt`.

## GEOMETRY 1

Set up the geometry that consists of two domains (positive porous electrode and separator). The negative lithium electrode surface is located at  $y = 0$  mm, with a small protrusion with a height of 40 mm, centered around  $x = 0$ .


### *Polygon 1 (pol1)*

- 1 In the **Geometry** toolbar, click  **Polygon**.
- 2 In the **Settings** window for **Polygon**, locate the **Coordinates** section.
- 3 In the table, enter the following settings:

<b>x (m)</b>	<b>y (m)</b>
0	H_prot
-W_prot/2	0
-W_cell/2	0


<b>x (m)</b>	<b>y (m)</b>
-W_cell/2	H_sep
W_cell/2	H_sep
W_cell/2	0
W_prot/2	0

#### *Rectangle 1 (r1)*



- 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 W\_cell.
- 4 In the **Height** text field, type H\_pos.
- 5 Locate the **Position** section. In the **x** text field, type -W\_cell/2.
- 6 In the **y** text field, type H\_sep.

#### *Fillet 1 (fil1)*


Round the corners by adding fillets.

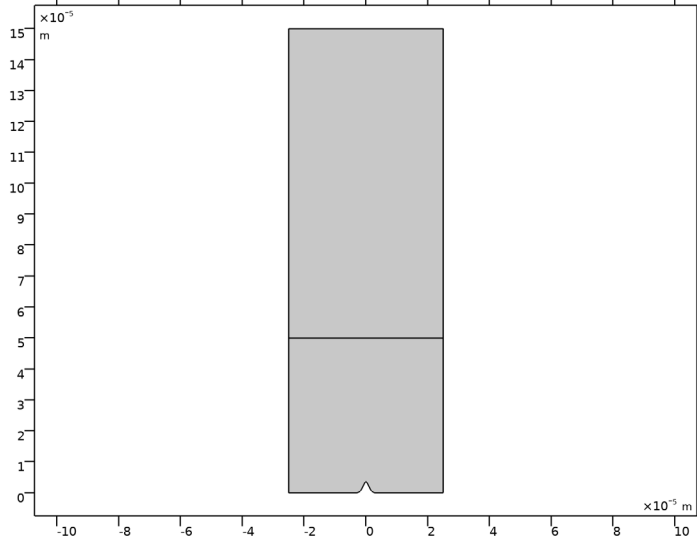
- 1 In the **Geometry** toolbar, click  **Fillet**.
- 2 On the object **poll**, select Point 4 only.
- 3 In the **Settings** window for **Fillet**, locate the **Radius** section.
- 4 In the **Radius** text field, type H\_prot/10.

#### *Fillet 2 (fil2)*

- 1 In the **Geometry** toolbar, click  **Fillet**.
- 2 On the object **fill**, select Points 3 and 6 only.
- 3 In the **Settings** window for **Fillet**, locate the **Radius** section.
- 4 In the **Radius** text field, type W\_prot/2.
- 5 In the **Geometry** toolbar, click  **Build All**.




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



#### ADD MATERIAL

The model has a lithium metal negative electrode, a NMC 622 positive electrode, and a LiPF6 3:7 EC:EMC electrolyte. Import the materials from the Battery Material Library.

- 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 **Battery>Electrolytes>LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery)**.
- 4 Click **Add to Component** in the window toolbar.

#### ADD MATERIAL


- 1 Go to the **Add Material** window.
- 2 In the tree, select **Battery>Electrodes>NMC 622, LiNi0.6Mn0.2Co0.2O2 (Positive, Li-ion Battery)**.
- 3 Click **Add to Component** in the window toolbar.

#### MATERIALS

*NMC 622, LiNi0.6Mn0.2Co0.2O2 (Positive, Li-ion Battery) (mat2)*


Select Domain 2 only.

## ADD MATERIAL

- 1 Go to the **Add Material** window.
- 2 In the tree, select **Battery>Electrodes>Lithium Metal, Li (Negative, Li-ion Battery)**.
- 3 Click **Add to Component** in the window toolbar.
- 4 In the **Home** toolbar, click  **Add Material** to close the **Add Material** window.

