

Diffusion-Induced Stress in a Lithium-Ion Battery

Introduction

Diffusion-induced stress in lithium-ion battery electrode materials can occur as a result of compositional inhomogeneities during lithium intercalation in the host material particles. These stresses are important since the electrode material can undergo significant volume changes during charging and discharging. The accumulated structural changes can induce electrode failure in the form of particle fracture.

In order to quantify the stress generated in the electrode, the elastic deformation of the material must be related to the intercalation process. Since atomic diffusion in solids is a much slower process than elastic deformation, mechanical equilibrium is established much faster than that of diffusion. Hence, mechanical equilibrium can be treated as a static equilibrium problem ([Ref. 1](#page-11-0) and [Ref. 2](#page-11-1)).

This application models diffusion-induced stress caused by concentration changes within the negative host material electrode particles during discharge and relaxation of a lithiumion battery. The application uses the Lithium-Ion Battery interface. The radial and tangential components of stress (considering spherical particles in the negative electrode) and von Mises stress inside a particle in the negative electrode are analyzed. It is seen that, during discharge, the von Mises stress is 0 at the center and reaches a maximum value at the surface of the particle. Similarly, the time evolution of radial and tangential components of the diffusion-induced strain at surface of particles along the length of the negative electrode is analyzed during discharge and relaxation. During de-intercalation of lithium ions from the negative electrode particles (discharge), the diffusion-induced surface strain decreases with time. Finally, the behavior and time evolution of the total elastic strain energy density stored in the negative electrode material particles is analyzed. Note that this quantity provides the driving force for particle fracture.

Model Definition

The model is set up for a graphite/LMO battery cell. The materials are available from the Battery Material Library and mainly default settings are selected. The model domains consist of:

- Negative porous electrode: Graphite (MCMB $Li_xC₆$) active material and electronic conductor.
- **•** Separator.
- Positive porous electrode: LMO (LiMn₂O₄) active material, electronic conductor, and filler.
- Electrolyte: 1.0 M LiPF₆ in EC:DEC (1:1 by weight).

This battery cell assembly gives a cell voltage around 4 V, depending on the state-of-charge (SOC) of the cell.

The model is set up using the Lithium-Ion Battery interface. The interface accounts for the following:

- electronic conduction in the electrodes,
- ionic charge transport in the electrodes and electrolyte/separator,
- **•** material transport in the electrolyte, allowing for the introduction of the effects of concentration on ionic conductivity and concentration overpotential,
- **•** material transport within the spherical particles that form the electrodes, and
- **•** Butler-Volmer electrode kinetics using experimentally measured discharge curves for the equilibrium potential.

Additionally, the model analyses diffusion-induced stress and strain generated in the negative electrode particles. Assuming the electrode particles to be isotropic linear elastic solids, analytical expressions are calculated at the Particle Intercalation node of the Porous Electrode feature, for several quantities such as stress, hydrostatic stress, von Mises stress, strain, total elastic strain energy density, etc. These expressions require the relative change in volume of the graphite electrode material, which is typically a function of concentration (i.e., state-of-charge) in the particle. For example, graphite material has a volumetric expansion of about 10% over state-of-charge values ranging from 0 to 1. Additionally, the stress and strain expressions require elastic properties such as the Young's modulus and Poisson's ratio (note that these elastic properties are assumed to be independent of concentration).

The applied current consists of a discharge current of 4 C that is applied for 850 s, followed by a relaxation period of 250 s.

Results and Discussion

The battery cell voltage profile is plotted as a function of time in [Figure 1](#page-3-0). Note that a discharge current of 4 C has been applied for 850 s, followed by a relaxation period of 250 s.

Figure 1: Battery cell voltage profile as a function of time.

[Figure 2](#page-4-0) shows the normalized lithium concentration in a particle at a particular position (center) in the negative electrode, at various times during discharge and relaxation. Note in all subsequent plots, the solid and dashed lines refer to the discharge and relaxation periods, respectively. During discharge, which involves de-intercalation of lithium ions from the negative electrode particles, it can be seen that the concentration in the particle

decreases with time. At the end of the relaxation period, the concentration settles at a final value.

