# The initial simulation on characteristic of lithium ion cells using COMSOL soft

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# Want to do

- Simulation on lithium ion cells
  - Simulation on charge-discharge behavior of lithium ion cells
  - Simulation on thermal and safety of lithium ion cells
  - Design for lithium ion cells – collector, stress
- Simulation on fuel cells
- Simulation on metal-air cells
- Simulation on solar cell
- Design for material

# Why?

For lithium-ion batteries, the risk of exploding has restricted the application

Thermal simulation is a useful way to understand and design safer batteries ！

# Initial simulation

- Electrochemical-thermal simulation on lithium-ion cells

  Simple simulation  J. Newman model  R. E. White model

- Thermal simulation on lithium-ion cells

  Adiabatic test  Oven test

- Others

  Electric current and temperature distribution on collector

  Electric current and temperature distribution on joint

  Stretch and stress

# Electrochemical-thermal simulation

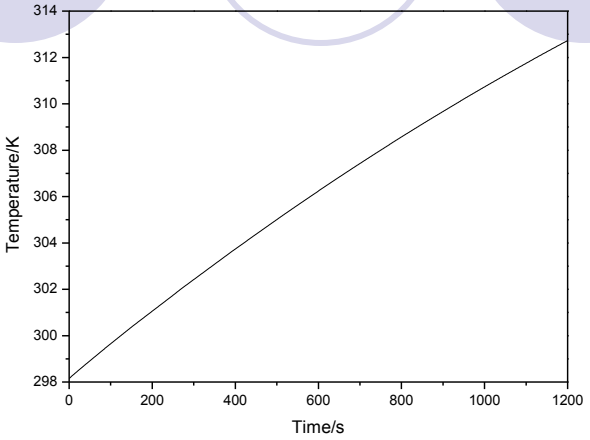
## Physical models：

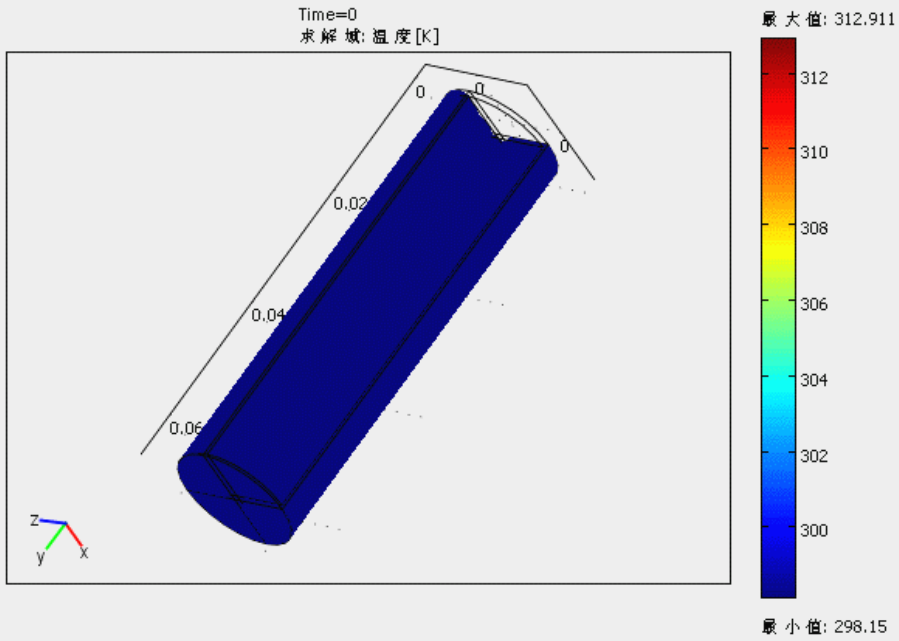
Heat transfer  or Heat transfer -Static electric

## Parameter：

Resistance/Conductance，dU/dT, Heat transfer coefficient，Thermal capacity ，Heat conduction coefficient ， Density

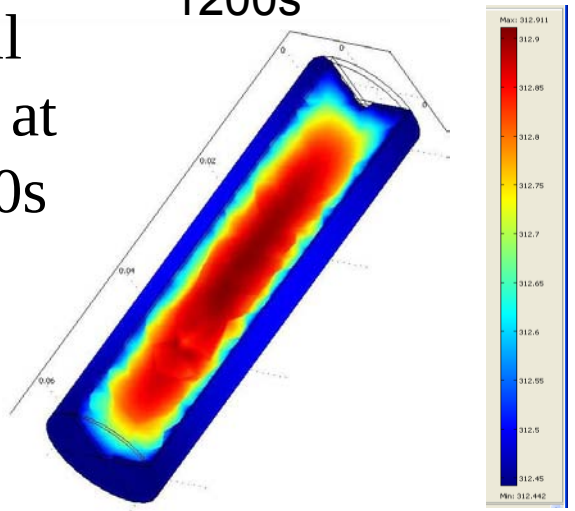
Simple simulation




18650 cell discharged at 3A for1200s

Temperature distribution at 1200s



# Electrochemical-thermal simulation

J. Newman model

Simulation the progress of charge-discharge，to understand the physical and chemical changes in cells

## Expressions:

$$\nabla\left(-\kappa_1^{\,eff}\nabla\phi_1\right)=-S_a i_{loc}$$

$$\nabla\left[-\kappa_2^{\,eff}\nabla\phi_2+\frac{2RT\kappa_2^{\,eff}}{F}\left(1+\frac{\partial\ln f}{\partial\ln c_2}\right)(1-t_+)\nabla(\ln c_2)\right]=S_a i_{loc}$$

$$\frac{dc_1}{dt}+\frac{1}{r_p^{\,2}}\frac{\partial}{\partial r_p}\left(-r_p^{\,2}D_1\frac{\partial}{\partial r_p}(c_1)\right)=0$$

$$\varepsilon_2\frac{dc_2}{dt}+\nabla\left(-D_2^{\,eff}\nabla c_2\right)=\frac{S_a i_{loc}}{F}(1-t_+)$$

$$\rho C_p\frac{\partial T}{\partial t}-\nabla(K\nabla T)=Q$$

$$Q=S_a i_{loc}(\phi_1-\phi_2-U)+S_a i_{loc}T\frac{\partial U}{\partial T}+\kappa_1^{\,eff}\nabla\phi_1\cdot\nabla\phi_1+\kappa_2^{\,eff}\nabla\phi_2\cdot\nabla\phi_2$$
$$+\frac{2RT\kappa_2^{\,eff}}{F}\left(1+\frac{\partial\ln f}{\partial\ln c_2}\right)(1-t_+)\nabla(\ln c_2)\cdot\nabla\phi_2$$

$$i_{loc}=kc_2^{\,\alpha_a}\left(c_1^{\,\max}-c_1\right)^{\alpha_a}c_1^{\,\alpha_c}\left\{\exp\left[\frac{\alpha_a F}{RT}(\phi_1-\phi_2-U)\right]-\exp\left[-\frac{\alpha_c F}{RT}(\phi_1-\phi_2-U)\right]\right\}$$

## Physical models：

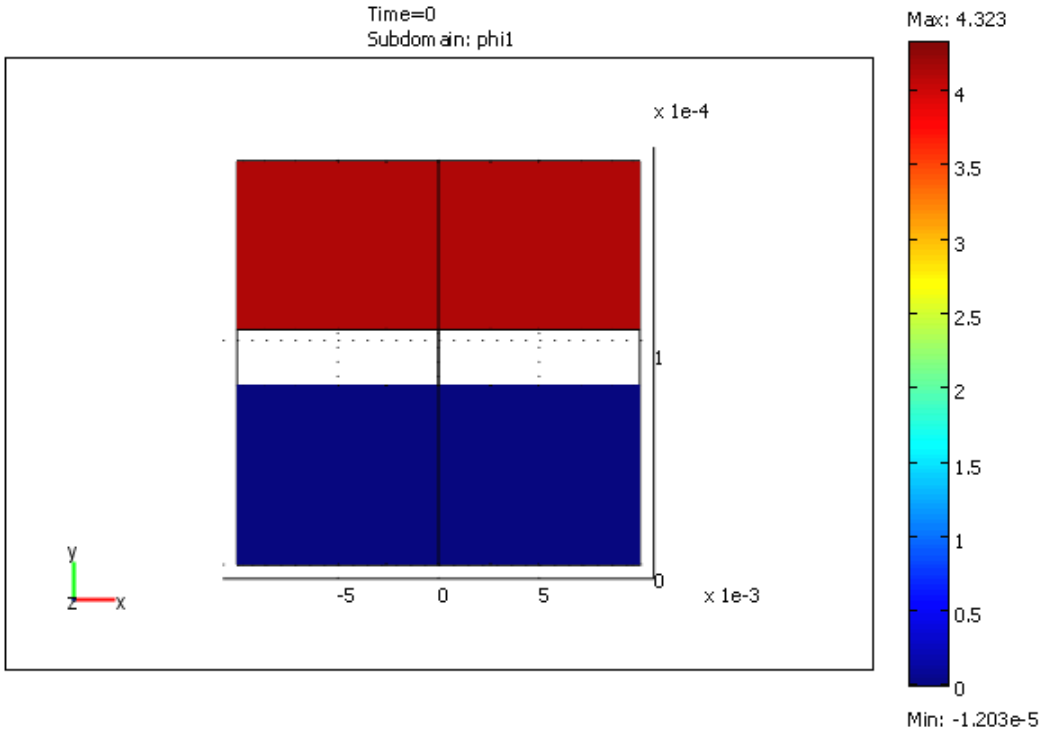
PDE（2）， Diffusion （2）， Heat transfer

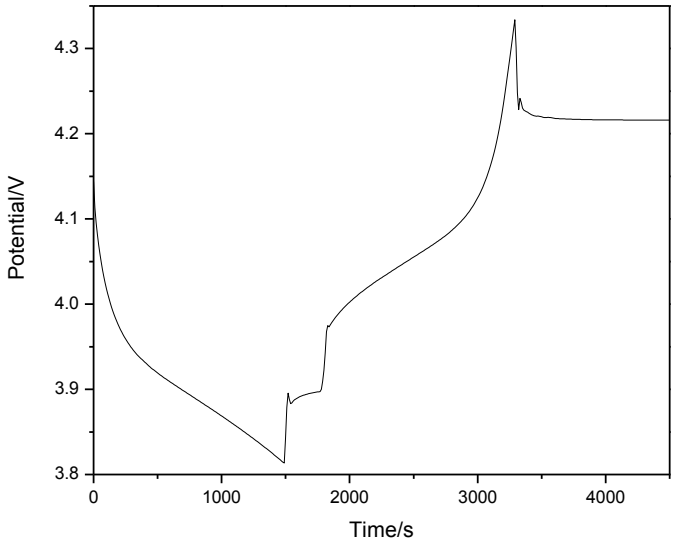
## Parameter：

Porosity， Radius， Surface area，dU/dT， Equilibrium potential， Diffusion coefficient ( liquid, solid), Conductance (liquid, solid)，Reaction rate coefficient, Heat transfer coefficient，Thermal capacity， Heat conduction coefficient， Density

# Electrochemical-thermal simulation

J. Newman model



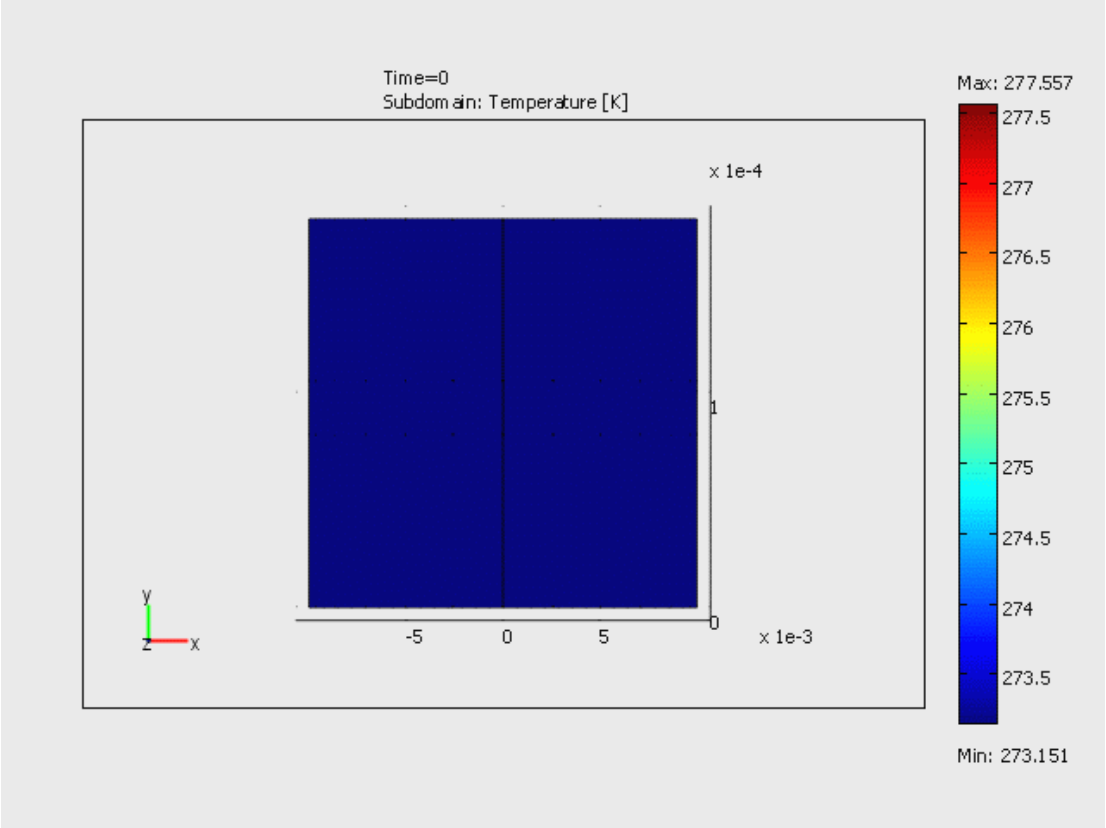



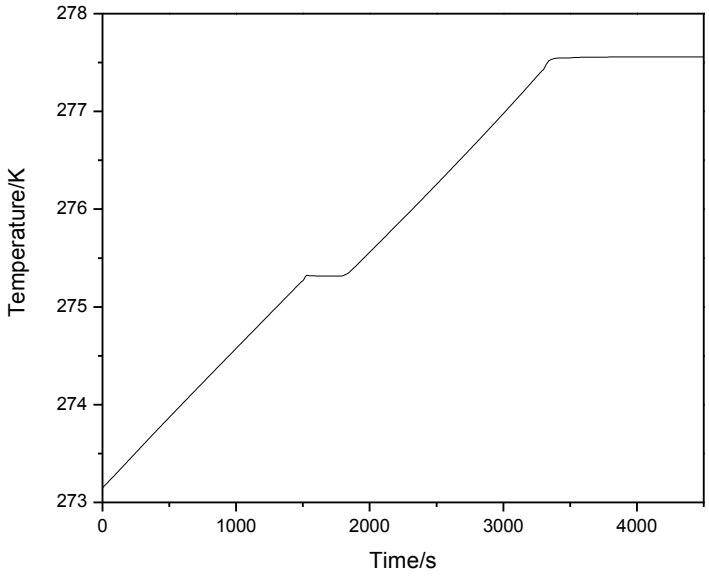

Cell voltage

2430 coin cell discharged at 9A/m$^2$ for 1500s， rest for 300s, and charged at 9A/m$^2$ for 1500s

