Analysis of Electro-Thermal Hot Spot Formation in Li-Ion-Battery-Cells

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Abstract: Thermal management is a key-factor for Li-Ion-Batteries in high power applications, to stabilize cell temperature within an optimum range- ensuring efficient, safe operation and low degradation [1]. Thermal cell behavior is controlled by interaction of various mechanisms: heat transport, electrical conduction, electrochemistry and a complex geometrical structure (multi-layer winding body, contact tabs, housing). Processes are coupled: reaction and Joule's heat acting as thermal sources and all processes and parameters showing an distinct temperature dependence. Experimental means to characterize the distribution of internal quantities (temperature, heat source and current density, state of charge) during operation are limited, impeding an detailed analysis of problems as, for instance, formation of internal thermal hot spots. Purpose of the model is to provide a simulation tool that gives virtual, localized, 3D insight into essential mechanisms within a Li-Ion Cell, accounting for coupled internal electrical and thermal processes and the geometrical design features on a practically relevant level of detail.

Keywords: Li-ion-cell, electro-thermal model, homogenisation approach, 3D analysis

1. Introduction

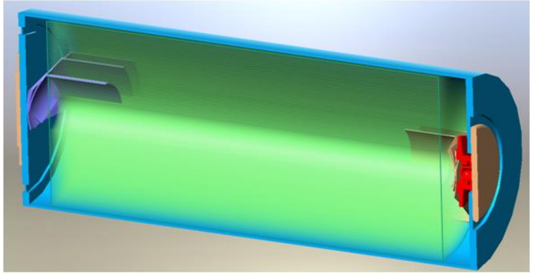

Figure 1. Geometry of a typical Li-Ion battery with winding body (green), embedded contact tabs and housing (light blue)

The formation of thermal hot spots as a possible source of thermal runaway is a worrying scenario in the operation of Li-Ion battery cells. General experience from preceding work in the thermal management of energy converters and chemical reactor components suggests, that local overheating is often emanating from design heterogeneities, acting as source for localized field concentrations. In the context of battery cells this especially applies to the internal cell contacting structure. The essential functional element of a battery is the cell laminate (consisting of 2 current collector + 2 electrode + 1 electrolyte filled separator layers) with a huge square dimension. To keep the cell within a reasonable outer dimension, the cell laminate is winded up in coils in most cases, building a winding body with dozens or hundreds of winding layers (figure 2).

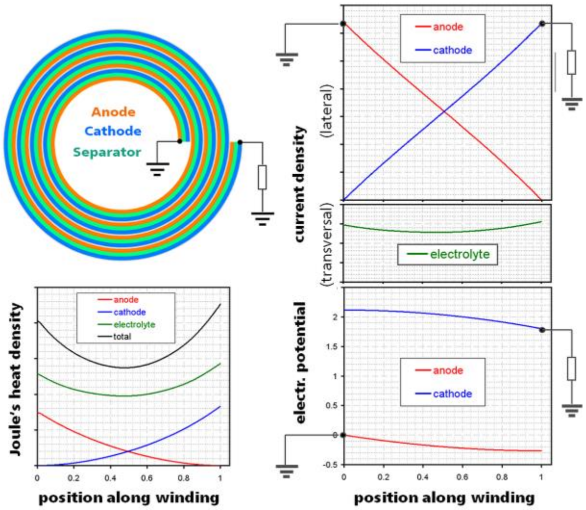

Figure 2. 2D Sketch of a section through a winded, end contacted cell laminate, with distributions of lateral and transversal current densities in the layers, electrode layer potential and Joule's heat.

The charge carriers of the battery current, crossing the electrolyte layer, have to be collected from all over the cell surface area by current collector layers and guided towards the internal contacting structure (tabs, wires, sheets). In a common design a few alternating metallic stripes are embedded between some individual windings as contact tabs, leaving large numbers of non-contacted layers between them (figure 1). The current from the total cell area is conducted to these widely separated contact tabs, following the helical winding structure and thereby accumulating and concentrating to a large lateral current density in the surrounding of the contact tabs. This process correspondingly results in concentrated sources of Joule's heat. The lateral current flow also brings on lateral gradients in the anode and cathode voltage potential (figure 2). Since the local electrode potential difference acts as a driving force for the transverse current flow through the electrolyte layer, the latter shows also an non-uniform distribution over the extent of the cell area. Cell current density is related to cell electro-chemistry and does control local distribution of reaction and Joule's heat from the electro-chemical processes. And last not least there is a strong coupling between the thermal and the various other processes by a strong temperature dependence of the material (conductivities) and process (thermodynamic) quantities, possibly influencing the intensity of field concentrations and hot spots.