Figure 2: Normalized lithium concentration in a particle at the center of the negative electrode, at various times during discharge (solid lines) and relaxation (dashed lines).

The radial component of the diffusion-induced stress in a particle at the center of the negative electrode, at various times during discharge and relaxation, is shown in [Figure 3](#page-5-0). During discharge (de-intercalation of lithium ions from the particle), the radial stress is compressive inside the spherical particle. At any given time, the compressive radial stress is highest at the center and decreases monotonically to 0 at the surface of the particle. During the relaxation period, the compressive radial stress inside the particle relaxes to 0.

Figure 3: Radial component of the diffusion-induced stress in a particle at the center of the negative electrode, at various times during discharge (solid lines) and relaxation (dashed lines).

Similarly, [Figure 4](#page-6-0) shows the tangential component of the diffusion-induced stress in a particle at the center of the negative electrode, at various times during discharge and relaxation. During discharge, the tangential stress is compressive at the center and tensile at the surface of the spherical particle. Note that at the center of the particle, the tangential and radial stresses always have the same magnitude so that the stress state at the center of the particle is purely hydrostatic. The crossover from compressive to tensile occurs at $r = 1/\sqrt{2}$, after the stress reaches steady state.

Figure 4: Tangential component of the diffusion-induced stress in a particle at the center of the negative electrode, at various times during discharge (solid lines) and relaxation (dashed lines).

[Figure 5](#page-7-0) shows the von Mises stress in a particle at the center of the negative electrode, at various times during discharge and relaxation. During discharge, the von Mises stress is 0

at the center of the particle and reaches a maximum value at the surface of the spherical particle. During the relaxation period, the stress inside the particle relaxes to 0.

Figure 5: von Mises stress in a particle at the center of the negative electrode, at various times during discharge (solid lines) and relaxation (dashed lines).

[Figure 6](#page-8-0) and [Figure 7](#page-9-0) shows the radial and tangential components, respectively, of the diffusion-induced strain at surface of particles along the length of the negative electrode, at various times during discharge and relaxation. During de-intercalation of lithium ions from the particle, the surface strain decreases with time in the negative electrode. Also, the surface value of strain is not uniform across the electrode because of variation in particle concentration across the electrode. The maximum value of surface strain is observed at the

current collector end. At the end of the relaxation period, the strain eventually reaches a value corresponding to the final particle concentration.

Figure 6: Radial component of diffusion-induced surface strain along the length of the negative electrode, at various times during discharge (solid lines) and relaxation (dashed lines).

Figure 7: Tangential component of diffusion-induced surface strain along the length of the negative electrode, at various times during discharge (solid lines) and relaxation (dashed lines).

The total elastic strain energy density that is stored in the negative electrode material particles provides the driving force for particle fracture. This quantity is plotted along the length of the negative electrode in [Figure 8,](#page-10-0) at various times during discharge. It can be seen that the total elastic strain energy density increases with time across the electrode. The value is initially higher at the separator end. The maximum value gradually moves across the electrode toward the current collector end at the end of discharge.

Figure 8: Total elastic strain energy density stored in the negative electrode material particles, plotted along the length of the negative electrode, at various times during discharge.

All the above plots show a quantity plotted either across the particle dimension or along the length of the negative electrode, at various times during discharge. Alternatively, it is useful to plot the time evolution of any quantity at different positions in the negative electrode. The von Mises stress at the surface of particles at two positions in the negative electrode (current collector end and separator end) is plotted versus time in [Figure 9](#page-11-2). The plot also includes the applied current for reference. The von Mises stress contains contribution from both the radial and tangential components of the diffusion-induced stress. As seen from [Figure 3](#page-5-0) and [Figure 4,](#page-6-0) the surface value of the radial component of the diffusion-induced stress is 0. So, the surface von Mises stress essentially mimics the behavior of the tangential component of the diffusion-induced surface stress. In [Figure 9](#page-11-2), it can be seen that the von Mises stress initially increases at the separator end and subsequently at the current collector end. The stress induced in the electrode particles varies at different positions along the negative electrode due to concentration gradients in the porous electrode. Similarly, it can be expected that the total elastic strain density, that provides the driving force for fracture, also varies at different positions along the negative electrode. It can be seen in [Figure 9](#page-11-2) that the surface von Mises stress is higher at the