# Electrochemical-thermal simulation

## J. Newman model

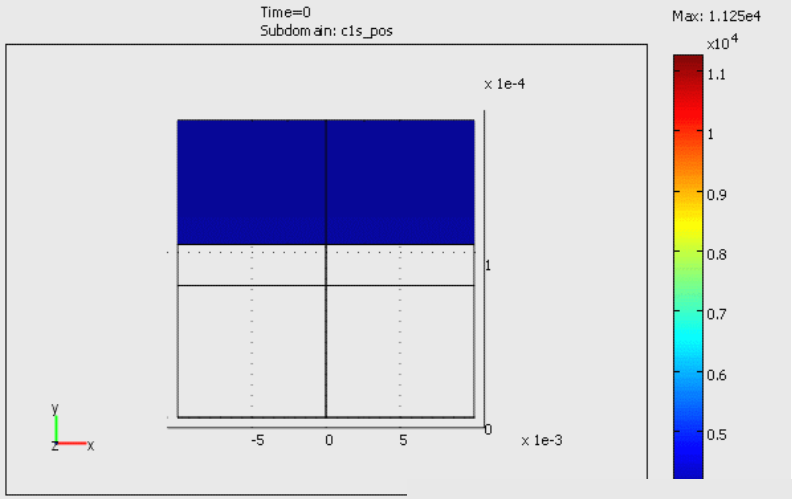


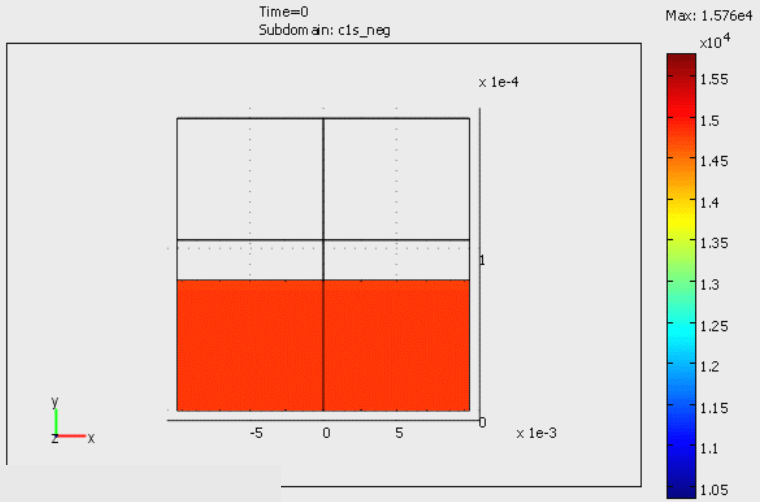




Cell temperature

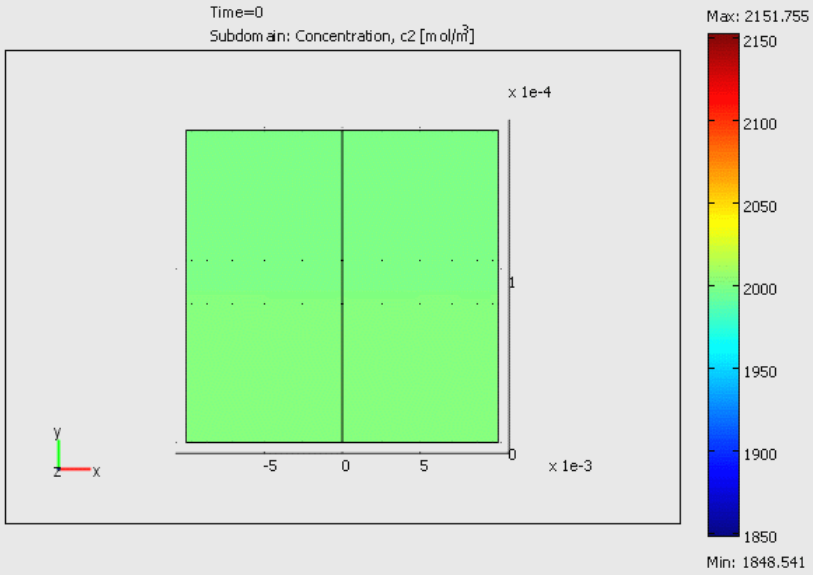
# Electrochemical-thermal simulation

J. Newman model




Positive concentration

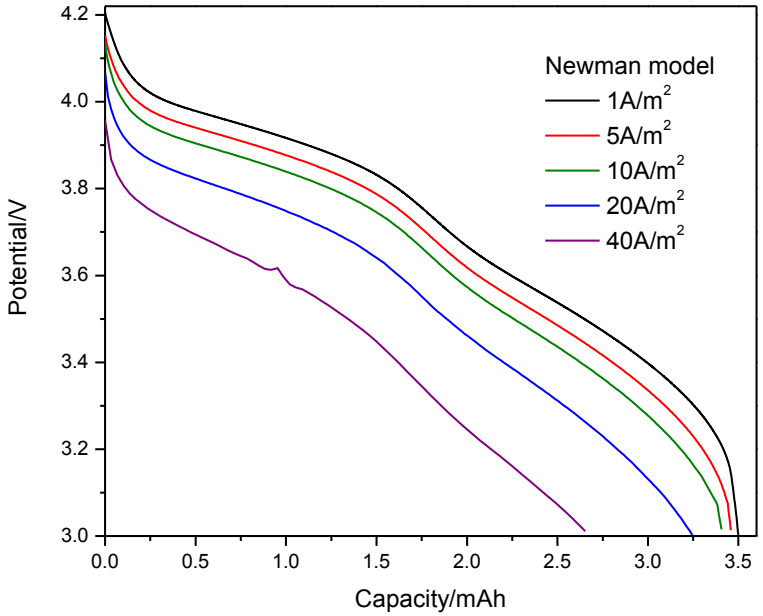


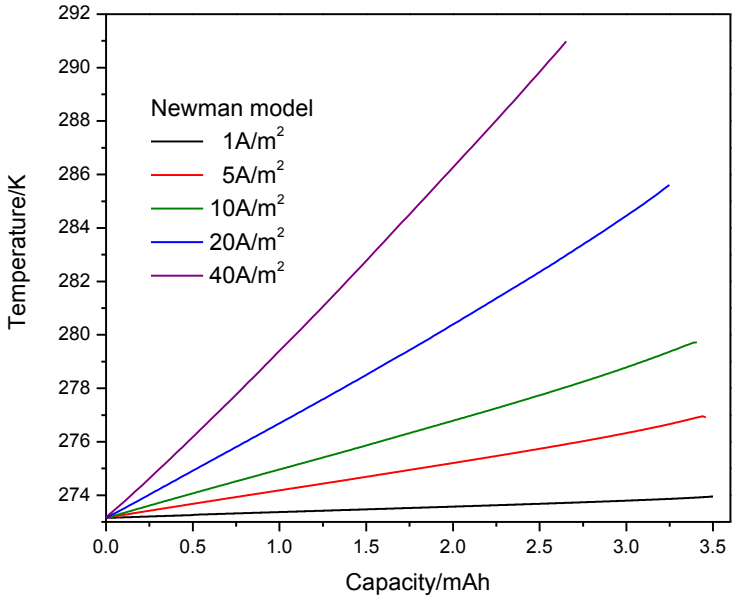

Negative concentration

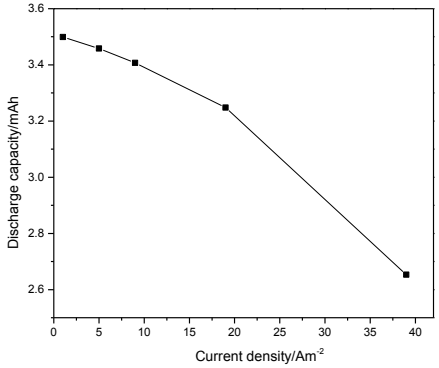
Electrolyte concentration

# Electrochemical-thermal simulation

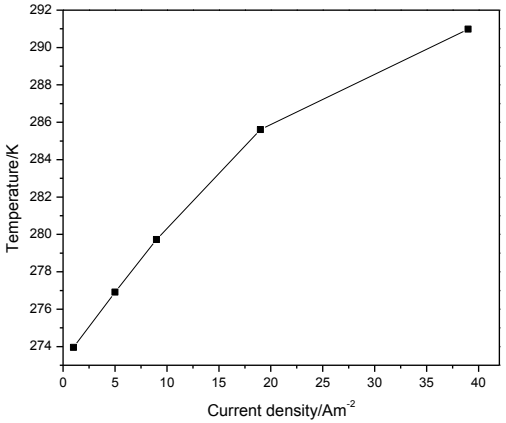
## J. Newman model




Discharged at different current densities



# Electrochemical-thermal simulation

R. E. White model

Simulate the progress of charge-discharge，to understand the physical and chemical changes in cells

## Expressions:

$$\nabla\left(-\kappa_1^{\,eff}\nabla\phi_1\right)=-S_a i_{loc}$$

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$$\frac{\partial c_1^{\,ave}}{\partial t}=-\frac{3S_a i_{loc}}{F}\qquad c_1^{\,ave}-c_1=\frac{i_{loc}r_p}{5FD_1}$$

$$\varepsilon_2\frac{dc_2}{dt}+\nabla\left(-D_2^{\,eff}\nabla c_2\right)=\frac{S_a i_{loc}}{F}(1-t_+)$$

$$\rho C_p\frac{\partial T}{\partial t}-\nabla(K\nabla T)=Q$$

$$Q=S_a i_{loc}\left(\phi_1-\phi_2-U\right)+S_a i_{loc}T\frac{\partial U}{\partial T}+\kappa_1^{\,eff}\nabla\phi_1\cdot\nabla\phi_1+\kappa_2^{\,eff}\nabla\phi_2\cdot\nabla\phi_2$$

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## Physical models：

PDE（3）， Diffusion（1）， Heat transfer

## Parameter：

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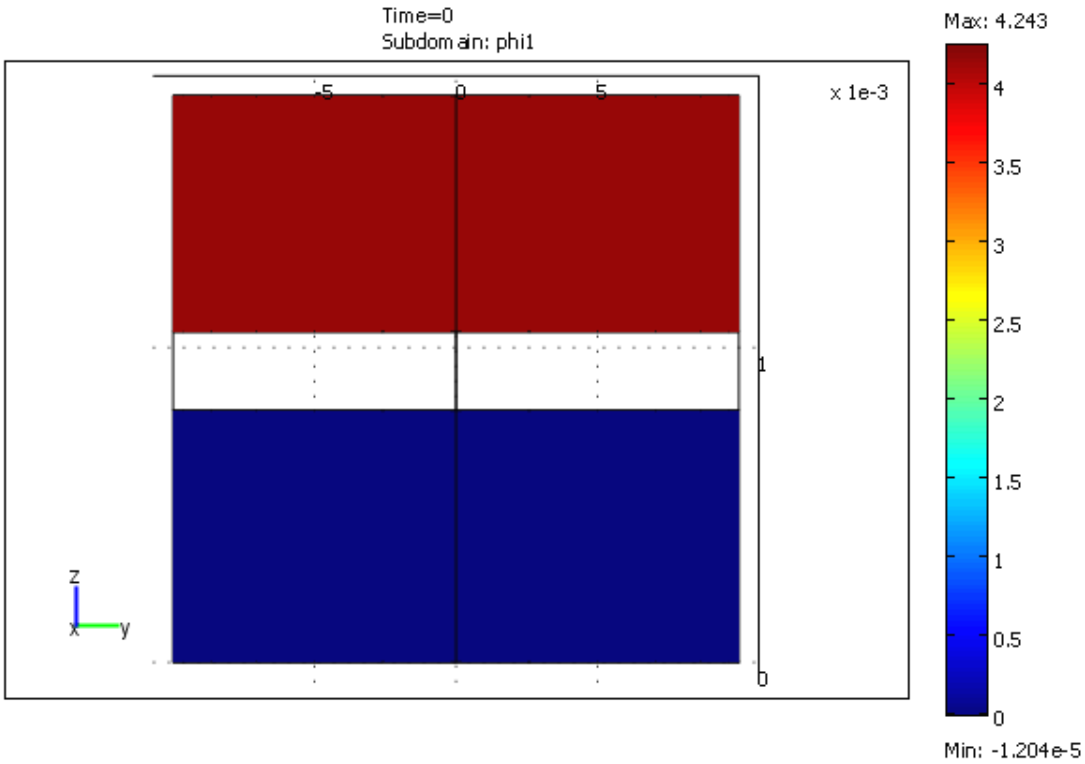
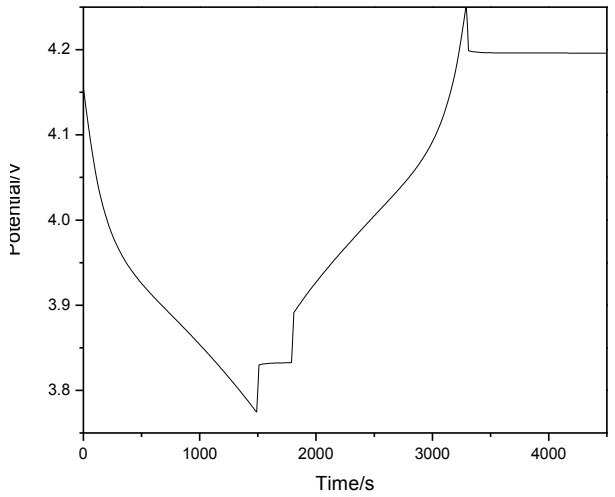
# Electrochemical-thermal simulation

## R. E. White model



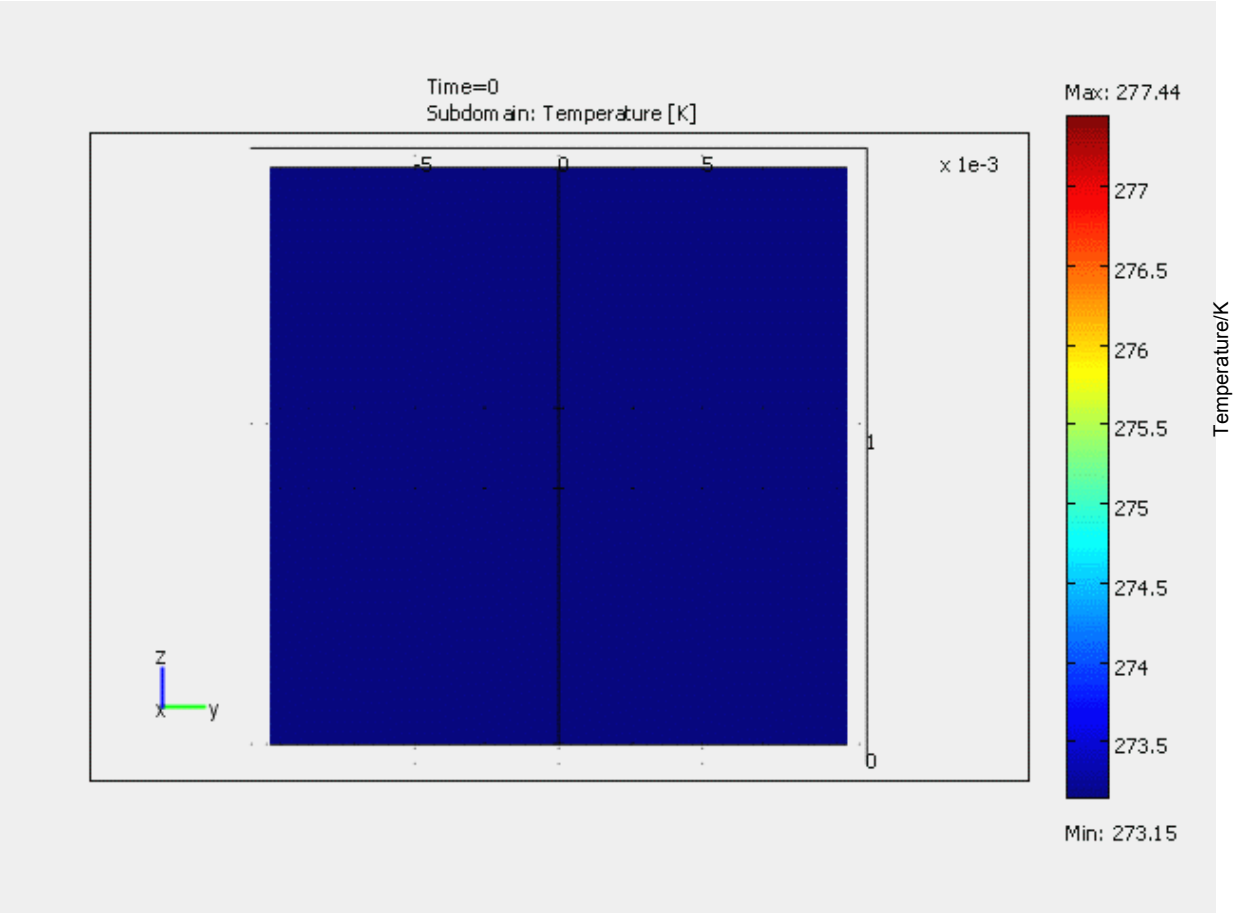



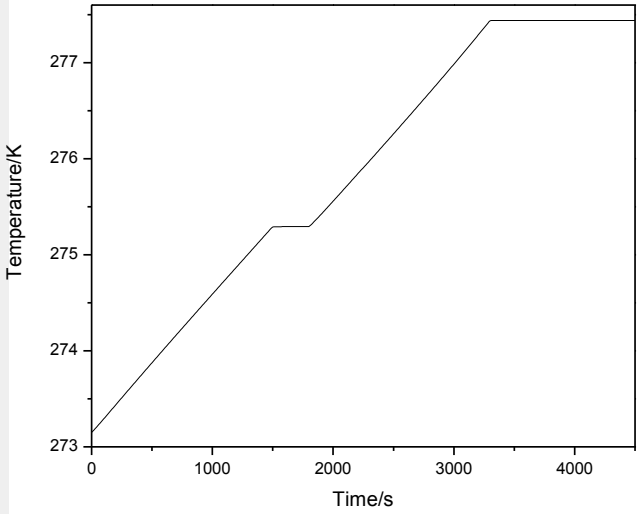

Cell voltage

2430 coin cell discharged at 9A/m$^2$ for 1500s， rest for 300s, and charged at 9A/m$^2$ for 1500s