The details of material and geometrical design of the cell are expected to have a strong and complex effect on the thermal management and the risk of thermal hot spot formation.

The possibilities of direct, interference-free experimental characterization and analysis of these processes in a actual cell configuration during operation mode are very limited due to the closed housing, the small structural dimensions and the tight windings. Modeling offers a chance to gain internal insight into a cell and to analyze the influence of design details on battery operation.

A model, focussed on thermal management of a individual cell design, should involve the aspects of electro-thermal coupling, anisotropic current flow and the influence of structural details (windings, contact tabs and structures). To include all mechanisms and structural features in full detail would become extremely computationally expensive. Especially the resolution of the winded cell laminate layer structure and a detailed description of the electrochemical processes (transport of Li-Ions,...) would dramatically increase the models complexity.

In the present model we apply model reduction techniques to reduce the models complexity, using a anisotropic continuum composite approach for the winding body (figure 3) and a simple empirical approach, based on experimental characterization, for the electro-chemical characteristics of the cell laminate, which will be described in the following section.

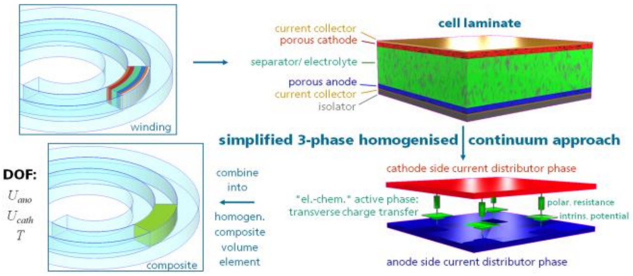

Figure 3. Homogenization approach for cell laminate

2. Use of COMSOL Multiphysics

2.1 Model geometry

A real cell (LiFePo4 38120, figure 1), analyzed by 3D x-ray tomography, served as template for the geometry model. The design consists of a cylindrical winding body for the laminate with 34 windings and 2*4 contact tabs, placed on both ends (representing batteries + and – terminals), embedded between distinct layers (being in contact with either the cathode or anode side current collector film) and connecting them to the external cell terminals by a wire and spring structure.

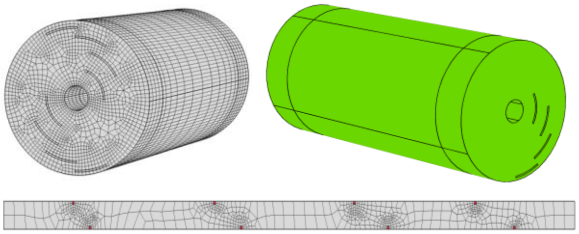

Figure 4. Geometry and mesh of the 3D thermal model node (top) and the unrolled 2D electrical model node (bottom, display axially shrinked) of the cell composite with contact tab domains (red in 2D)

In a first step the model approach was confined to the winding body with the contact tabs, using an elaborate composite approach. In a final step the model was completed by the remaining geometrical compounds (contacting terminals and housing), externally generated and imported by the CAD-interface as an separate assembly and coupled to that of the winding body.

The 3D geometry of the winding body was implemented with a parameterized approach directly using COMSOL's built-in geometry generator (figure 4). The helical structure of the windings was neglected in the mesh but was respected in the positioning of the contact tabs, which domains followed exactly the positions of the corresponding windings of the section. This was essential, because the electric model was based on a 2D domain of the unrolled cell composite and a bi-directional mapping between a distinct position at the winding in the 3d model and its projection on the 2D unrolled laminate was employed. The precision of the mapping was especially important in terms of the positioning of the tabs.

The 3D geometry of the remaining elements as housing and contacting wires was imported as an assembly from an external CAD-generator via the CAD-interface (figure 5).

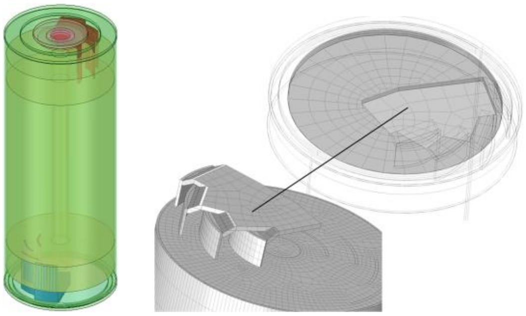

Figure 5. Model of the full cell with housing and contact structures using coupled assemblies

2.2 Hybrid Model description

Comsol 4.2a was used for the analysis. In an initial attempt a straight forward- both thermal and electric- 3d anisotropic composite approach was implemented for the winding body. For the thermal part, the simplification of the helical winding structure by a circular anisotropy of the thermal conductivity proved adequate. For the electrical part, due to the large discrepancy between transversal (through electrolyte and between neighbored winding layers) and lateral (along current collector layers) electrical conductivity, current flow does proceed on a helical path, following the tight winding structure. A helical- slightly tilted with relation to circular-anisotropy was expected to reproduce the helical current flow on a mesh, coarser than the individual windings. This did not work, causing unstable behavior and inadequate results.