current collector end as compared to the separator end, toward the end of the discharge period. Finally, the stress in the particles relaxes to 0 during the relaxation period.

Figure 9: Time evolution of the von Mises stress at the surface of the particles at two positions in the negative electrode. The applied current is also plotted for reference.

References

1. Y-T. Cheng, and M.W. Verbrugge, "Evolution of stress within a spherical insertion electrode particle under potentiostatic and galvanostatic operation," *Journal of Power Sources*, vol. 190, pp. 453–460, 2009.

2. V. Malave, J.R. Berger, and P.A. Martin, "Concentration-dependent chemical expansion in lithium-ion battery cathode particles," *Journal of Applied Mechanics*, vol. 81, pp. 091005 1–9, 2014.

Application Library path: Battery_Design_Module/Batteries,_Lithium-Ion/ diffusion_induced_stress

Modeling Instructions

Start this tutorial by opening a template file that contains a 1D battery model. Alternatively, you may build the template model yourself by following the instructions found in the template model.

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

Browse to the model's Application Libraries folder and double-click the file li_battery_seed.mph.

GLOBAL DEFINITIONS

Parameters 1

The template model already contains a few parameters. Change the value of the initial cell voltage and add a few parameters for the Young's modulus and reference exchange current densities.

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

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

3 In the table, enter the following settings:

Step 1 (step1)

Define a step function that will be used later to set up the applied current.

- **1** In the **Home** toolbar, click $f(x)$ **Functions** and choose **Global>Step**.
- **2** In the **Settings** window for **Step**, locate the **Parameters** section.
- **3** In the **From** text field, type 1.
- **4** In the **To** text field, type 0.

Relative volume change as function of soc

Define an interpolation function that defines the relative expansion of graphite material as a function of state-of-charge.

- **1** In the **Home** toolbar, click $f(x)$ **Functions** and choose **Global>Interpolation**.
- **2** In the **Settings** window for **Interpolation**, type Relative volume change as function of soc in the **Label** text field.
- **3** Locate the **Definition** section. In the table, enter the following settings:

- **4** In the **Function name** text field, type fvol.
- **5** Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Piecewise cubic**.
- **6** Locate the **Units** section. In the **Arguments** text field, type 1.
- **7** In the **Function** text field, type 1.

DEFINITIONS (COMP1)

Load the variables for this model from a text file.

Variables 1

- **1** In the **Home** toolbar, click $\partial = \mathbf{Variable}$ and choose **Local Variables**.
- **2** In the **Settings** window for **Variables**, locate the **Variables** section.
- **3** Click **Load from File**.
- **4** Browse to the model's Application Libraries folder and double-click the file diffusion_induced_stress_variables.txt.

LITHIUM-ION BATTERY (LIION)

The physics has already been set up in the template model. Next, set up the inputs required for stress and strain calculations in the **Particle Intercalation** node of the porous electrode domain corresponding to the negative electrode (graphite material). Also, specify the reference exchange current density for the electrode kinetics in the **Porous Electrode Reaction** nodes of the negative and positive electrodes. Finally, specify the applied current (that corresponds to a discharge current of 4C for 850 s followed by a relaxation period for the next 250 s) in the **Electrode Current** node.

Particle Intercalation 1

- **1** In the **Model Builder** window, expand the **Porous Electrode 1** node, then click **Particle Intercalation 1**.
- **2** In the **Settings** window for **Particle Intercalation**, click to expand the **Stress and Strain** section.
- **3** Select the **Calculate stress and strain** check box.
- **4** In the *E* text field, type E.
- **5** In the $\Delta V/V_0$ text field, type $fvol($ liion.cs_pce1/liion.csmax).