# Electrochemical-thermal simulation

## R. E. White model

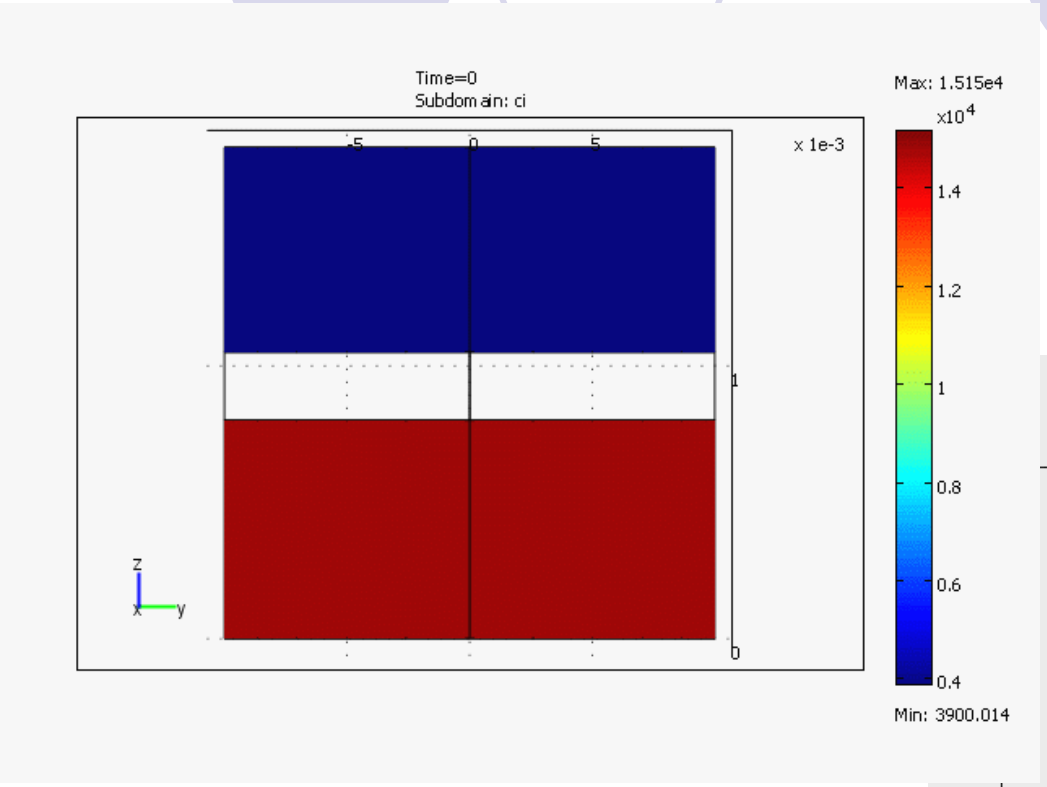



Cell temperature

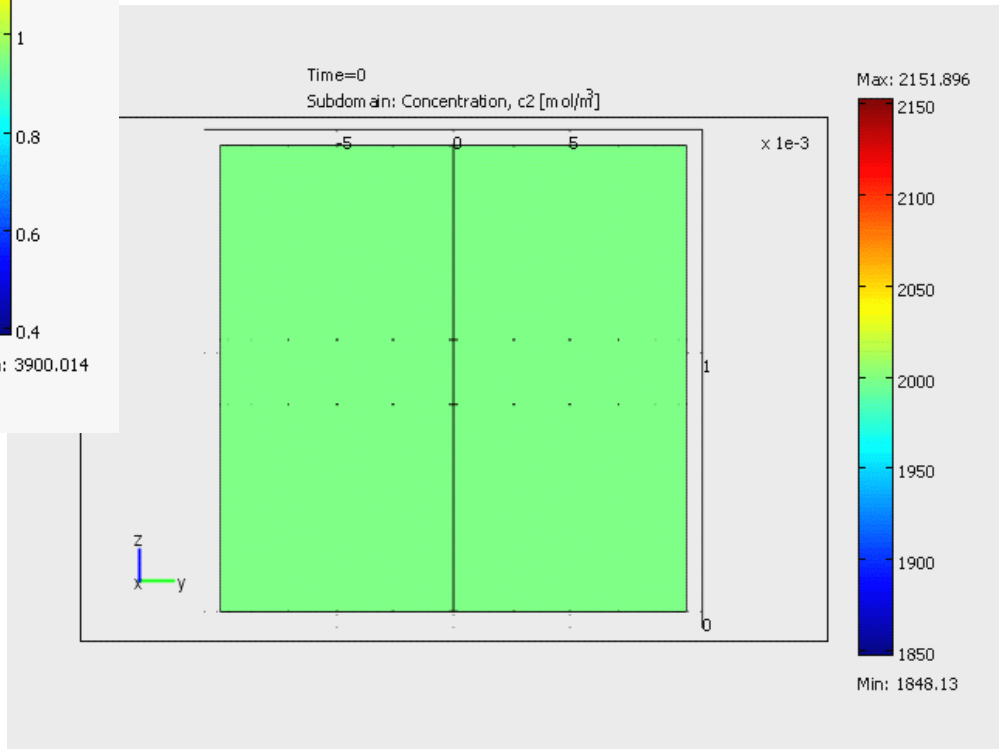
# Electrochemical-thermal simulation

R. E. White model



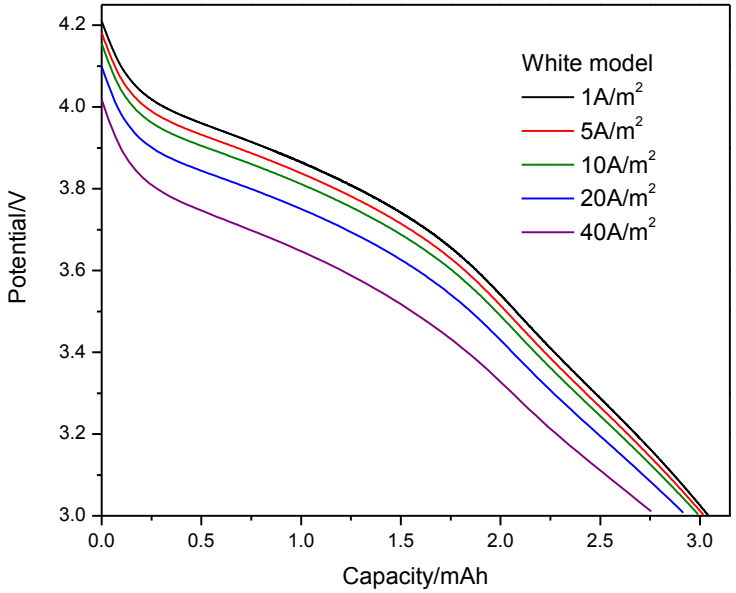

Positive/negative concentration

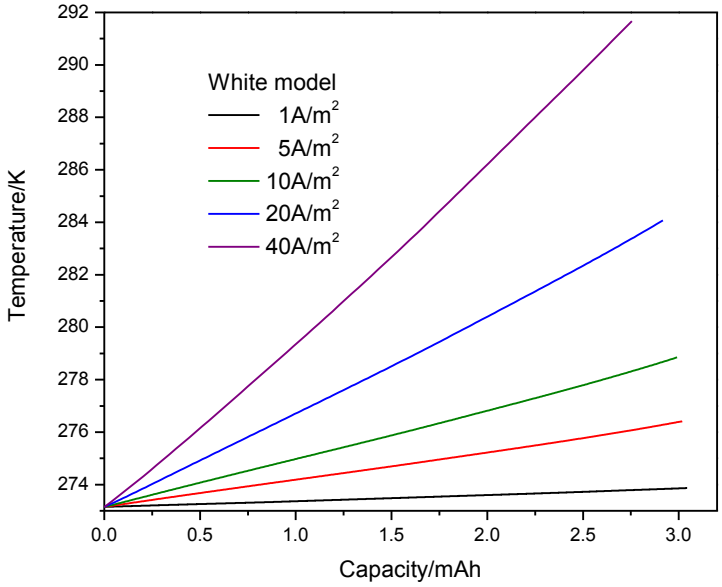
Electrolyte concentration

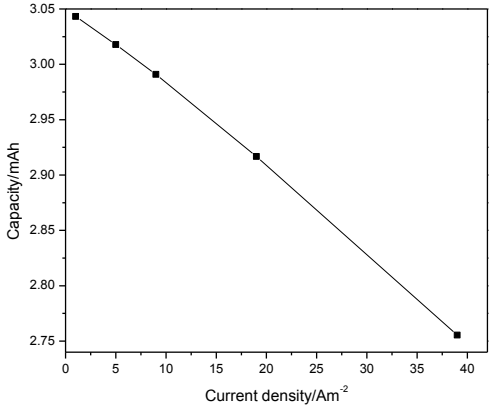


# Electrochemical-thermal simulation

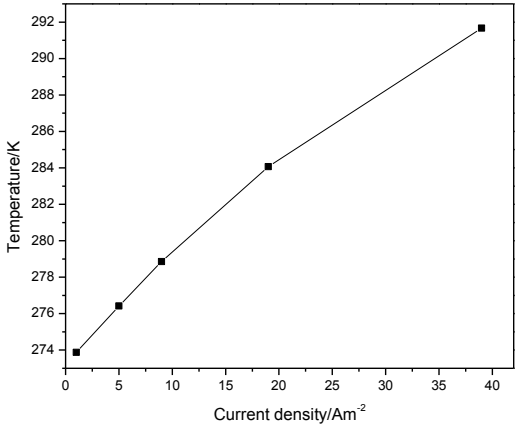
## R. E. White model



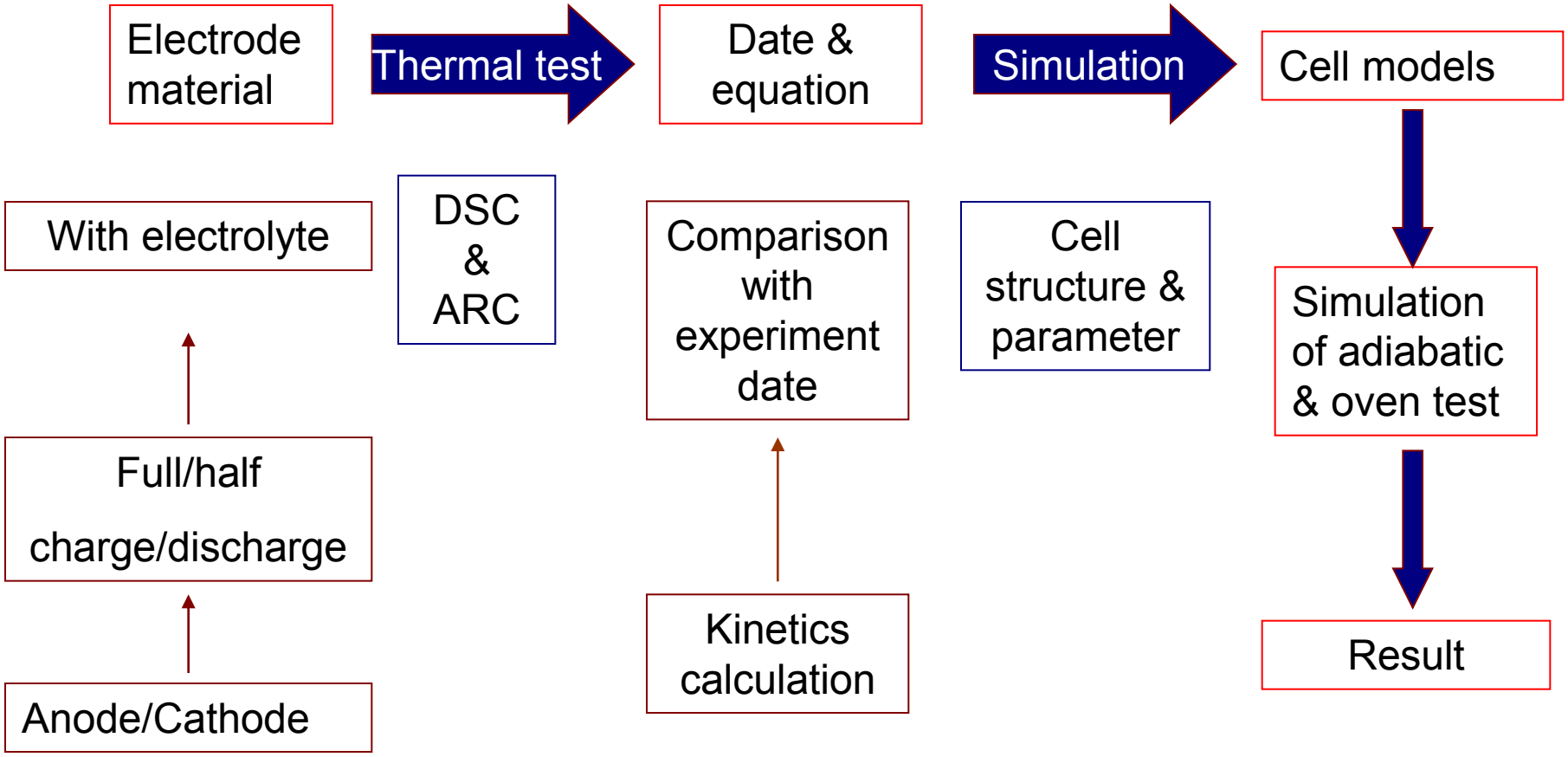




Discharged at different current densities



# Thermal simulation



# Thermal simulation

Simulate the thermal behavior and safety of lithium ion cells

## Expressions:

$$\delta\rho_i C_{pi}\frac{\partial T}{\partial t}-\nabla(K_i\nabla T)=Q$$

$$\frac{dx_1}{dt}=-A\exp\left(-\frac{E_a}{RT}\right)x_1{}^n(1-x_1)^a$$

$$\frac{dx_2}{dt}=-A\exp\left(-\frac{E_a}{RT}\right)x_2{}^n(1-x_2)^a$$

.....