We therefore developed an hybrid approach (figure 6) for the winding body domain with a

- 2D description of the electrical problem on the cell laminate, unrolled to a plane electrical composite and a
- 3D description of the thermal problem with a 3D circular anisotropic thermal composite

The two model nodes were coupled and simultaneously solved taking full advantage of the embedded COMSOL features (simultaneous model nodes and coupling variables via general extrusion).

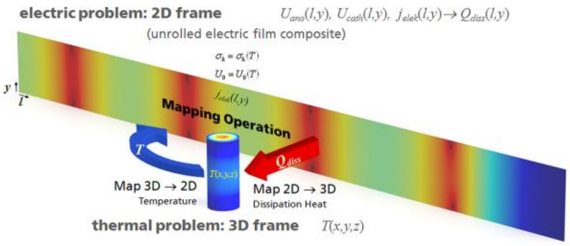

Figure 6. Hybrid 2D electric- 3D thermal composite approach with mapping of temperature (3D→2D) and Joule's heat (2D→3D) information between the model nodes.

The thermal model node of the winding body (with contact tabs) applies a thermal conduction mode with circular anisotropy in the original 3D-domain (eq. 1). The electrical model node on the 2D domain of the unrolled battery film (with contact tabs) distinguishes 2 DOF's for the electrical potential distribution along the anode and the cathode electrode film, solving a 2D PDE for electrical conduction within each electrode plane (eq. 2 and 3). Both PDE's are connected by specific charge carrier source terms, accounting for distributed charge transfer through the electrochemically active electrolyte layer (eq. 4). These terms reflect the electrochemical characteristics (electrolyte current density as function of anode-cathode voltage difference, temperature and state of charge). For that we used an simple empirical model approach (Shepherd's model [2]) (eq. 5) for battery cells, based on analytical terms which are weighted by a set of scalar, temperature dependent parameters. The latter were obtained by fitting from elaborate experimental characterization of example cells. The simple approach was able to nicely reproduce real cell behavior over a wide range of temperature (figure 7) and discharging rates [3].

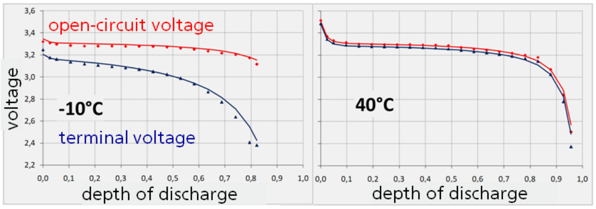

Figure 7. Evaluation of the empirical Shepherd model (lines: model, points: exp.) for the electrical characteristics from discharging of a sample cell.

To couple the 2D electrical and the 3D thermal model nodes, information on local temperature (3D→2D) and local heat production (2D→3D) had to be simultaneously mapped and transferred between the models during solution process. The mapping follows the helical path of the center line of the winding helix and assigns a (x,y,z) position in the 3D-model of the winding body the corresponding length (and height) position (l,h) on the unrolled 2D-model of the cell laminate. It was implemented employing analytical description functions for an Archimedean spiral, making use of coupling variables with general extrusion. For the opposite direction (2D→3D) an inverse approach was used, but had to be complemented by a linear interpolation process for the mapped quantities, to fill the coordinate space in 3D left undefined between the mapped center line of the spiral.

Anisotropic material properties were obtained from a composite approach for the cell laminate, using bulk literature values for the various layer materials. The thermal composite properties include all layers while the electrical properties distinguish a anode side sub-composite (anode layer + anode side current collector layer) and a cathode side sub-composite (cathode layer + cathode side current collector layer). Properties of the separator layer are used for the formulation of the source terms. Within the domains of the contact tabs (assumed as copper), the excellent conductivity of that material dominates the composite properties,

As electrical boundary conditions the cell terminal potential values were applied to the corresponding end faces of the contact tabs. As thermal boundary conditions free convection to air and surface to ambient radiation was assumed at the external surfaces.