It is essential to have a finer resolution along the graphite particle dimension and this can be done by setting a linear distribution with 30 elements.

- **6** Click to expand the **Particle Discretization** section. From the **Distribution** list, choose **Linear**.
- **7** In the N_{el} text field, type 30.

Porous Electrode Reaction 1

- **1** In the **Model Builder** window, click **Porous Electrode Reaction 1**.
- **2** In the **Settings** window for **Porous Electrode Reaction**, locate the **Electrode Kinetics** section.
- **3** In the $i_{0,\text{ref}}(T)$ text field, type i0ref_neg.

Porous Electrode Reaction 1

- **1** In the **Model Builder** window, expand the **Porous Electrode 2** node, then click **Porous Electrode Reaction 1**.
- **2** In the **Settings** window for **Porous Electrode Reaction**, locate the **Electrode Kinetics** section.
- **3** In the $i_{0,\text{ref}}(T)$ text field, type i0ref_pos.

Electrode Current 1

- **1** In the **Model Builder** window, click **Electrode Current 1**.
- **2** In the **Settings** window for **Electrode Current**, locate the **Electrode Current** section.
- **3** In the $I_{\text{s,total}}$ text field, type Iapp.

STUDY 1

Step 2: Time Dependent

- **1** In the **Model Builder** window, expand the **Study 1** node, then click **Step 2: Time Dependent**.
- **2** In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
- **3** In the **Output times** text field, type range(0,10,1100).
- **4** In the **Model Builder** window, click **Study 1**.
- **5** In the **Settings** window for **Study**, locate the **Study Settings** section.
- **6** Clear the **Generate default plots** check box.
- **7** In the **Home** toolbar, click **Compute**.

RESULTS

Battery cell voltage

The probe plot show the battery cell voltage [\(Figure 1\)](#page-3-0).

- **1** In the **Model Builder** window, under **Results** click **Probe Plot Group 1**.
- **2** In the **Settings** window for **1D Plot Group**, type Battery cell voltage in the **Label** text field.
- **3** Click to expand the **Title** section. From the **Title type** list, choose **Label**.
- **4** Locate the **Plot Settings** section. Select the **y-axis label** check box.
- **5** In the associated text field, type Battery cell voltage (V).
- **6** Locate the **Legend** section. Clear the **Show legends** check box.
- **7** In the **Battery cell voltage** toolbar, click **O** Plot.

Study 1/Solution 1 (sol1)

To plot along the graphite particle dimension, you need to create a Solution dataset that refers to the extra dimension that is set up by the Porous Electrode node corresponding to the negative electrode.

Study 1/Solution 1 (4) (sol1)

- **1** In the **Model Builder** window, expand the **Results>Datasets** node.
- **2** Right-click **Results>Datasets>Study 1/Solution 1 (sol1)** and choose **Duplicate**.
- **3** In the **Settings** window for **Solution**, locate the **Solution** section.
- **4** From the **Component** list, choose

Extra Dimension from Particle Intercalation 1 (liion_pce1_pin1_xdim).

Negative particle concentration

Next, follow the steps below to plot the normalized lithium concentration in a particle at a particular position (say center) in the negative electrode, at various times during discharge and relaxation. Note in all the subsequent plots in the model, the solid and dashed lines refer to the discharge period and the relaxation period, respectively. [\(Figure 2\)](#page-4-0).

- In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
- In the **Settings** window for **1D Plot Group**, type Negative particle concentration in the **Label** text field.

Line Graph 1

- Right-click **Negative particle concentration** and choose **Line Graph**.
- In the **Settings** window for **Line Graph**, locate the **Data** section.
- From the **Dataset** list, choose **Study 1/Solution 1 (4) (sol1)**.
- From the **Time selection** list, choose **Interpolated**.
- In the **Times (s)** text field, type 0,100,300,400,500,600,700,850.
- Locate the **Selection** section. From the **Selection** list, choose **All domains**.
- Locate the **y-Axis Data** section. In the **Expression** text field, type comp1.atxd1(15e-6, liion.cs_pce1/liion.csmax).
- Click to expand the **Legends** section. Select the **Show legends** check box.