$$\frac{dx}{dt}=-R$$

$$Q=\sum_i H_i\rho_i R_i$$

## Physical models：

PDE（n），Heat transfer (1)

## Parameter：

Heat transfer coefficient，Thermal capacity，Heat conduction coefficient，Density, Activation energy, frequency factor , enthalpy，reaction order

6 group of reaction rate expressions used in the example：

Positive 1， Negative 2， Electrolyte 3

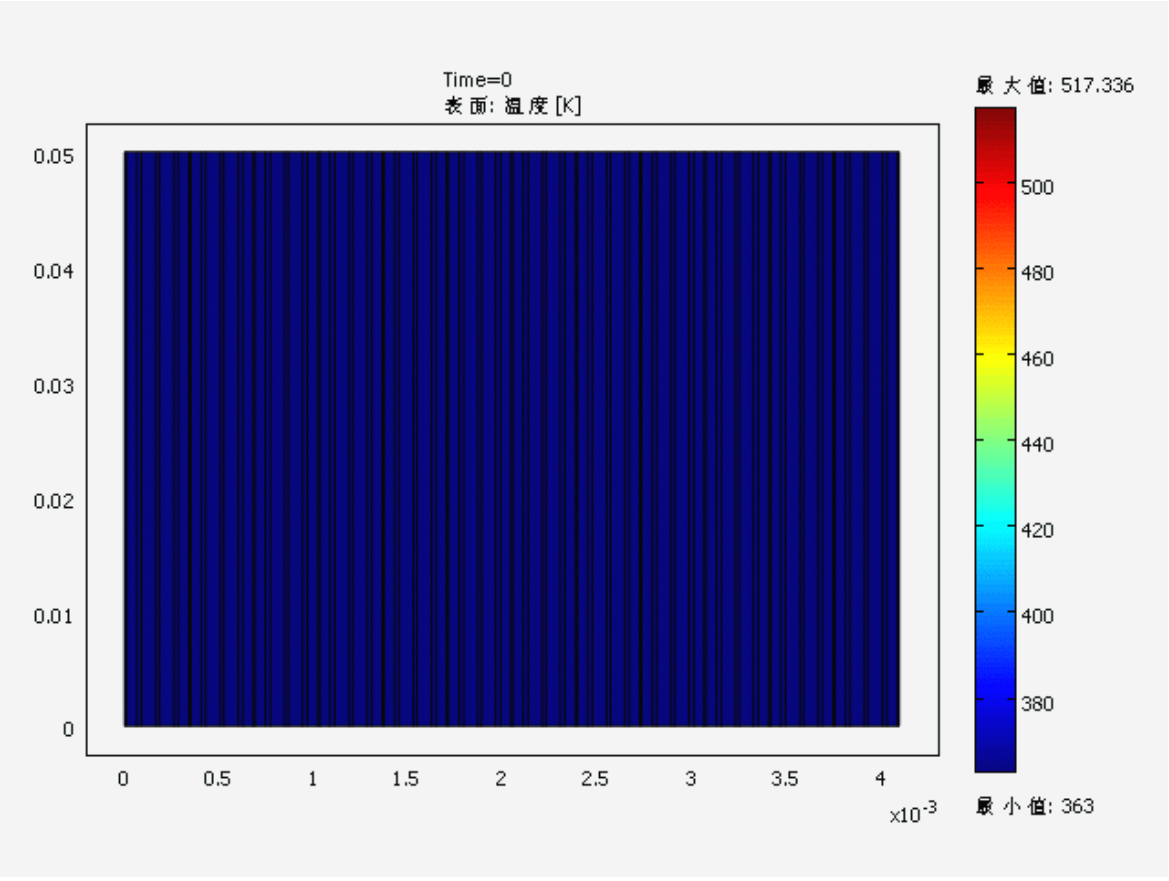
# Thermal simulation

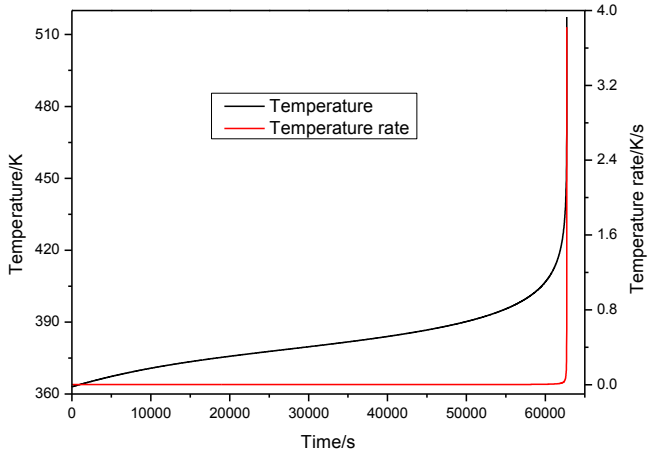
Adiabatic

Li-Co-O/C cell

363K

Temperature



# Thermal simulation

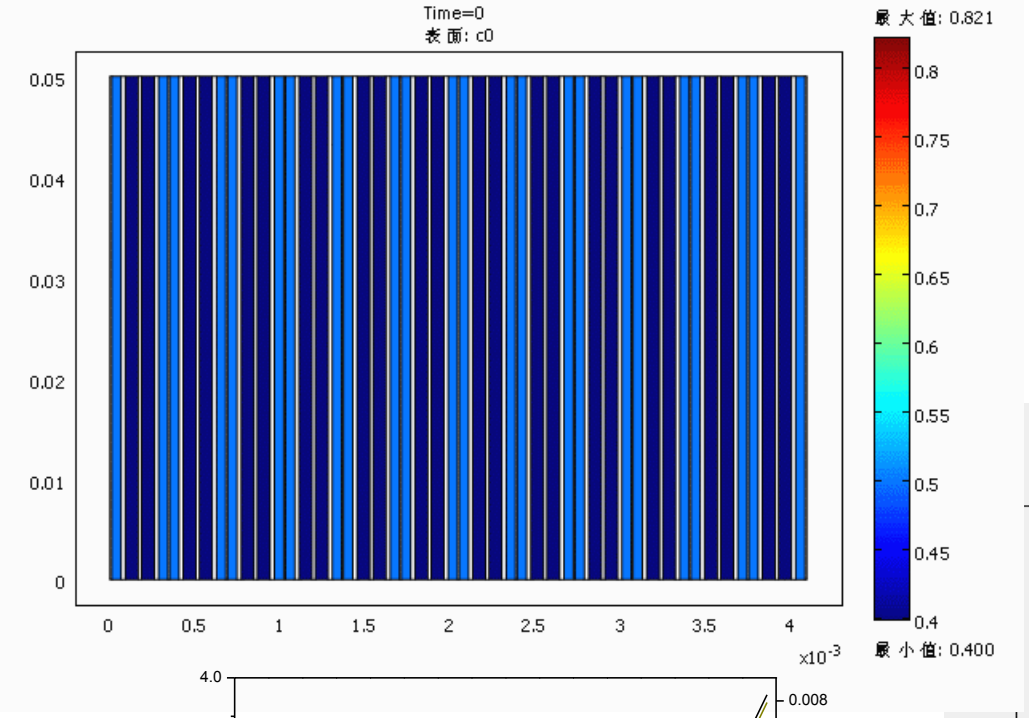
Adiabatic

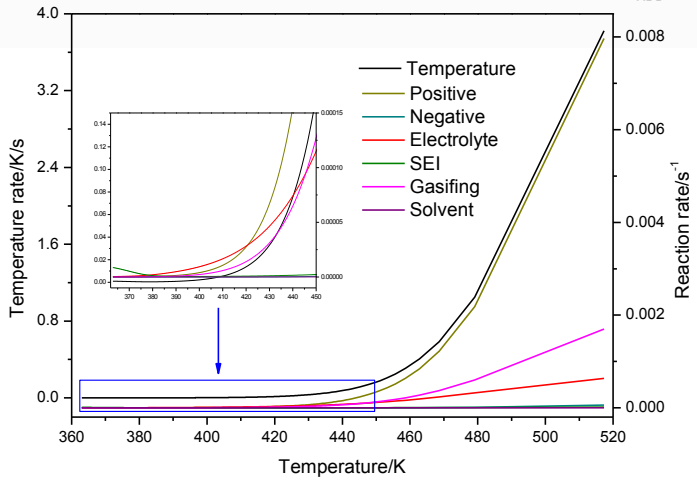
Li-Co-O/C cell

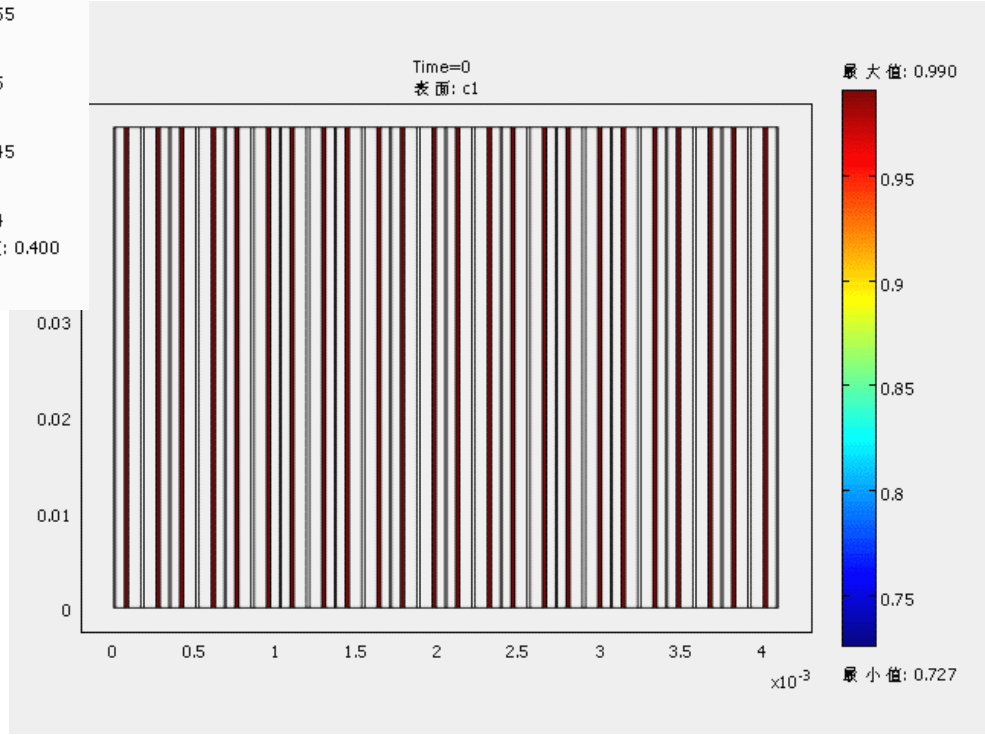
363K

Electrode concentration

Electrolyte concentration