For the full model including external contact structures and housing, the winding body was coupled at all external faces to the housing. The end faces of the tabs were thermally and electrically coupled to the corresponding ends of the terminal contact structures. Free convection/ radiation was assumed at the housing external boundaries together with prescribed potential values at the external terminal faces.

2.3 Governing Equations

Thermal balance with Joule's heat source term:

$$\rho \cdot c_{p,eff} \cdot \dot{T} - \nabla \cdot \left(\boldsymbol{\lambda}_{eff} \cdot \nabla \cdot T \right) = \sum_{k=elec,ano,cath} (\boldsymbol{\sigma}_{eff,k}^{-1} \cdot \mathbf{j}_{el,k}) \cdot \mathbf{j}_{el,k} + \ldots \tag{1}$$

Cathode sub-composite layer charge balance:

$$-\nabla \cdot \left(\boldsymbol{\sigma}_{eff,cath} \cdot \nabla \cdot U_{cath} \right) = + \frac{j_{elec}}{h_{uc}} \tag{2}$$

Anode sub-composite layer charge balance:

$$-\nabla \left(\boldsymbol{\sigma}_{eff,ano} \cdot \nabla U_{ano} \right) = - \frac{j_{elec}}{h_{uc}} \tag{3}$$

Transverse electrode current density characteristics:

$$j_{el,elec} = \frac{U_{cath} - U_{ano} + U_0(T, \ldots)}{R_{el}^{A}(T, j, \ldots)} \tag{4}$$

Shepherd's empirical model approach:

$$j_{el,elec} = \frac{U_{cath} - U_{ano} - U_s + a(T) \cdot e^{-b \cdot DoD} - \left(d'(T) + \frac{k'(T)}{1 - DoD} \right) \cdot DoD}{\frac{k(T)}{1 - DoD} + l(T)} \tag{5}$$

$\boldsymbol{\sigma}_{eff,cath}$	anisotropic electrical composite conductivity tensor for component k
$\boldsymbol{\lambda}_{eff}$	anisotropic composite thermal conductivity tensors for component k
h_{uc}	total thickness of cell lamuinate
DoD	Depth of Discharge of the cell
a, b, d', k, k'	parameter set for Shepherd model

3. Model Results

We started the investigation with a stationary analysis of the cell under different operation conditions. Exemplary results are shown in figure 8 for the Joule's heat, obtained from 2D electric model node and simultaneously mapped to the 3D thermal model node, where it provides the thermal source term. The mapping approach worked fine and precise. Joule's heat production takes place over the whole cell laminate area but there are strong concentrations (up to 400%) in the vicinity of the contact tabs from the current collection effects. In the 3D domain this sources remain restricted to the thickness of one winding layer plane, while the neighbored windings are not concerned.

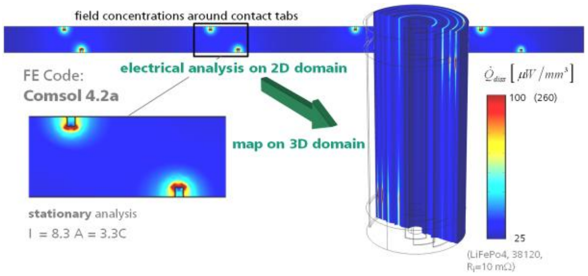

Figure 8. Model Results for Joule's heat from a stationary load case.

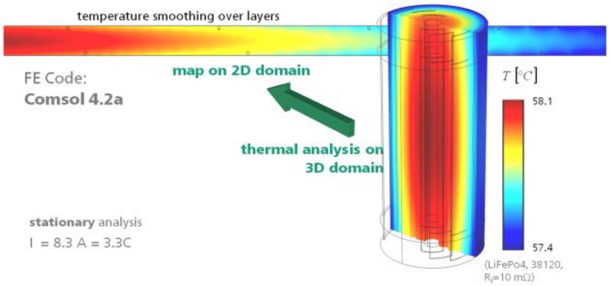

Figure 9. Model Results for temperature from a stationary load case.

The thermal results for the stationary load case are shown in figure 9. It was surprising, that the strong concentration of the thermal sources around the contact tabs did not become reflected correspondingly by hot spots in the temperature distribution. In the stationary case the tightly localized heat may apparently easily diffuse away from the tab regions to neighbored windings without inducing appreciable temperature gradients.