## MATERIALS

*Lithium Metal, Li (Negative, Li-ion Battery) (mat3)*

- 1 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.
- 2 From the **Geometric entity level** list, choose **Boundary**.  
Use a box selection to select all the (lower) boundaries pertaining to the lithium electrode surface, including the protrusion.
- 3 Select Boundaries 2, 6–8, and 11–13 only.
- 4 Click  **Create Selection**.  
By creating a selection in this way you can conveniently select the same set of boundaries again later on.
- 5 In the **Create Selection** dialog box, type **Lithium Electrode Surface** in the **Selection name** text field.
- 6 Click **OK**.


## LITHIUM-ION BATTERY (LIION)

Now start setting up the forward cycle lithium-ion battery model.

*Separator 1*

- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Lithium-Ion Battery (liion)** and choose **Separator**.
- 2 Select Domain 1 only.

*Porous Electrode 1*


- 1 In the **Physics** toolbar, click  **Domains** and choose **Porous Electrode**.
- 2 Select Domain 2 only.
- 3 In the **Settings** window for **Porous Electrode**, locate the **Electrolyte Properties** section.
- 4 From the **Electrolyte material** list, choose **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat1)**.

- 5 Locate the **Electrode Properties** section. From the  $\sigma_s$  list, choose **User defined**. In the associated text field, type `sigmas_pos`.
- 6 Locate the **Porous Matrix Properties** section. In the  $\varepsilon_s$  text field, type `epss_pos`.

#### *Particle Intercalation I*

- 1 In the **Model Builder** window, click **Particle Intercalation I**.
- 2 In the **Settings** window for **Particle Intercalation**, locate the **Species Settings** section.
- 3 In the  $c_{s,init}$  text field, type `cs_init_pos`.
- 4 Locate the **Particle Transport Properties** section. In the  $r_p$  text field, type `rp_pos`.

#### *Electrode Surface I*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Electrode Surface**.
- 2 In the **Settings** window for **Electrode Surface**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Lithium Electrode Surface**.
- 4 Click to expand the **Dissolving-Depositing Species** section. Use a **Dissolving-Depositing Species** to define the growth velocity of the lithium electrode surface.
- 5 Click **+ Add**.
- 6 In the table, enter the following settings:

Species	Density (kg/m <sup>3</sup> )	Molar mass (kg/mol)
Li	rho_Li	M_Li


- 7 Clear the **Solve for surface concentration variables** check box.

#### *Electrode Reaction I*

- 1 In the **Model Builder** window, click **Electrode Reaction I**.
- 2 In the **Settings** window for **Electrode Reaction**, locate the **Stoichiometric Coefficients** section.
- 3 In the **Stoichiometric coefficients for dissolving-depositing species:** table, enter the following settings:

Species	Stoichiometric coefficient (I)
Li	1

#### *Electrode Current: Forward Cycle*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Electrode Current**.
- 2 In the **Settings** window for **Electrode Current**, type **Electrode Current: Forward Cycle** in the **Label** text field.

- 3 Select Boundary 5 only.
- 4 Locate the **Electrode Current** section. From the list, choose **Average current density**.
- 5 In the  $i_{s,average}$  text field, type `i_app_fwd`.

## DEFORMED GEOMETRY

Select the separator domain as the **Deforming Domain**.

### *Deforming Domain 1*

- 1 In the **Model Builder** window, expand the **Deformed Geometry** node, then click **Deforming Domain 1**.
- 2 Select Domain 1 only.

## MULTIPHYSICS

### *Nondeforming Boundary 1 (ndbdg1)*

Set zero normal displacement at the vertical nondeforming boundaries.

- 1 In the **Model Builder** window, expand the **Multiphysics** node, then click **Nondeforming Boundary 1 (ndbdg1)**.
- 2 In the **Settings** window for **Nondeforming Boundary**, locate the **Nondeforming Boundary** section.
- 3 From the **Boundary condition** list, choose **Zero normal displacement**.

## LITHIUM-ION BATTERY (LIION)

Set linear elements for all the dependent variables in the **Lithium-Ion Battery** interface to speed up computation time.

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Lithium-Ion Battery (liion)**.
- 2 In the **Settings** window for **Lithium-Ion Battery**, click to expand the **Discretization** section.
- 3 From the **Electrolyte potential** list, choose **Linear**.
- 4 From the **Electrolyte salt concentration** list, choose **Linear**.
- 5 From the **Electric potential** list, choose **Linear**.

## MESH 1

Modify the mesh as follows to get more mesh elements along the lithium electrode surface.