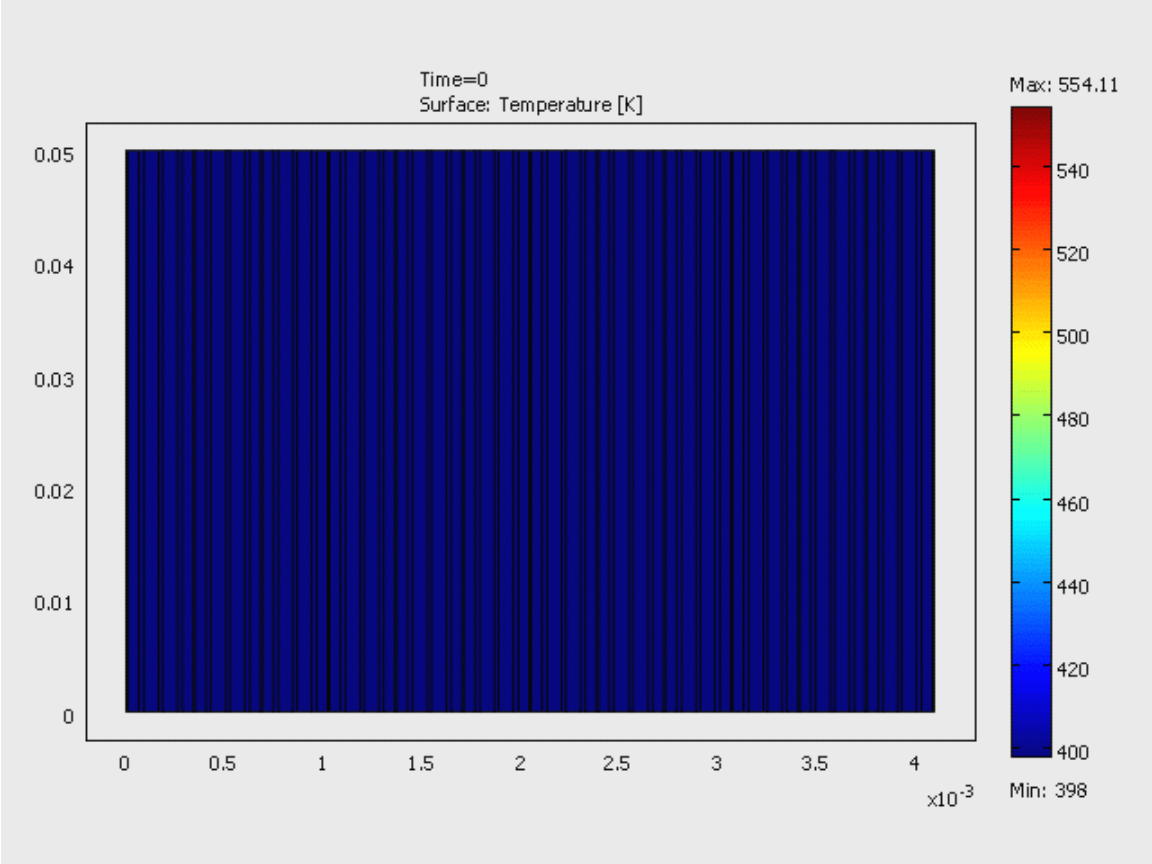



# Thermal simulation

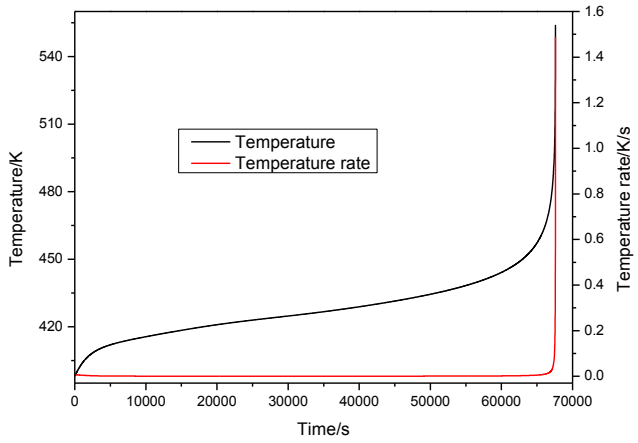
Adiabatic

$LiFePO_4$/C cell

398K




Temperature



# Thermal simulation

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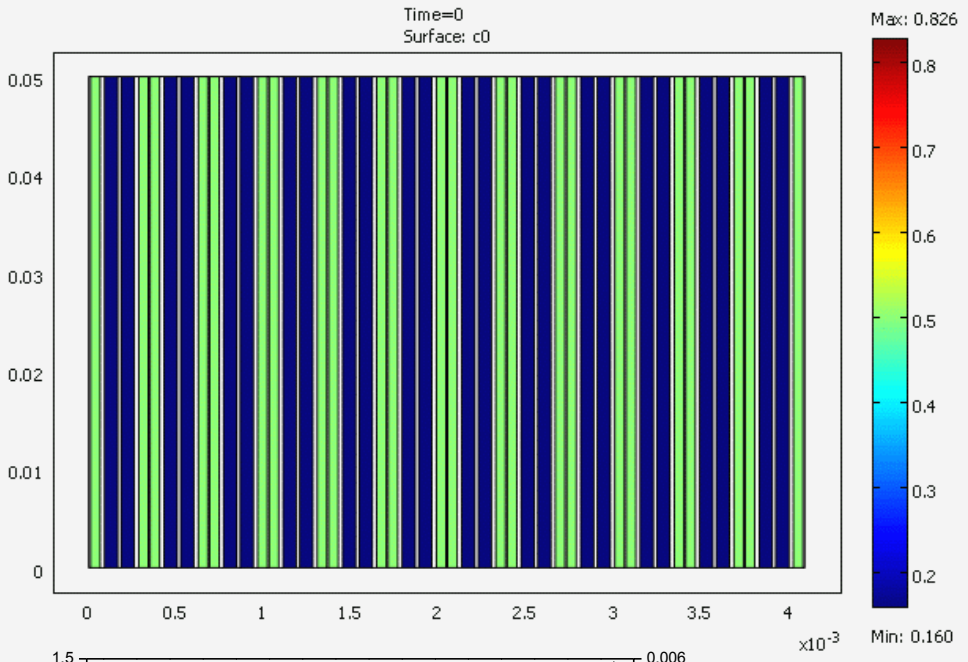
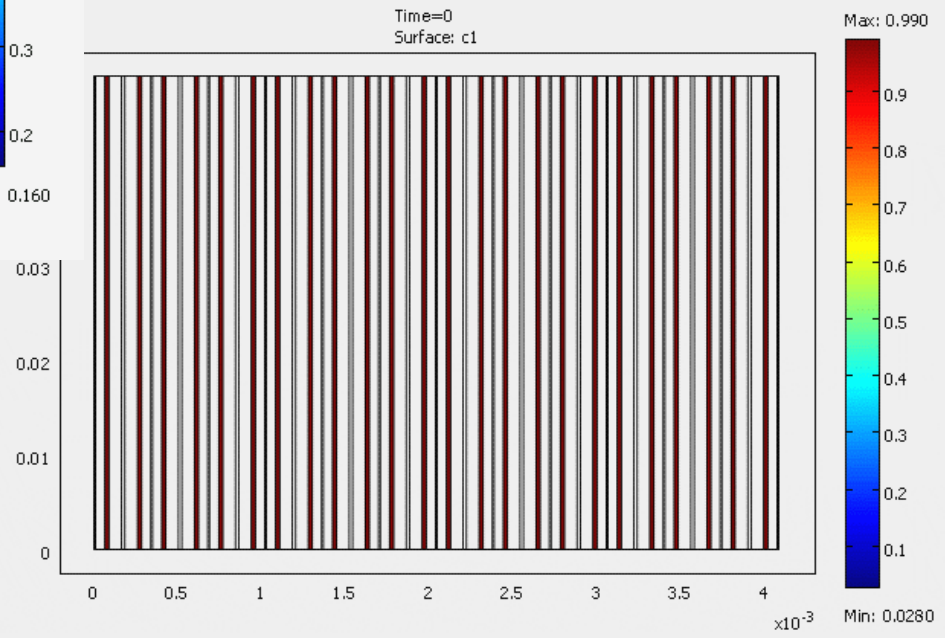
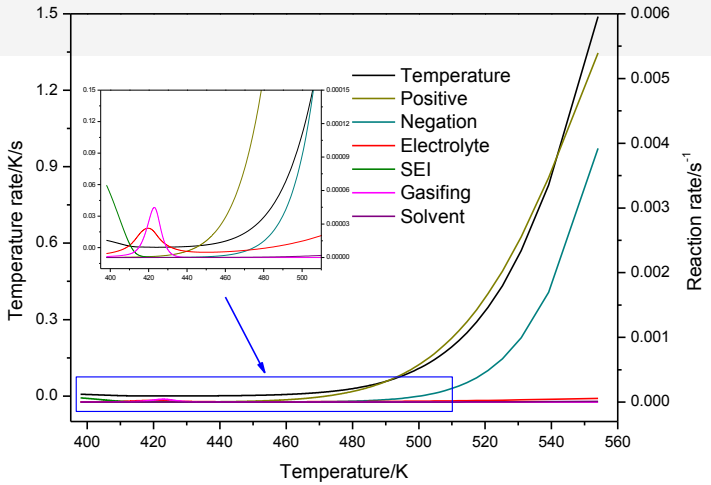
Electrode concentration




Electrolyte concentration



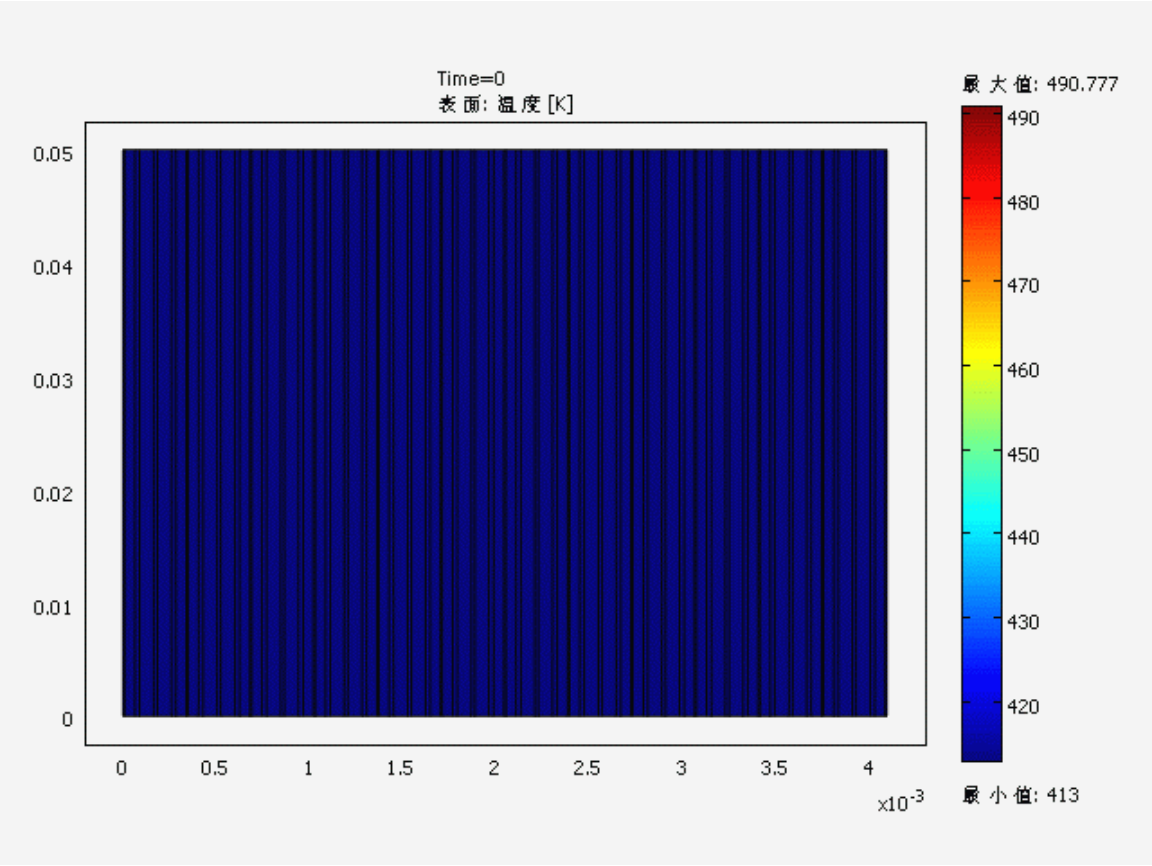



# Thermal simulation

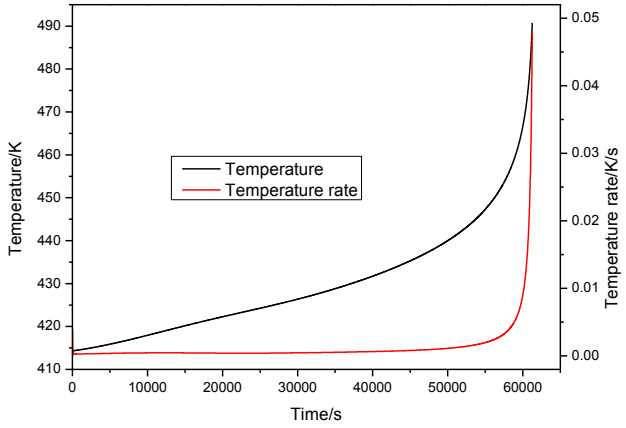
Adiabatic

$LiFePO_4$/Li-Ti-O cell

413K




Temperature



# Thermal simulation

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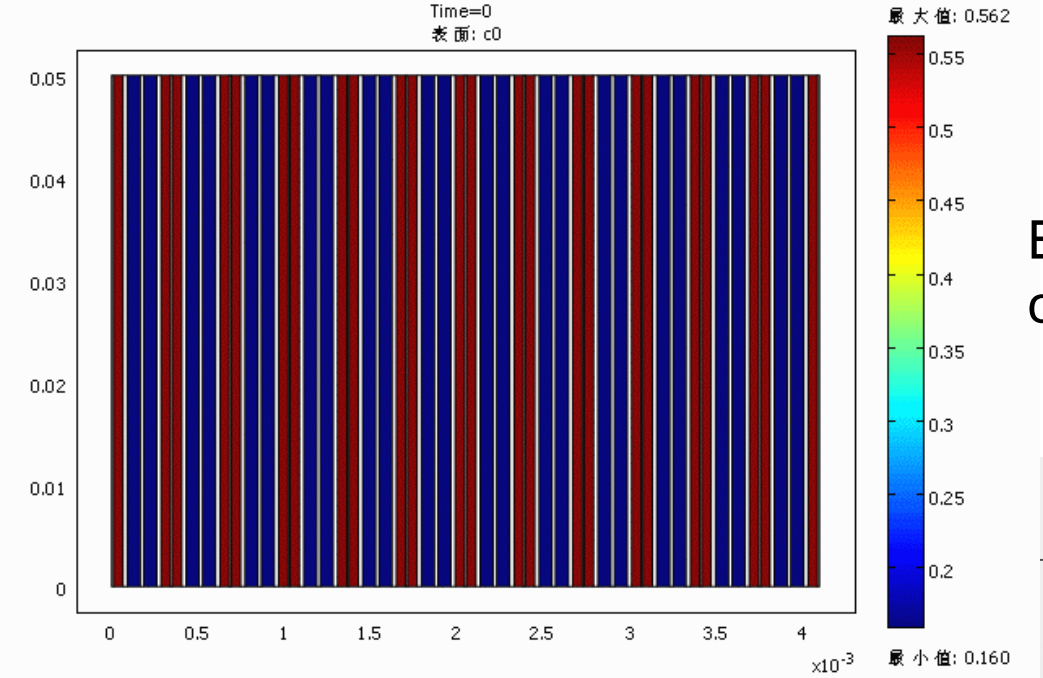
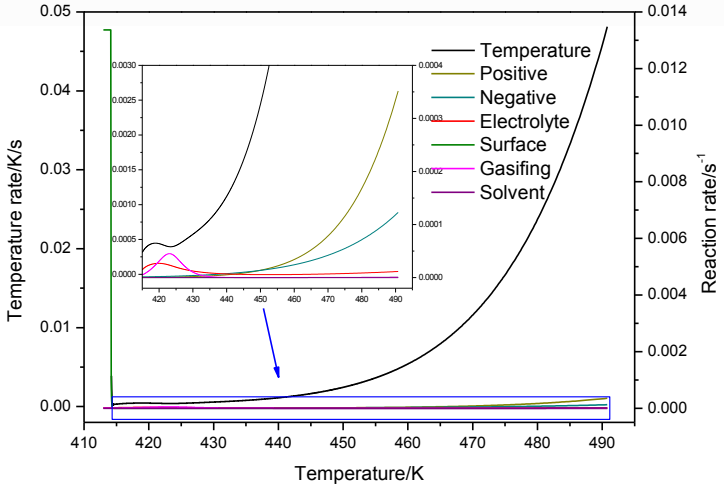