During operation in high power applications battery cells have to sustain strong, short current pulses (<10 s) with discharging rates up to 40-60 C. Such a case was employed as a template scenario for a transient analysis load case (figure 10). Figure 11 and 12 display the effect of a strong (40 C), short (5 s) discharging current pulse on temperature behavior. The model indicates for strong transient current loads, that the contacting structure may act as a possible source for the formation of temperature hot spots, which will also advance to the neighboring layers. The effect is limited to some K in the current model but may be much larger in reality due to the effect of additional heat source mechanisms from electro-chemistry and thermodynamics (reaction heat, reversible heat), not yet considered in the analysis. Another possible reason is that the inserted contact tabs may perturb the tight winding structure between the windings in that regions, inducing voids with reduced thermal conductivity, thereby contributing to local overheating.

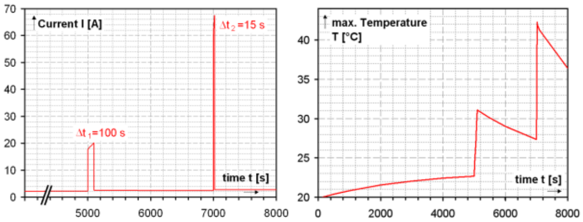

Figure 10. Analysed transient discharging scenario with short current pulses.

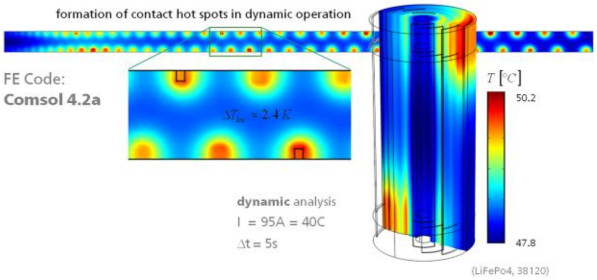

Figure 11. Model results for temperature from the transient analysis (current pulse).

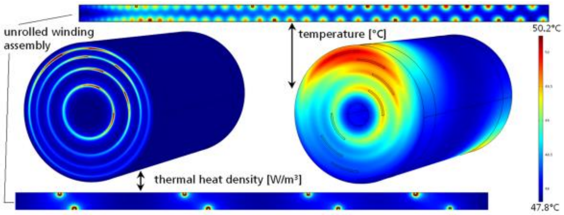

Figure 12. Model results for temperature from the transient analysis (current pulse).

In a final stage, the model was extended to the analysis of a complete cell geometry that includes housing and terminal structure (figure 13). The model proved its capability to do that job successfully, providing comparable results to the foregoing analyses for the separate winding body.

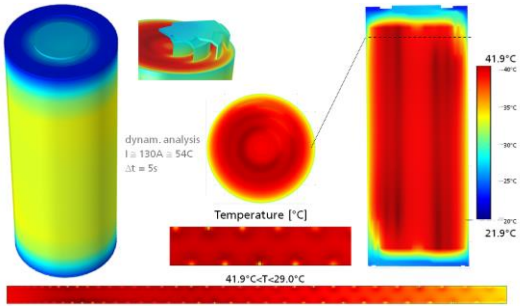

Figure 13. Model results for temperature distribution from a transient analysis with the full cell model .

4. Conclusions and Outlook

The presented model approach offers a computational efficient tool to analyze the influences of geometrical design details, material selection and operational conditions on the electro-thermal behavior of a full Li ion battery cell geometry. It considers typical aspects as anisotropic winding structure, electro-thermal coupling and nonlinear electrical characteristics for moderate computational costs. That becomes possible by employing elaborate model reduction strategies, taking full advantage of the flexible features offered by the COMSOL code: using an homogenized 3 DOF phase composite model for electric and thermal conduction in the cell laminate, a simple empirical, experimental based, submodel for the electro-chemical characteristics and a hybrid coupled 2D-3D approach for the electrical and thermal interactions in the winding body. The model proves the responsibility of the heterogeneities of the contact structure for the formation of localized thermal sources in the winding body, that may result in the formation of dangerous thermal hot-spots, especially for dynamic operation scenarios with high rate current pulses.

In future work the model may be extended by considering the influence of additional thermal sources as reaction and reversible heat, linked to the electro-chemical nature of battery operation. Also transient effects in the electrical characteristics, related to electro-capacitive mechanisms, should be included. All this could be more or less easily included into the frame of the presented model under the premise of the availability of corresponding detailed data, which must be drawn from elaborate experimental characterization and evaluation. Also a better knowledge over the details of geometrical design, obtained by direct communication with the manufacturer could further improve the quality of the model description. If all that information can obtained for a specific real cell sample, the model predictions should be evaluated by an elaborate electro-thermal experimental characterization campaign.

8. References

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