### *Free Triangular 1*

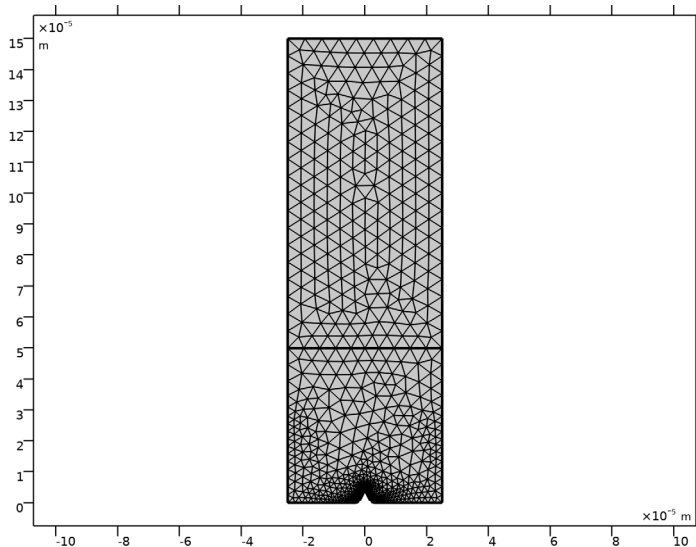
In the **Mesh** toolbar, click  **Free Triangular**.

### Size 1

- 1 Right-click **Free Triangular 1** and choose **Size**.
- 2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Boundary**.
- 4 From the **Selection** list, choose **Lithium Electrode Surface**.
- 5 Locate the **Element Size** section. From the **Predefined** list, choose **Finer**.
- 6 Click the **Custom** button.
- 7 Locate the **Element Size Parameters** section. Select the **Maximum element growth rate** check box.
- 8 In the associated text field, type 1.1.

### Size

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Size**.
- 2 In the **Settings** window for **Size**, locate the **Element Size** section.
- 3 From the **Predefined** list, choose **Finer**.
- 4 Click  **Build All**.




### STUDY: FORWARD CYCLE

The forward cycle problem is now ready for solving. Update the time unit and output times before solving.

- 1 In the **Model Builder** window, click **Study 1**.
- 2 In the **Settings** window for **Study**, type Study: Forward Cycle in the **Label** text field.


#### *Step 2: Time Dependent*

- 1 In the **Model Builder** window, expand the **Study: Forward Cycle** node, then click **Step 2: Time Dependent**.
- 2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
- 3 From the **Time unit** list, choose **h**.
- 4 In the **Output times** text field, type  $\text{range}(0, 0.05/C\_rate\_avg, 0.75/C\_rate\_avg)$ .
- 5 In the **Home** toolbar, click  **Compute**.

## **RESULTS**

Create a line plot for the shape of the lithium electrode surface at different times during the forward cycle (Figure 2) as follows.

#### *Electrode Shape: Forward Cycle*

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Electrode Shape: Forward Cycle in the **Label** text field.
- 3 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.
- 4 In the **Title** text area, type Electrode Shape: Forward Cycle.

#### *Line Graph 1*

- 1 Right-click **Electrode Shape: Forward Cycle** and choose **Line Graph**.
- 2 In the **Settings** window for **Line Graph**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Lithium Electrode Surface**.
- 4 Locate the **y-Axis Data** section. In the **Expression** text field, type  $y$ .
- 5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
- 6 In the **Expression** text field, type  $x$ .

#### *Electrode Shape: Forward Cycle*



- 1 In the **Model Builder** window, click **Electrode Shape: Forward Cycle**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Axis** section.
- 3 Select the **Manual axis limits** check box.
- 4 In the **y minimum** text field, type  $-5.5e-7$ .
- 5 In the **y maximum** text field, type  $1.7e-5$ .

6 In the **Electrode Shape: Forward Cycle** toolbar, click  **Plot**.

## ADD PHYSICS

You have now completed the first part of this tutorial where the applied current included only the forward current duty cycle. We will now set up the second part of the tutorial where the applied current includes both the forward and reverse current duty cycles.

Start by adding an **Events** interface and set up an **Event Sequence** consisting of the forward and reverse current duty cycles.

- 1 In the **Home** toolbar, click  **Add Physics** to open the **Add Physics** window.
- 2 Go to the **Add Physics** window.
- 3 In the tree, select **Mathematics>ODE and DAE Interfaces>Events (ev)**.
- 4 Click **Add to Component 1** in the window toolbar.
- 5 In the **Home** toolbar, click  **Add Physics** to close the **Add Physics** window.