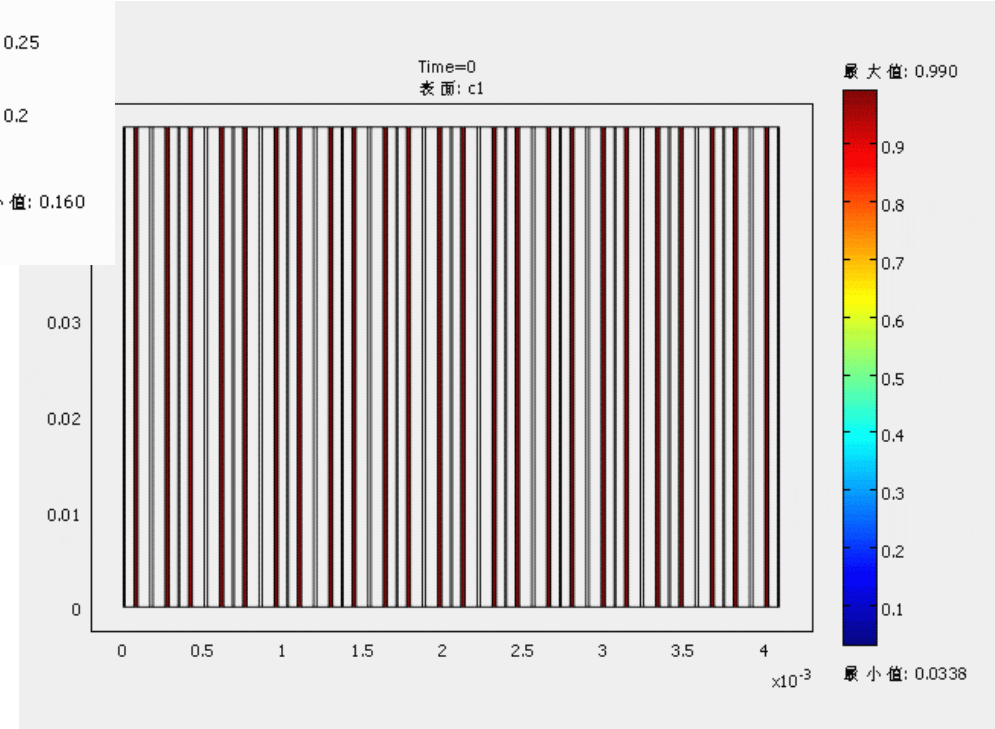

$LiFePO_4$/Li-Ti-O cell

413K

Electrode concentration

Electrolyte concentration



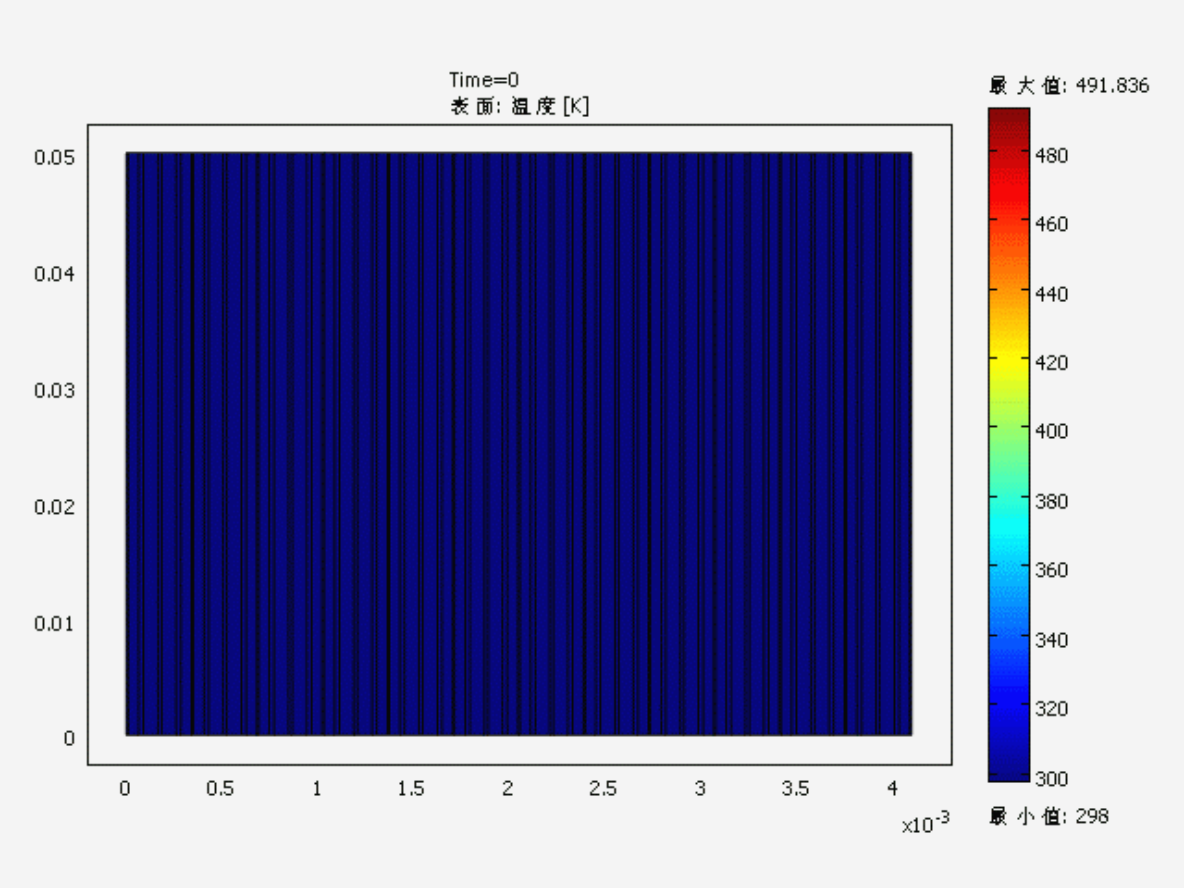



# Thermal simulation

Oven test

Li-Co-O/C cell

413K

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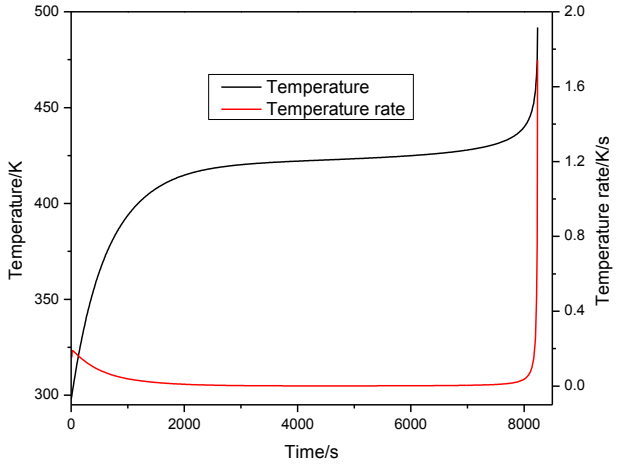

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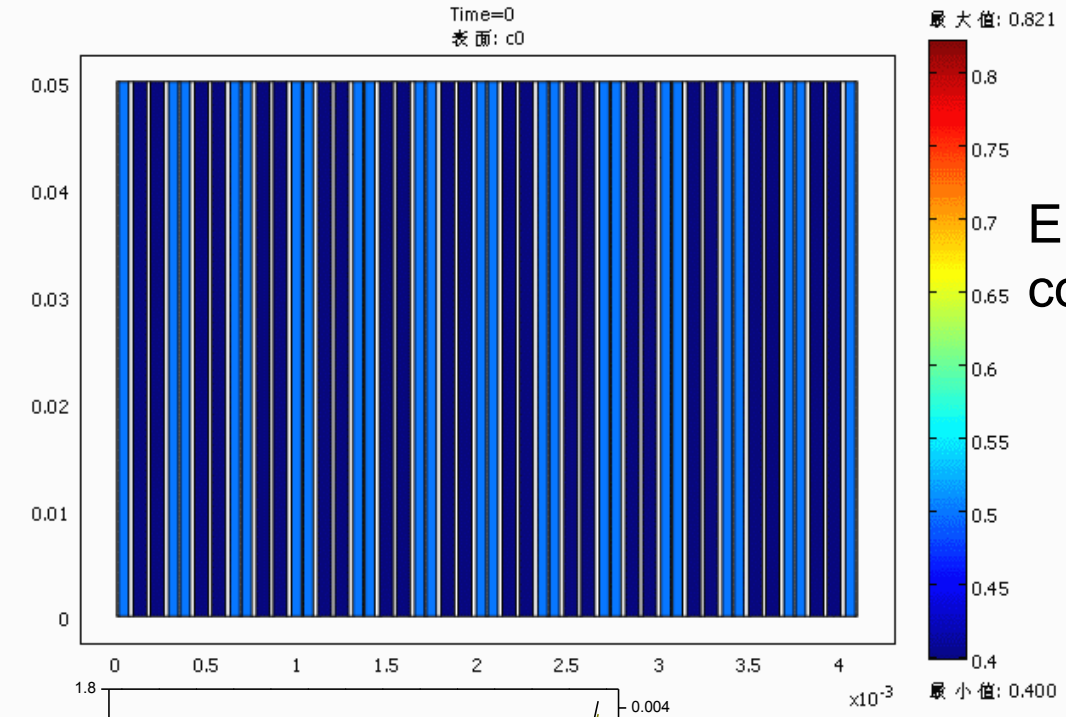
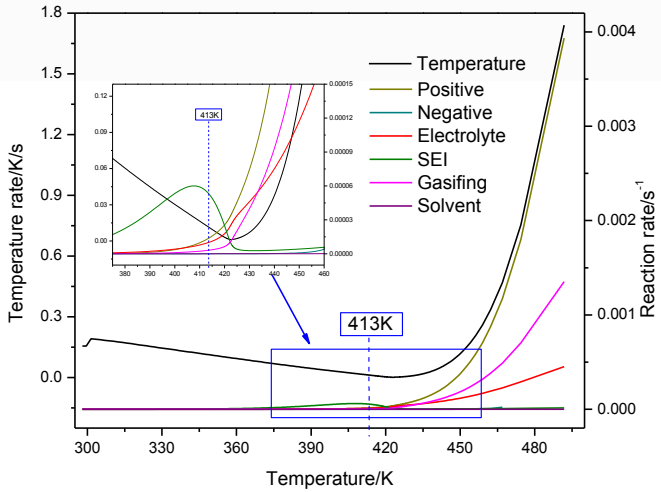
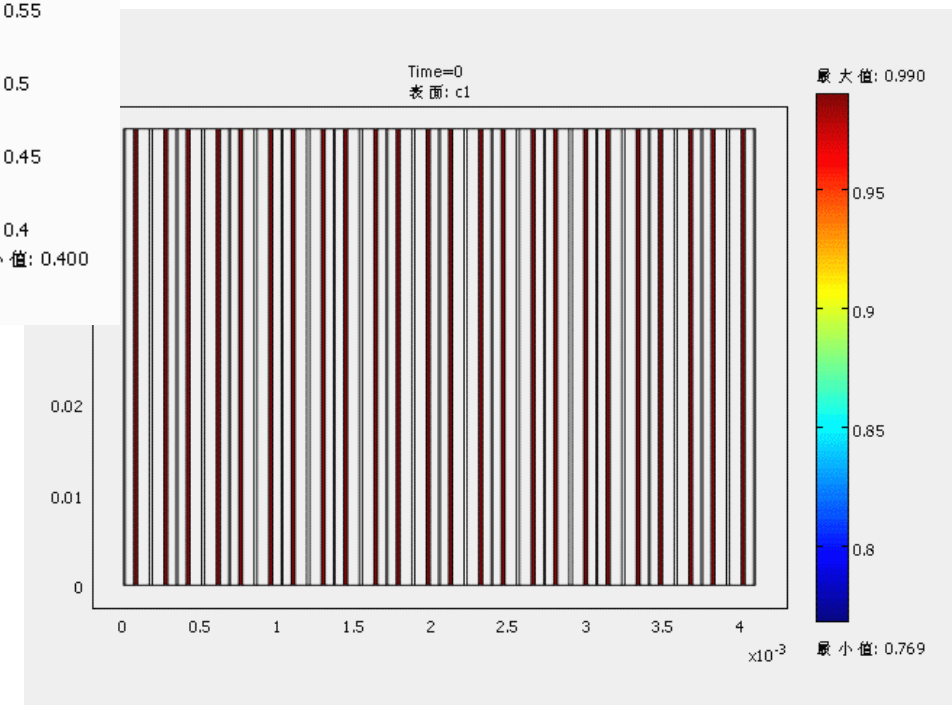


