

A 'Microscopic' Structural Mechanics FE Model of a Lithium-Ion Pouch Cell for Quasi-Static Load Cases

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ABSTRACT

This study deals with the experimental investigation of the mechanical properties of a lithium-ion pouch cell and its modelling in an explicit finite element simulation code. One can distinguish between 'macroscopic' and 'microscopic' modelling approaches. In the 'macroscopic' approach, one material model approximates the behaviour of multiple inner cell layers. In the 'microscopic' approach, which is used in the present study, all layers and their interactions are modelled separately.

The cell under study is a pouch-type lithium-ion cell with a liquid electrolyte. With its cell chemistry, design, size and capacity it is usable for automotive applications and can be assembled into traction batteries.

One cell sample was fully discharged and disassembled, and its components (anode, cathode, separator and pouch) were examined and measured by electron microscopy. Components were also tensile tested. In this way, each component was fully characterised with respect to the properties needed for explicit finite element models.

Multiple quasi-static mechanical tests at different state of charge (SOC) levels under various load cases were conducted. Test results were used to validate the numerical cell model.

Simulation of the mechanical behaviour of individual cell layers and the entire cell showed a very reasonable correlation with experimental testing. The developed structural mechanics model for quasi-static load cases is a solid starting point for future analyses, and opens the possibility to predict cell damages with explicit finite element simulations.

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INTRODUCTION

Due to the global warming partially caused by emissions of conventional motor vehicles, alternative vehicle concepts are gaining importance in order to preserve individual mobility. Approaches to reduce emissions in vehicle operation include hybrid and fully electric vehicles. Many of these vehicle concepts need an electric energy storage system (EESS). The main research topics in this field are battery lifetime, the driving range of electric vehicles and safety. Improvements to battery technology are very important for wide acceptance of alternative traction concepts.

Improvements also concern the robustness of the battery against fire, venting or spill in case of a crash. In vehicle safety research, finite element simulations - combined with as few physical tests as possible - are state-of-the-art to keep development costs low. Physical tests are expensive and are a potential hazard to human health, equipment and environment [1]. Hence reliable finite element models of the EESS for crash calculations are imperatively needed.

There are two approaches for modelling lithium-ion cells in an explicit finite element crash code: 'microscopic' and 'macroscopic'. This study deals with a 'microscopic' modelling approach. This means that all layers (pouch,

separator, copper anode, aluminium cathode and active materials) are modelled separately. This study is the first, to the knowledge of the authors, to attempt a 'microscopic' modelling of an EESS. Other publications, e.g. [2], [3] and [4], deal with the 'macroscopic' approach, where one element layer represents more cell layers (sometimes referred as a 'representative volume element'). In these publications ([2], [3] and [4]), various test methods for cell model validation have been described, which were adopted and applied in the present study. The aim of the present study is the development of a single model applicable to arbitrary mechanical load cases. In previous publications, separate models had been created for different load cases.

For 'microscopic' modelling, mechanical testing of each component is necessary to obtain data for defining material cards (the input deck for material parameters) and validating the material behaviour. The thickness of each layer was measured by electron microscopy. Conventional thickness measurement (e.g. micrometre) was not applicable, as the active material could not be detached from the metallic foil.

Further, the active material layers were found to be very compliant and vulnerable, thus non-contact measuring techniques were preferred. Electron microscopy enabled non-contact thickness measurements of the electrodes (consisting of metallic current collector and attached active material) and pouch (consisting of aluminium foil as well plastic coating). At the same time, electron microscopy allowed the analysis of the surface condition of each layer.

Tensile tests of the components (anode, cathode, separator, and pouch) were conducted to obtain material parameters. Mechanical tests with the entire cell - charged, uncharged and fully discharged - were performed to validate the structural behaviour of the cell model, which is very important for the modelling of the interactions between the single layers.

Currently, original equipment manufacturers', e.g. Audi's, requirements for the vehicle structure do not allow any EESS deformation in internal, legislative or consumer crash tests [5].

Profound knowledge of EESS behaviour under crash loading and advancements in the modelling of EESS are key features for a lightweight design of electric vehicles. This leads to a permission of EESS deformation to a certain extent without exceeding a predefined hazard level.

DESCRIPTION OF THE METHODOLOGY

For this study, a lithium-ion polymer pouch cell with LiMn_2O_4 as cathode active material was used. During disassembly, safety measures for human and environment were taken. Detailed technical cell data are summarized in Table 1. This cell is similar to cells applied as vehicle traction batteries, but has a relatively small capacity. This means a low risk in mechanical tests [1], but results are still comparable to other automotive pouch cells.