Line Graph 2

- Right-click **Line Graph 1** and choose **Duplicate**.
- In the **Settings** window for **Line Graph**, locate the **Data** section.
- In the **Times (s)** text field, type 860,875,900,1100.
- Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- From the **Color** list, choose **Cycle (reset)**.

Negative particle concentration

- In the **Model Builder** window, click **Negative particle concentration**.
- In the **Settings** window for **1D Plot Group**, locate the **Title** section.
- From the **Title type** list, choose **Label**.
- Locate the **Plot Settings** section. Select the **x-axis label** check box.
- In the associated text field, type Normalized particle dimension (1).
- Select the **y-axis label** check box.
- In the associated text field, type Normalized lithium concentration (1).
- In the **Negative particle concentration** toolbar, click **O** Plot.

Now, create a plot of the radial component of the diffusion-induced stress in a particle [\(Figure 3\)](#page-5-0) at the center of the negative electrode, at various times during discharge and relaxation. This can be done by duplicating the previous plot.

Diffusion-induced stress, radial component

- Right-click **Negative particle concentration** and choose **Duplicate**.
- In the **Settings** window for **1D Plot Group**, type Diffusion-induced stress, radial component in the **Label** text field.
- Locate the **Plot Settings** section. In the **y-axis label** text field, type Diffusion-induced stress, radial component (Pa).

Line Graph 1

- In the **Model Builder** window, expand the **Diffusion-induced stress, radial component** node, then click **Line Graph 1**.
- In the **Settings** window for **Line Graph**, locate the **Data** section.
- In the **Times (s)** text field, type 100,300,400,500,600,700,850.
- Locate the **y-Axis Data** section. In the **Expression** text field, type comp1.atxd1(15e-6, liion.sr_pce1).
- Click to expand the **Quality** section. From the **Resolution** list, choose **No refinement**.

Line Graph 2

- In the **Model Builder** window, click **Line Graph 2**.
- In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- In the **Expression** text field, type comp1.atxd1(15e-6,liion.sr_pce1).
- Locate the **Quality** section. From the **Resolution** list, choose **No refinement**.

Diffusion-induced stress, radial component

- In the **Model Builder** window, click **Diffusion-induced stress, radial component**.
- In the **Settings** window for **1D Plot Group**, locate the **Axis** section.
- Select the **Manual axis limits** check box.
- In the **x minimum** text field, type 0.05.
- In the **x maximum** text field, type 1.
- In the **y minimum** text field, type -1.5E7.
- **7** In the **y maximum** text field, type 0.2E7.
- **8** Locate the **Legend** section. From the **Position** list, choose **Lower right**.
- **9** In the **Diffusion-induced stress, radial component** toolbar, click **Plot**.

Now, create a plot of the tangential component of the diffusion-induced stress in a particle [\(Figure 4\)](#page-6-0) at the center of the negative electrode, at various times during discharge and relaxation. This can be done by duplicating the previous plot.

Diffusion-induced stress, tangential component

- **1** Right-click **Diffusion-induced stress, radial component** and choose **Duplicate**.
- **2** In the **Settings** window for **1D Plot Group**, type Diffusion-induced stress, tangential component in the **Label** text field.
- **3** Locate the **Plot Settings** section. In the **y-axis label** text field, type Diffusion-induced stress, tangential component (Pa).

Line Graph 1

- **1** In the **Model Builder** window, expand the **Diffusion-induced stress, tangential component** node, then click **Line Graph 1**.
- **2** In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- **3** In the **Expression** text field, type comp1.atxd1(15e-6,liion.stheta_pce1).

Line Graph 2

- **1** In the **Model Builder** window, click **Line Graph 2**.
- **2** In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- **3** In the **Expression** text field, type comp1.atxd1(15e-6,liion.stheta_pce1).