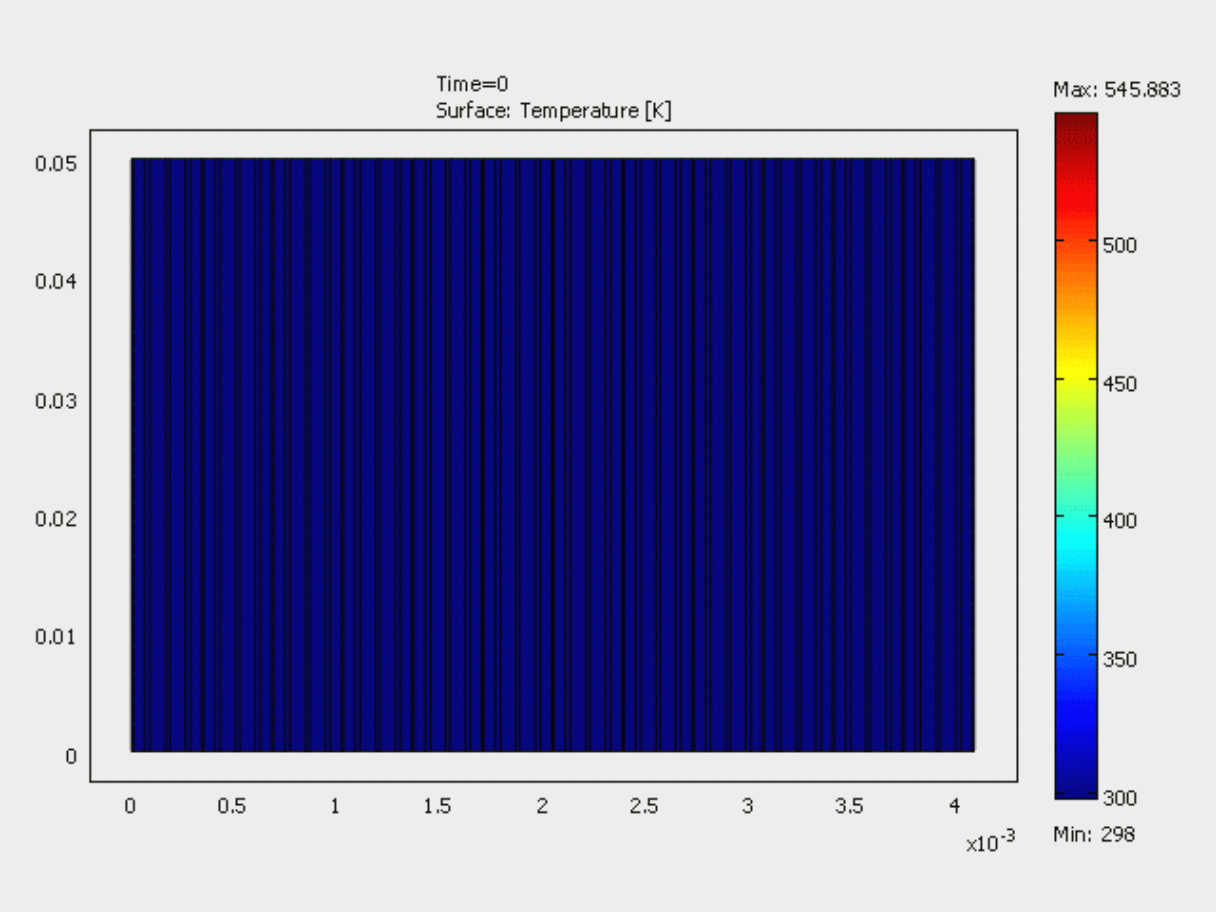



# Thermal simulation

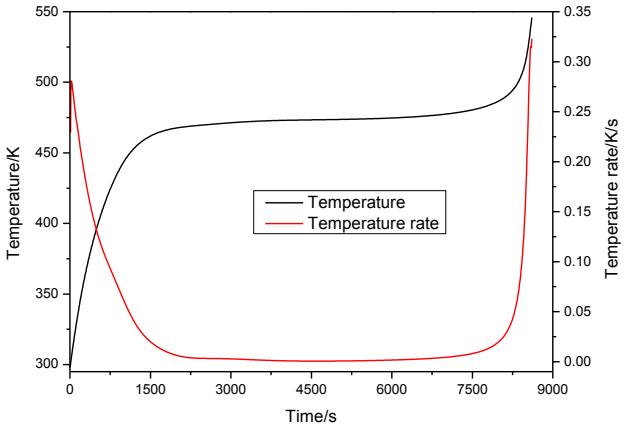
Oven test

$LiFePO_4$/C cell

468K




Temperature



# Thermal simulation

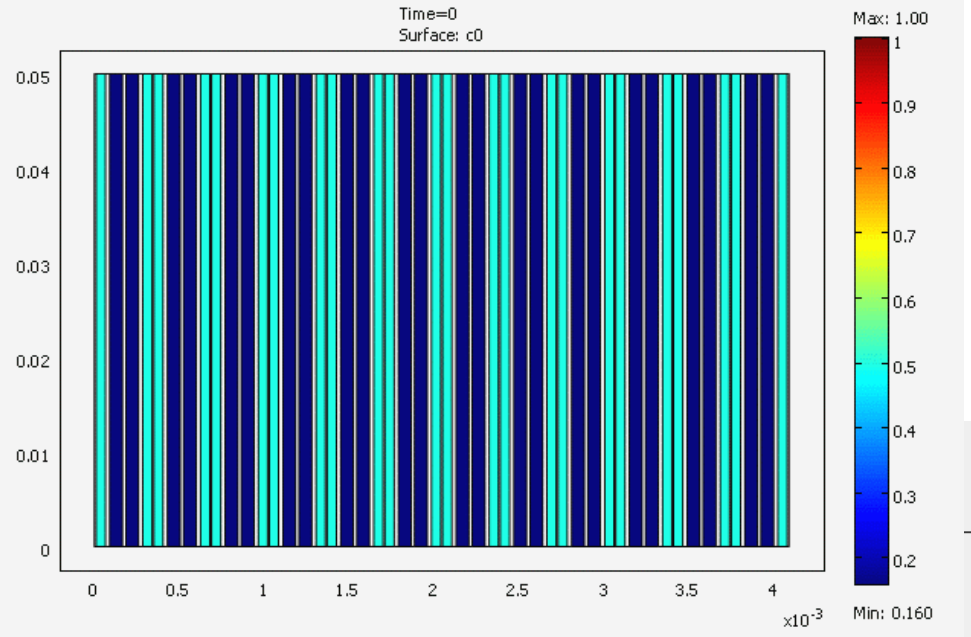
## Oven test

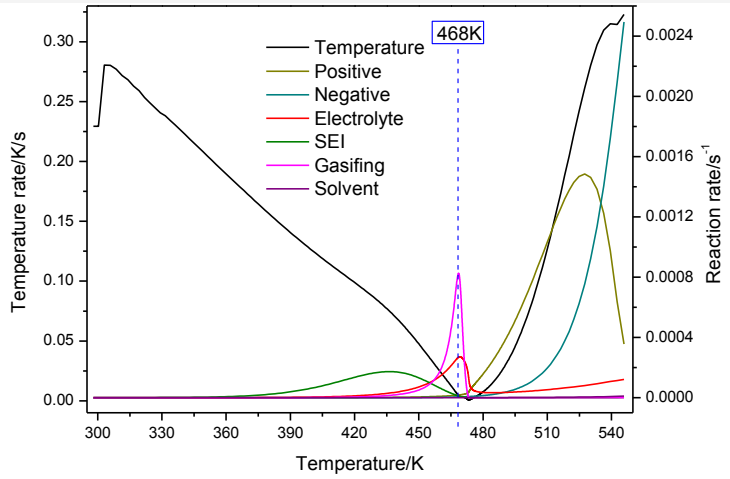
$LiFePO_4$/C cell

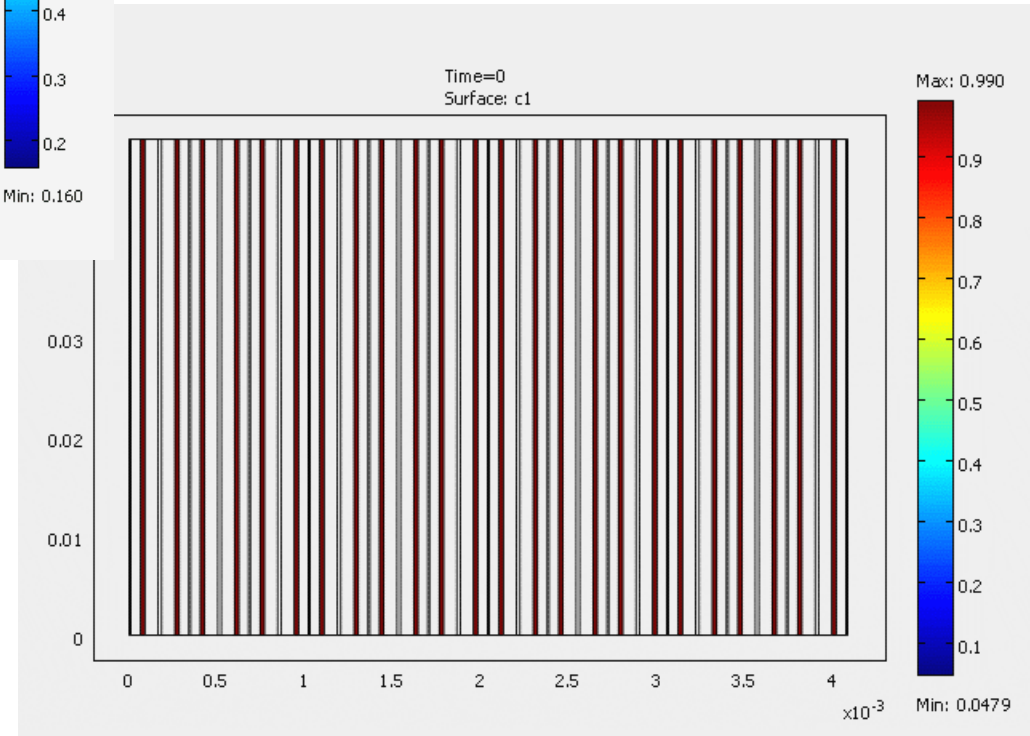
468K

Electrode concentration

Electrolyte concentration



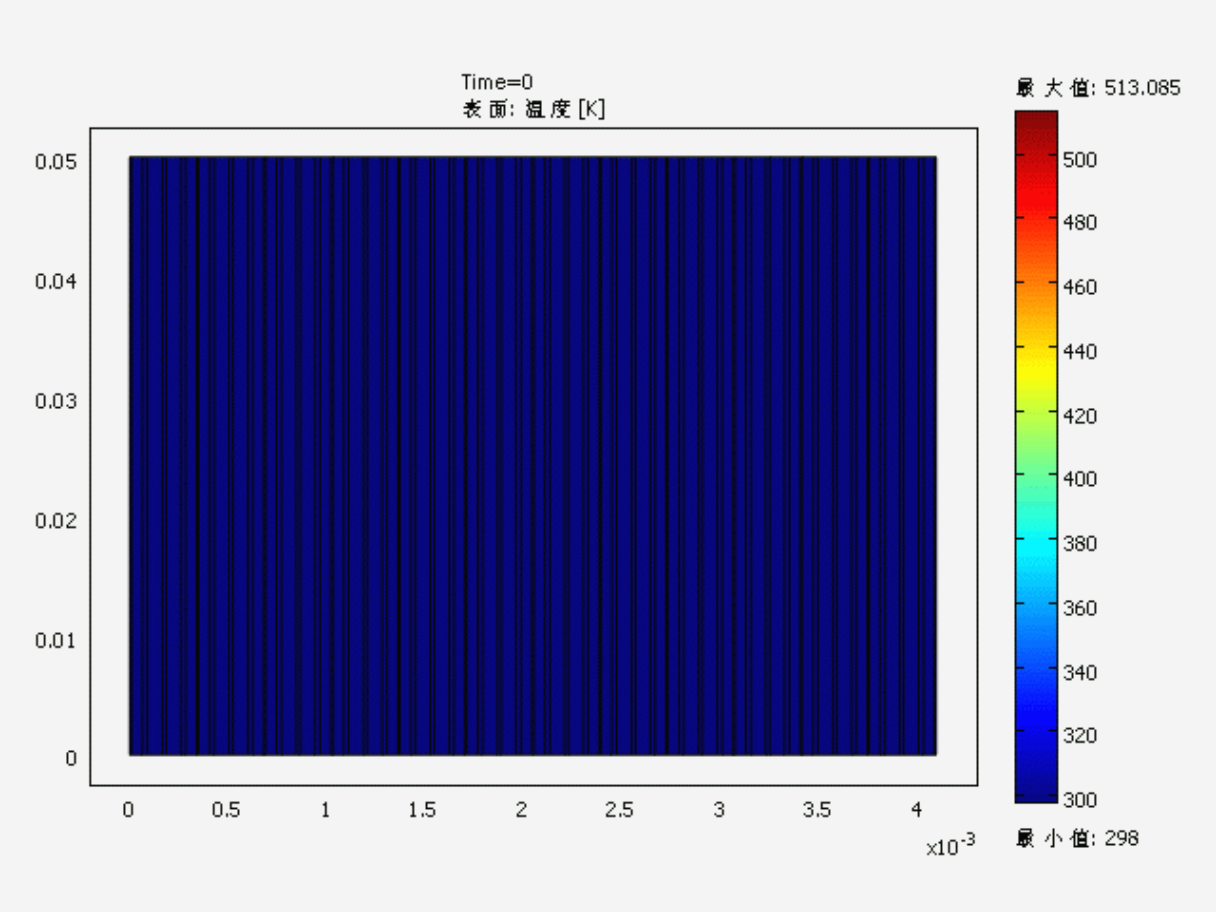



# Thermal simulation

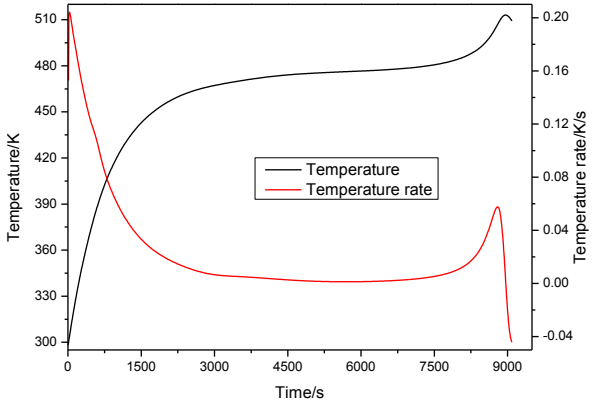
Oven test

$LiFePO_4$/Li-Ti-O cell

468K




Temperature



# Thermal simulation

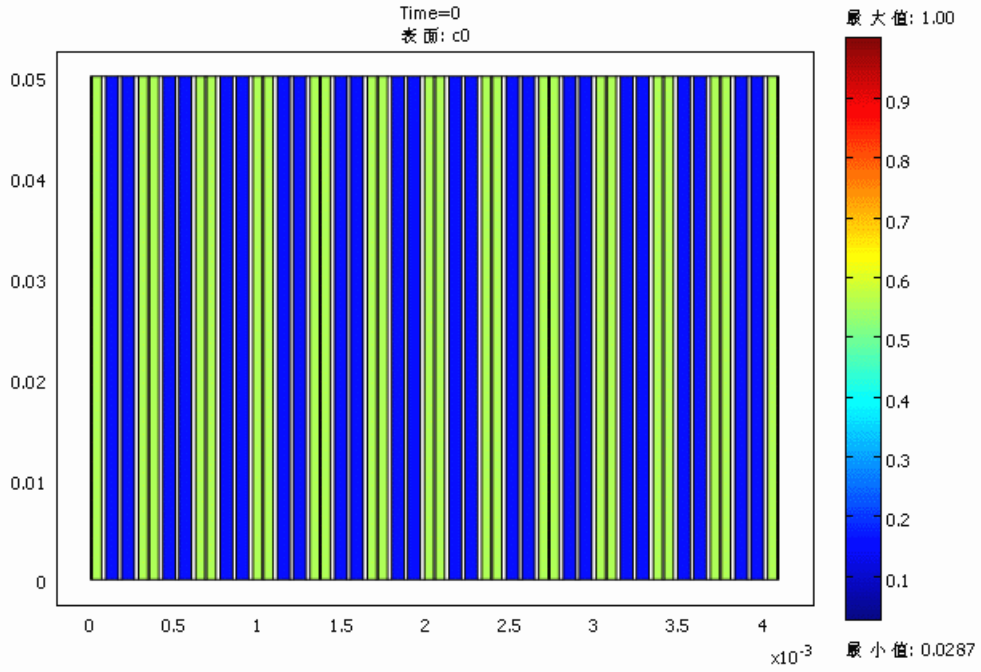
## Oven test

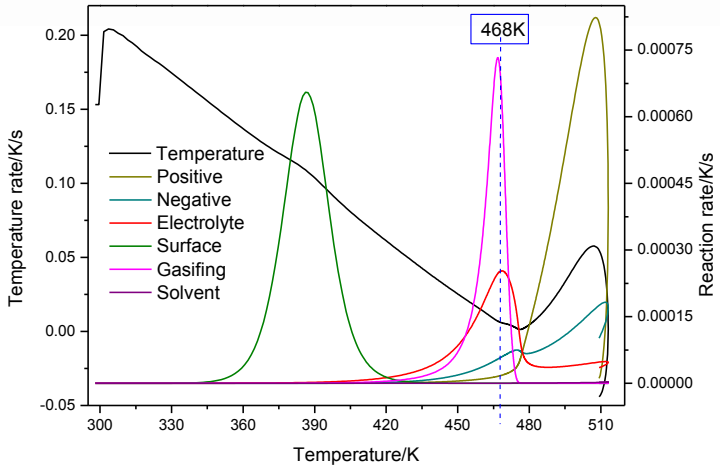
$LiFePO_4$/Li-Ti-O cell

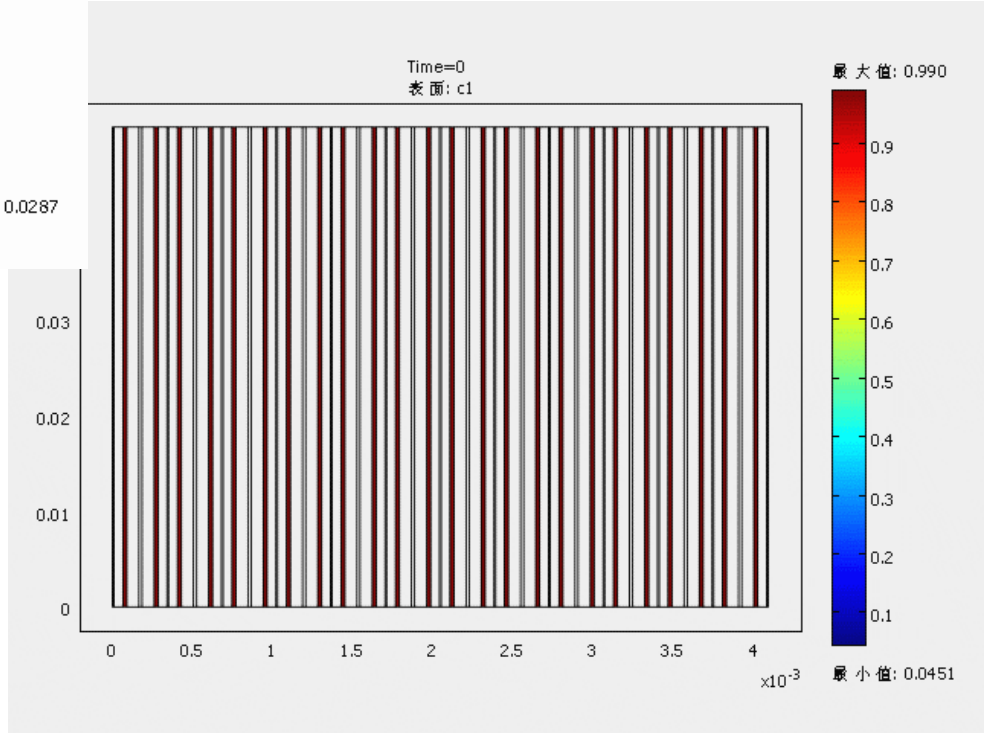
468K

Electrode concentration

Electrolyte concentration

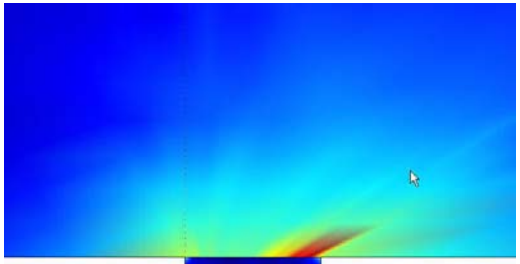


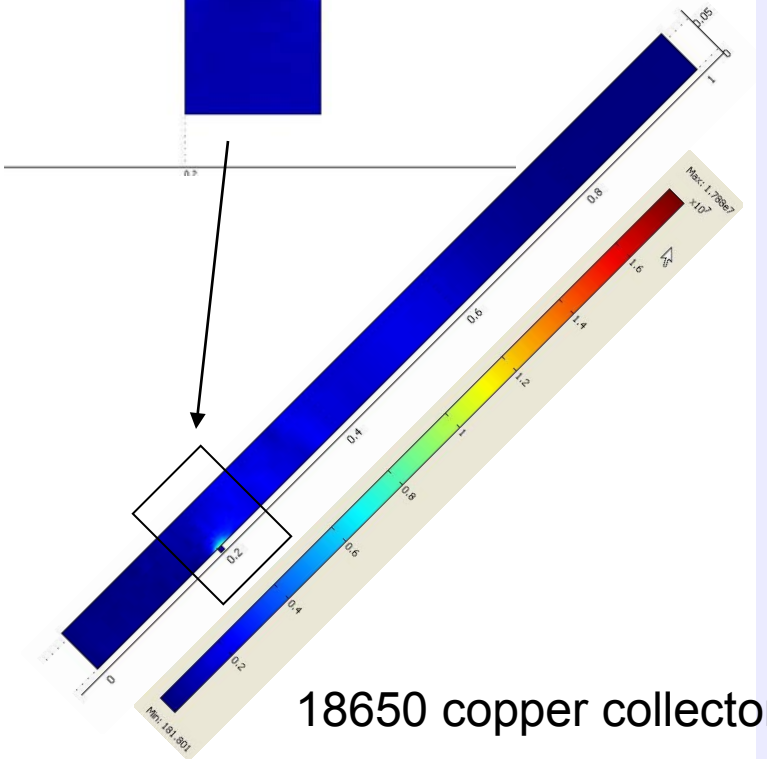



# Electric current and temperature distribution on collector

Electric current





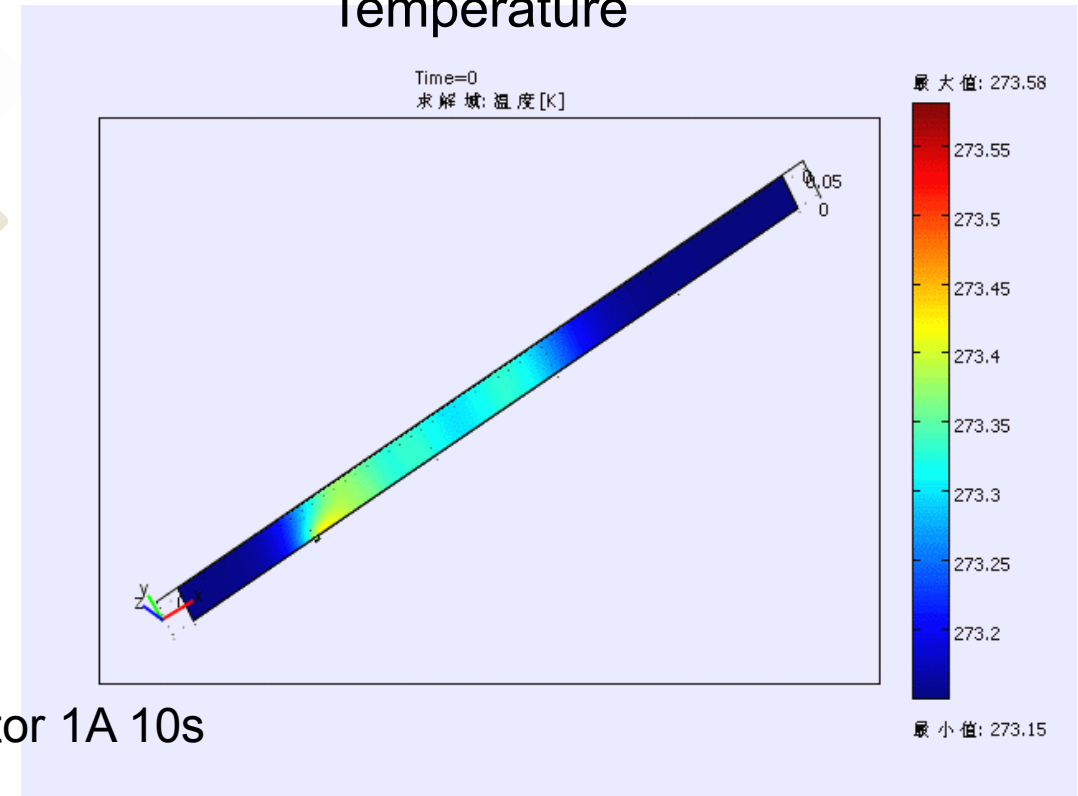
## Physical models：

Heat transfer , Static electric

## Parameter：

Conductance， , Heat transfer coefficient， Thermal capacity ， Heat conduction coefficient ， Density

Temperature




18650 copper collector 1A 10s

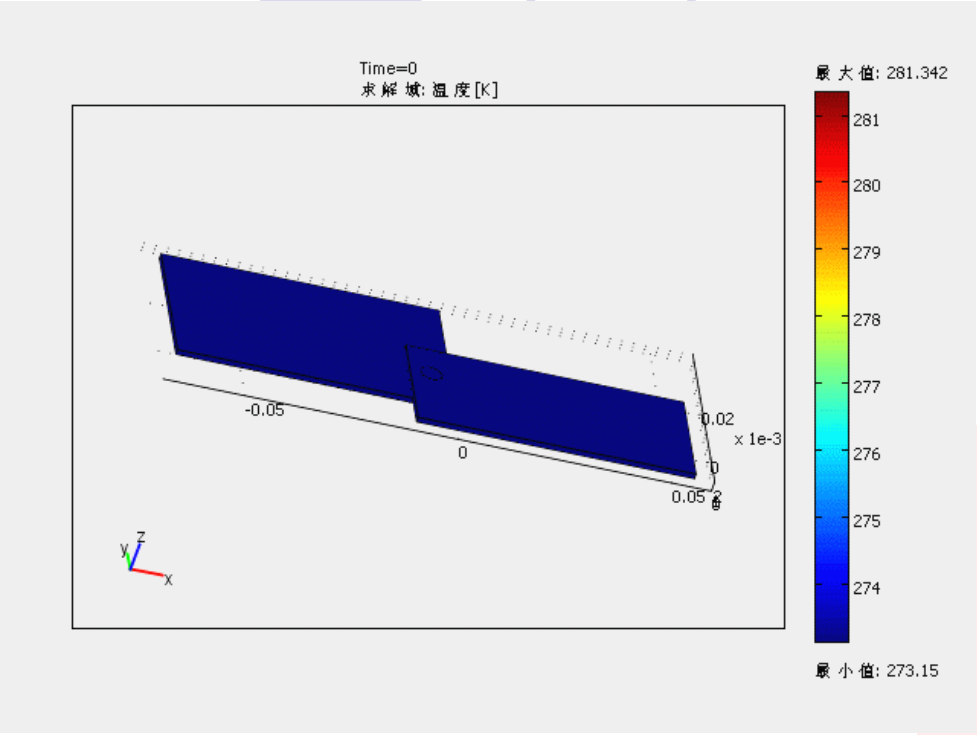