## EVENTS (EV)

### *Event Sequence 1*

- 1 Right-click **Component 1 (comp1)>Events (ev)** and choose **Event Sequence**.
- 2 In the **Settings** window for **Event Sequence**, locate the **Sequence Control** section.
- 3 Select the **Loop** check box.


### *Sequence Member 1*

- 1 In the **Model Builder** window, expand the **Event Sequence 1** node, then click **Sequence Member 1**.
- 2 In the **Settings** window for **Sequence Member**, locate the **Sequence Member** section.
- 3 In the **Discrete state name** text field, type `state_fwd`.
- 4 From the **End condition** list, choose **Duration**.
- 5 In the **Duration** text field, type `T_cycle*t_fwd`.

### *Event Sequence 1*

In the **Model Builder** window, click **Event Sequence 1**.

### *Sequence Member 2*

- 1 In the **Physics** toolbar, click  **Attributes** and choose **Sequence Member**.
- 2 In the **Settings** window for **Sequence Member**, locate the **Sequence Member** section.
- 3 In the **Discrete state name** text field, type `state_rev`.

- 4 From the **End condition** list, choose **Duration**.
- 5 In the **Duration** text field, type  $T_{\text{cycle}}*t_{\text{rev}}$ .

### DEFINITIONS (COMPI)

Next, set up the variable for the applied current density for the forward and reverse cycle and use this variable to set the electrode current for the battery.

#### 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
i_app	state_fwd*i_fwd+ state_rev*i_rev	A/m <sup>2</sup>	Applied current density (forward and reverse cycle)



### LITHIUM-ION BATTERY (LIION)

#### Electrode Current: Forward and Reverse Cycle

- 1 In the **Model Builder** window, right-click **Electrode Current: Forward Cycle** and choose **Duplicate**.
- 2 In the **Settings** window for **Electrode Current**, type Electrode Current: Forward and Reverse Cycle in the **Label** text field.
- 3 Locate the **Electrode Current** section. In the  $i_{s,average}$  text field, type i\_app.

### ADD STUDY

The forward and reverse cycle model is now ready for solving. Use a **Parametric Sweep** to simulate different lengths of the forward plating duty cycle.



- 1 In the **Home** toolbar, click  **Add Study** to open the **Add Study** window.
- 2 Go to the **Add Study** window.
- 3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Lithium-Ion Battery>Time Dependent with Initialization**.
- 4 Click **Add Study** in the window toolbar.
- 5 In the **Home** toolbar, click  **Add Study** to close the **Add Study** window.



## STUDY: FORWARD AND REVERSE CYCLE

- 1 In the **Model Builder** window, click **Study 2**.
- 2 In the **Settings** window for **Study**, type Study: Forward and Reverse Cycle in the **Label** text field.


### *Parametric Sweep*

- 1 In the **Study** toolbar, click  **Parametric Sweep**.
- 2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.
- 3 Click  **Add**.
- 4 In the table, enter the following settings:


Parameter name	Parameter value list	Parameter unit
$\tau_{\text{fwd}}$ (Forward current duty cycle)	0.95 0.9 0.85	

### *Step 1: Current Distribution Initialization*

Also, disable **Electrode Current: Forward Cycle** node in this study.

- 1 In the **Model Builder** window, click **Step 1: Current Distribution Initialization**.
- 2 In the **Settings** window for **Current Distribution Initialization**, locate the **Physics and Variables Selection** section.
- 3 Select the **Modify model configuration for study step** check box.
- 4 In the tree, select **Component 1 (Comp1)>Lithium-Ion Battery (Liion)>Electrode Current: Forward Cycle**.
- 5 Click  **Disable**.


### *Step 2: Time Dependent*

- 1 In the **Model Builder** window, click **Step 2: Time Dependent**.
- 2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
- 3 From the **Time unit** list, choose **h**.
- 4 In the **Output times** text field, type  $\text{range}(0, 0.05/C_{\text{rate\_avg}}, 0.75/C_{\text{rate\_avg}})$ .
- 5 Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** check box.
- 6 In the tree, select **Component 1 (Comp1)>Lithium-Ion Battery (Liion)>Electrode Current: Forward Cycle**.
- 7 Click  **Disable**.

## STUDY: FORWARD CYCLE

Before solving the forward and reverse cycle study, disable appropriate nodes in the forward cycle study for completeness.