Diffusion-induced stress, tangential component

- **1** In the **Model Builder** window, click **Diffusion-induced stress, tangential component**.
- **2** In the **Settings** window for **1D Plot Group**, locate the **Axis** section.
- **3** In the **y maximum** text field, type 1.2E7.
- **4** In the **Diffusion-induced stress, tangential component** toolbar, click **P** Plot.

Now, create a plot of the von Mises stress in a particle ([Figure 5](#page-7-0)) at the center of the negative electrode, at various times during discharge and relaxation. This can be done by duplicating the previous plot.

von Mises Stress

- **1** Right-click **Diffusion-induced stress, tangential component** and choose **Duplicate**.
- **2** In the **Settings** window for **1D Plot Group**, type von Mises Stress in the **Label** text field.

 Locate the **Plot Settings** section. In the **y-axis label** text field, type von Mises stress (Pa).

Line Graph 1

- In the **Model Builder** window, expand the **von Mises Stress** node, then click **Line Graph 1**.
- In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- In the **Expression** text field, type comp1.atxd1(15e-6,liion.mises_pce1).

Line Graph 2

- In the **Model Builder** window, click **Line Graph 2**.
- In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- In the **Expression** text field, type comp1.atxd1(15e-6,liion.mises_pce1).

von Mises Stress

- In the **Model Builder** window, click **von Mises Stress**.
- In the **Settings** window for **1D Plot Group**, locate the **Axis** section.
- In the **y minimum** text field, type -0.1E7.
- Locate the **Legend** section. From the **Position** list, choose **Upper left**.
- In the **von Mises Stress** toolbar, click **Plot**.

Next, create a plot of the radial component of the diffusion-induced surface strain [\(Figure 6\)](#page-8-0) along the length of the negative electrode.

Diffusion-induced surface strain, radial component

- In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
- In the **Settings** window for **1D Plot Group**, type Diffusion-induced surface strain, radial component in the **Label** text field.

Line Graph 1

- Right-click **Diffusion-induced surface strain, radial component** and choose **Line Graph**.
- In the **Settings** window for **Line Graph**, locate the **Data** section.
- From the **Dataset** list, choose **Study 1/Solution 1 (1) (sol1)**.
- From the **Time selection** list, choose **Interpolated**.
- In the **Times (s)** text field, type 100,300,400,500,600,700,850.
- Select Domain 1 only.
- Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Lithium-Ion Battery>Stress and strain> liion.er_surface_pce1 - Diffusion-induced surface strain, radial component**.

Locate the **Legends** section. Select the **Show legends** check box.

Line Graph 2

- Right-click **Line Graph 1** and choose **Duplicate**.
- In the **Settings** window for **Line Graph**, locate the **Data** section.
- In the **Times (s)** text field, type 860,875,900,1100.
- Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- From the **Color** list, choose **Cycle (reset)**.

Diffusion-induced surface strain, radial component

- In the **Model Builder** window, click **Diffusion-induced surface strain, radial component**.
- In the **Settings** window for **1D Plot Group**, locate the **Title** section.
- From the **Title type** list, choose **Manual**.
- In the **Title** text area, type Diffusion-induced surface strain, radial component.
- Locate the **Plot Settings** section. Select the **x-axis label** check box.
- In the associated text field, type Distance along negative electrode (m).
- Locate the **Legend** section. From the **Position** list, choose **Lower middle**.
- In the **Diffusion-induced surface strain, radial component** toolbar, click **Plot**.

Next, create a plot of the tangential component of the diffusion-induced surface strain [\(Figure 7\)](#page-9-0) along the length of the negative electrode. This can be done by duplicating the previous plot.

Diffusion-induced surface strain, tangential component

- Right-click **Diffusion-induced surface strain, radial component** and choose **Duplicate**.
- In the **Settings** window for **1D Plot Group**, type Diffusion-induced surface strain, tangential component in the **Label** text field.
- Locate the **Title** section. In the **Title** text area, type Diffusion-induced surface strain, tangential component.