# Electric current and temperature distribution on joint

## Physical models：

Heat transfer , Static electric

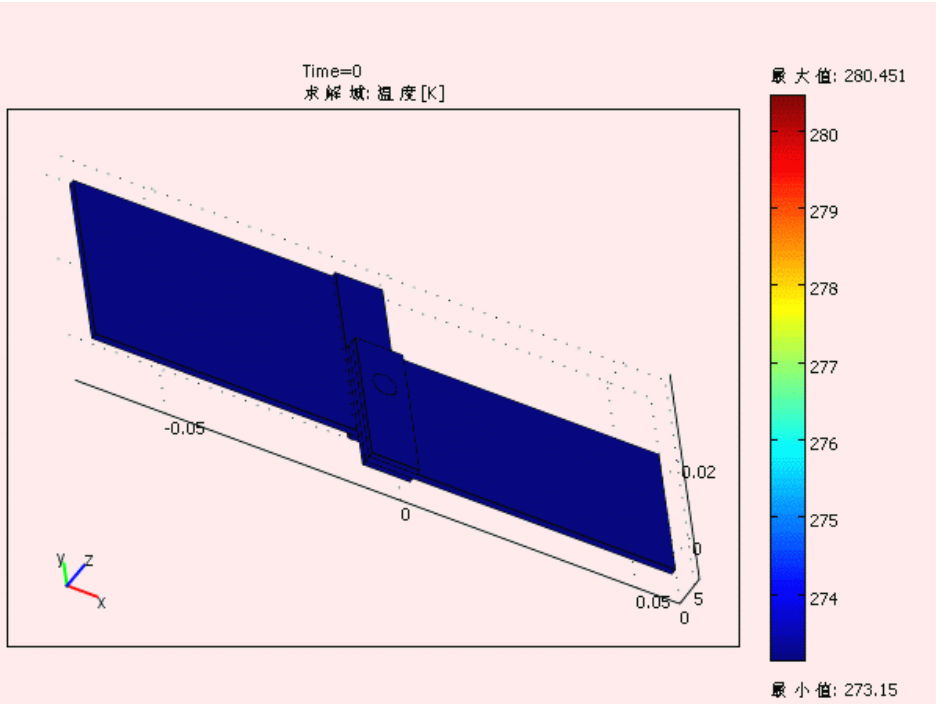
## Parameter：

Conductance，, Heat transfer coefficient，Thermal capacity，Heat conduction coefficient， Density



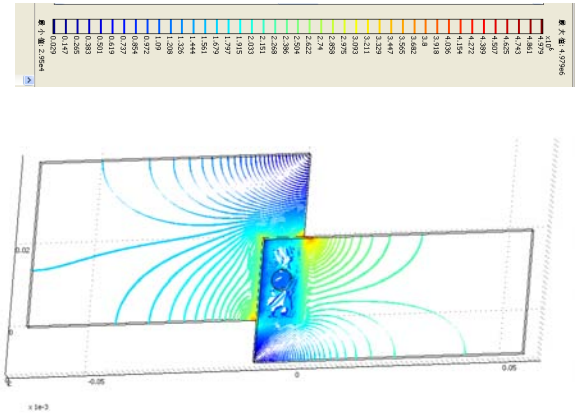

80A for 1200s

Temperature

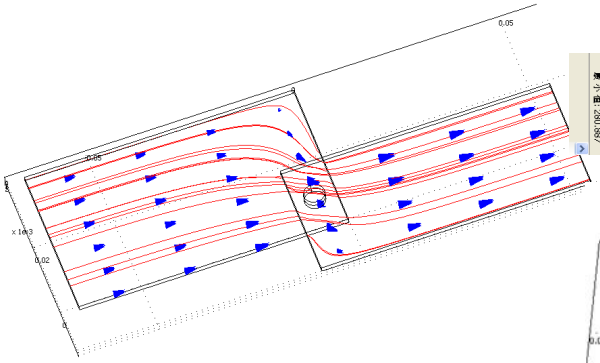


# Electric current and temperature distribution on joint

Electric current grads

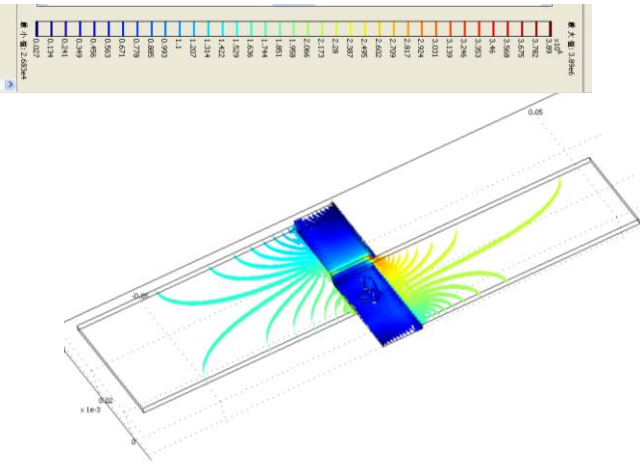


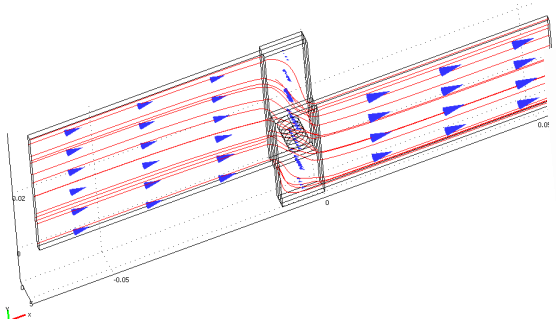
Electric current arrow

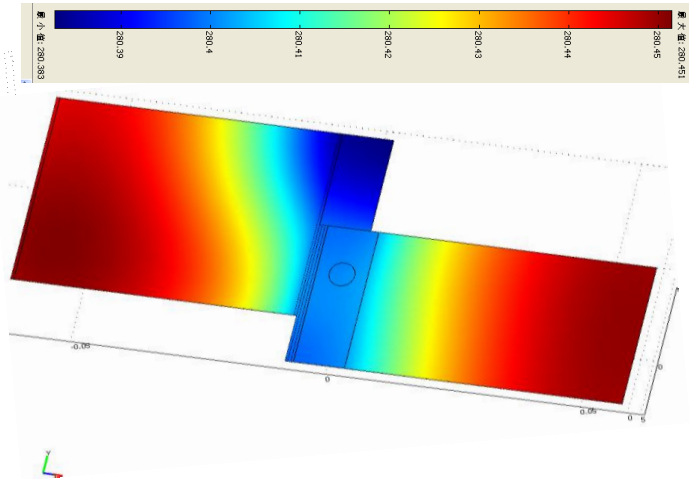


Temperature(1200s)









# Stretch and stress

18650 cell

**Physical models：**

Structure

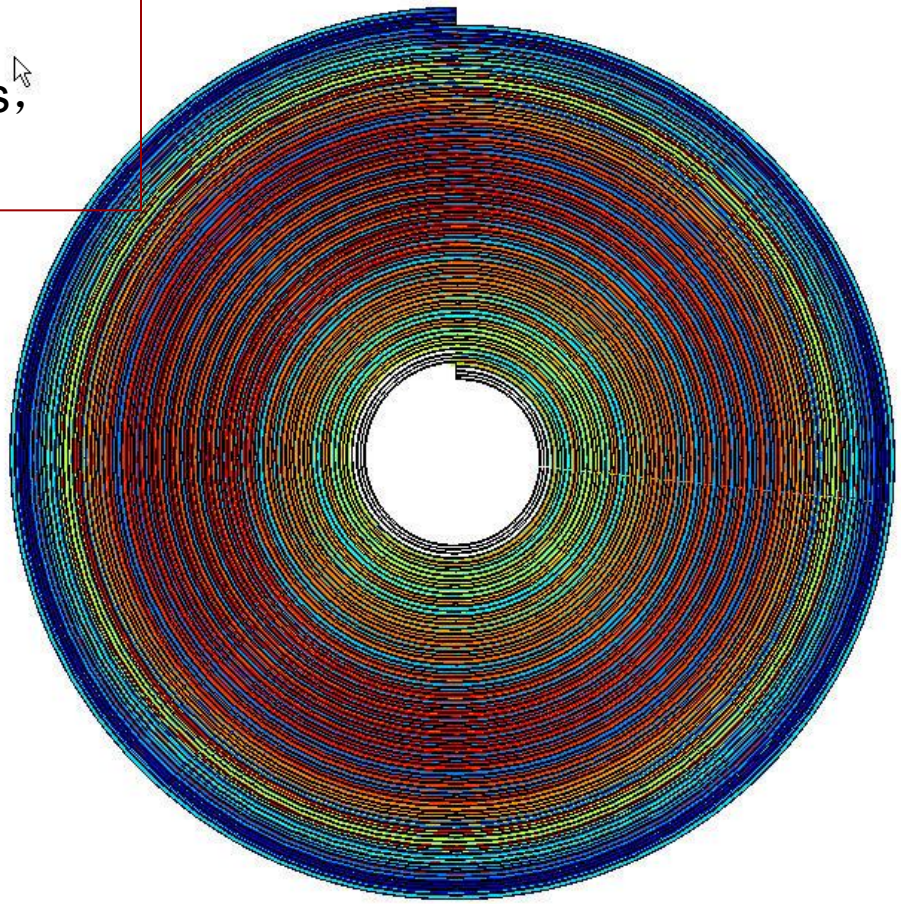
**Parameter：**

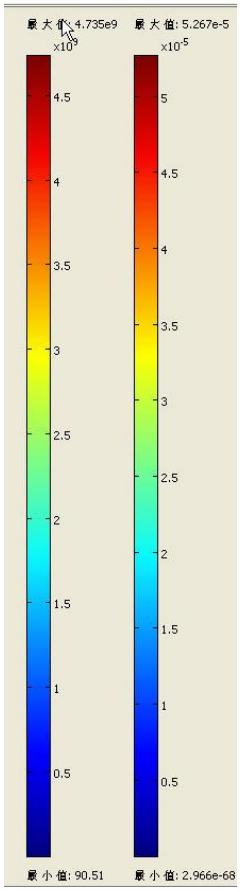
Young’s modulus,

Poisson’s ratio

Positive expanding 3%

Negative expanding 5%





# Conclusion

## Using COMSOL soft

- Simulation on charge-discharge behavior of lithium ion cells： the precision depends on models and conditions；
- Simulation on thermal and safety of lithium ion cells： availability, to forecast the cells safety under different conditions！
- Design for lithium ion cells structure： To direct the design for cell with high capacity and high rate, by analyzing the collector , stress, et al