### Step 1: Current Distribution Initialization

- 1 In the **Model Builder** window, under **Study: Forward Cycle** click **Step 1: Current Distribution Initialization**.
- 2 In the **Settings** window for **Current Distribution Initialization**, locate the **Physics and Variables Selection** section.
- 3 Select the **Modify model configuration for study step** check box.
- 4 In the tree, select **Component 1 (Comp 1)>Lithium-Ion Battery (Liion)>Electrode Current: Forward and Reverse Cycle**.
- 5 Click  **Disable**.

### Step 2: Time Dependent


- 1 In the **Model Builder** window, click **Step 2: Time Dependent**.
- 2 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.
- 3 In the table, enter the following settings:

Physics interface	Solve for	Equation form
Events (ev)		Automatic (Time dependent)

- 4 Select the **Modify model configuration for study step** check box.
- 5 In the tree, select **Component 1 (Comp 1)>Lithium-Ion Battery (Liion)>Electrode Current: Forward and Reverse Cycle**.
- 6 Click  **Disable**.

## STUDY: FORWARD AND REVERSE CYCLE


Finally, solve the forward and reverse cycle model.

- 1 In the **Model Builder** window, click **Study: Forward and Reverse Cycle**.
- 2 In the **Settings** window for **Study**, locate the **Study Settings** section.
- 3 Clear the **Generate default plots** check box.
- 4 In the **Study** toolbar, click  **Compute**.

## RESULTS


As before, create a line plot for the shape of the lithium electrode surface at different times during the forward and reverse cycle (Figure 3).

### *Electrode Shape: Forward and Reverse Cycle*

- 1 In the **Model Builder** window, right-click **Electrode Shape: Forward Cycle** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, type Electrode Shape: Forward and Reverse Cycle in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study: Forward and Reverse Cycle/ Parametric Solutions 1 (sol5)**.
- 4 From the **Parameter selection (t\_fwd)** list, choose **From list**.
- 5 In the **Parameter values (t\_fwd)** list, select **0.85**.
- 6 Click to expand the **Title** section. In the **Title** text area, type Electrode Shape: t\_fwd = eval(t\_fwd).
- 7 Locate the **Data** section. From the **Time selection** list, choose **Interpolated**.
- 8 In the **Times (h)** text field, type range (0, 0.05, 0.75).
- 9 In the **Electrode Shape: Forward and Reverse Cycle** toolbar, click  **Plot**.

### *Electrode Shape Comparison*

Finally, create a line plot for the shape of the lithium electrode surface at the last time step for different values of the forward plating duty cycle (Figure 4).

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Electrode Shape Comparison in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **None**.
- 4 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.
- 5 In the **Title** text area, type Electrode Shape Comparison.

### *Line Graph 1*


- 1 Right-click **Electrode Shape Comparison** and choose **Line Graph**.
- 2 In the **Settings** window for **Line Graph**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study: Forward Cycle/Solution 1 (sol1)**.
- 4 From the **Time selection** list, choose **Last**.
- 5 Locate the **Selection** section. From the **Selection** list, choose **Lithium Electrode Surface**.

- 6 Locate the **y-Axis Data** section. In the **Expression** text field, type  $y$ .
- 7 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
- 8 In the **Expression** text field, type  $x$ .
- 9 Click to expand the **Legends** section. Select the **Show legends** check box.
- 10 From the **Legends** list, choose **Evaluated**.
- 11 In the **Legend** text field, type  $t\_fwd = 1$ .

#### *Line Graph 2*

- 1 Right-click **Line Graph 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Line Graph**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study: Forward and Reverse Cycle/ Parametric Solutions 1 (sol5)**.
- 4 From the **Time selection** list, choose **Last**.
- 5 Locate the **Legends** section. In the **Legend** text field, type  $t\_fwd = \text{eval}(t\_fwd)$ .

#### *Electrode Shape Comparison*

- 1 In the **Model Builder** window, click **Electrode Shape Comparison**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Axis** section.
- 3 Select the **Manual axis limits** check box.
- 4 In the **y minimum** text field, type  $-5.5e-7$ .
- 5 In the **y maximum** text field, type  $1.7e-5$ .
- 6 Locate the **Legend** section. From the **Position** list, choose **Lower right**.
- 7 In the **Electrode Shape Comparison** toolbar, click  **Plot**.