Line Graph 1

- In the **Model Builder** window, expand the **Diffusion-induced surface strain, tangential component** node, then click **Line Graph 1**.
- In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Lithium-**

Ion Battery>Stress and strain>liion.etheta_surface_pce1 - Diffusion-induced surface strain, tangential component.

Line Graph 2

- **1** In the **Model Builder** window, click **Line Graph 2**.
- **2** In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Lithium-Ion Battery>Stress and strain>liion.etheta_surface_pce1 - Diffusion-induced surface strain, tangential component**.

Diffusion-induced surface strain, tangential component

- **1** In the **Model Builder** window, click **Diffusion-induced surface strain, tangential component**.
- **2** In the **Diffusion-induced surface strain, tangential component** toolbar, click **Plot**.

Total elastic strain energy density

Next, create a plot of the total elastic strain energy density stored in the negative electrode material particles [\(Figure 8](#page-10-0)) along the length of the negative electrode.

- **1** In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
- **2** In the **Settings** window for **1D Plot Group**, type Total elastic strain energy density in the **Label** text field.

Line Graph 1

- **1** Right-click **Total elastic strain energy density** and choose **Line Graph**.
- **2** In the **Settings** window for **Line Graph**, locate the **Data** section.
- **3** From the **Dataset** list, choose **Study 1/Solution 1 (1) (sol1)**.
- **4** From the **Time selection** list, choose **Interpolated**.
- **5** In the **Times (s)** text field, type 100,300,400,500,600,700,850.
- **6** Select Domain 1 only.
- **7** Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Lithium-Ion Battery>Stress and strain> liion.Ws_tot_pce1 - Total elastic strain energy density - J/m³**.
- **8** Locate the **Legends** section. Select the **Show legends** check box.

Total elastic strain energy density

- **1** In the **Model Builder** window, click **Total elastic strain energy density**.
- **2** In the **Settings** window for **1D Plot Group**, locate the **Title** section.
- **3** From the **Title type** list, choose **Label**.
- **4** Locate the **Plot Settings** section. Select the **x-axis label** check box.
- **5** In the associated text field, type Distance along negative electrode (m).
- **6** In the **Total elastic strain energy density** toolbar, click **Plot**.

Surface von Mises stress versus time

Finally, create a plot that shows the time evolution of the von Mises stress at the surface of the particles ([Figure 9](#page-11-2)) at two positions in the negative electrode (current collector end and separator end). Also include the applied current on the same plot for reference.

- **1** In the Home toolbar, click **Add Plot Group** and choose **1D Plot Group**.
- **2** In the **Settings** window for **1D Plot Group**, type Surface von Mises stress versus time in the **Label** text field.

Point Graph 1

- **1** Right-click **Surface von Mises stress versus time** and choose **Point Graph**.
- **2** Select Boundaries 1 and 2 only.
- **3** In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Lithium-Ion Battery>Stress and strain>liion.mises_surface_pce1 - Surface von Mises stress - Pa**.
- **4** Click to expand the **Legends** section. Select the **Show legends** check box.
- **5** From the **Legends** list, choose **Manual**.
- **6** In the table, enter the following settings:

Legends

Current collector end

Separator end

Global 1

- **1** In the **Model Builder** window, right-click **Surface von Mises stress versus time** and choose **Global**.
- **2** In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions> Variables>Iapp - Applied current - A**.

Surface von Mises stress versus time

- **1** In the **Model Builder** window, click **Surface von Mises stress versus time**.
- **2** In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.
- Select the **Two y-axes** check box.
- In the table, select the **Plot on secondary y-axis** check box for **Global 1**.
- Locate the **Title** section. From the **Title type** list, choose **Manual**.
- In the **Title** text area, type Surface von Mises stress and Applied current.
- Locate the **Legend** section. From the **Position** list, choose **Upper left**.
- In the **Surface von Mises stress versus time** toolbar, click **Plot**.