Table 1. Technical data of the lithium-ion polymer pouch cell

Positive Material		LiMn_2O_4
Negative Material		Graphite
Voltage	Average	3.8V
	Maximum	4.2V
	Minimum	2.8V
Capacity		8.2 Ah
Cycle Life Time		1700
Weight		200g
Internal Resistance		<4m Ω
Energy		31.4Wh
Energy Density	Per Weight	157Wh/kg
	Per Volume	316Wh/l
Maximum C-Rate	Charge	3C
	Discharge	5C
Dimensions	Thickness	7.7-8.05mm
	Width	98.0mm
	Length	130.0mm
Operating Temperature	Charging	0-45°C
	Discharging	-20-55°C
Storage Temperature		-20-40°C

The following subchapters describe in greater detail the methods which were used to develop a 'microscopic' structural mechanics FE model of a lithium-ion pouch cell for quasi-static load cases. The challenges were:

1. Testing (e.g. thin materials, hazards)
2. Quality of the measured data
3. Ratio between thickness and length/width of components
4. Calculation time step
5. Interaction modelling between the layers

Determination of Geometry

A fully discharged cell (with 0 volts) was completely disassembled to identify the layers. It is noteworthy that the cell is made up of one more anode than cathode. The separator is wrapped around the electrodes in an s-shaped pattern, see Figure 1. The electrode separator stack is held together with six strips of adhesive tape. The separator is moistened with liquid electrolyte. The stack-up is enclosed in a flexible pouch cover (Figure 2). The electrodes, i.e. anode and cathode, are interconnected by tags for current collection. The terminals are placed on the shorter cell edge - see Figure 2.

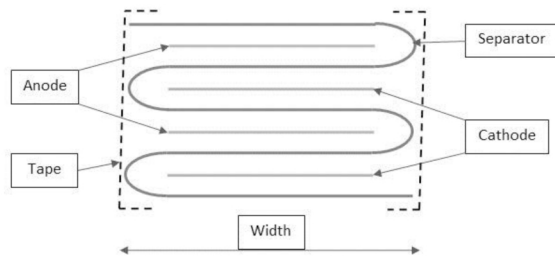


Figure 1. Principal inner build-up of a lithium-ion pouch cell

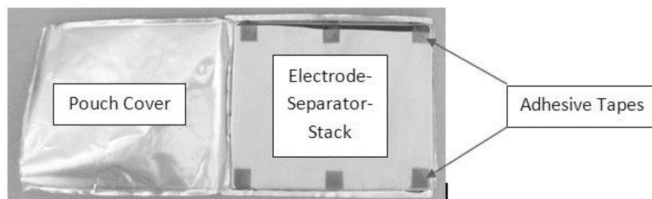


Figure 2. Picture of the outer build-up of a lithium-ion pouch cell

The thicknesses of the disassembled components were measured by electron microscopy to achieve maximum accuracy. This method permits a discrimination between active materials and metallic current collectors (i.e. copper or aluminium). At the same time, the microstructure (e.g. grain size, voids, irregularities, bonding, surface quality) was analysed. Figure 3 shows snapshots of the cathode under electron microscopy.

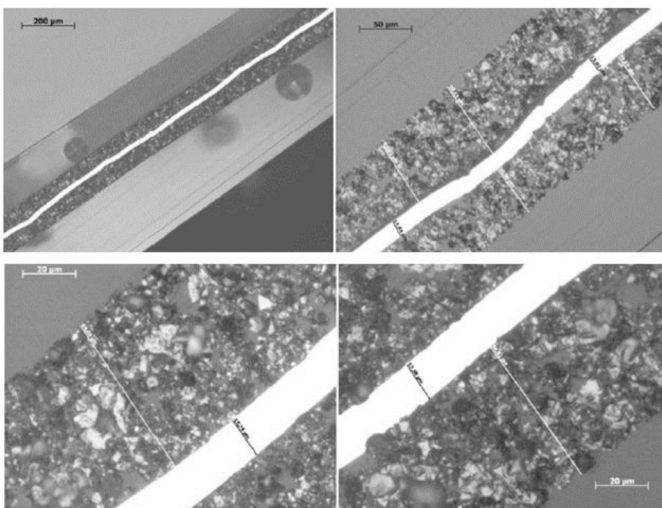


Figure 3. Electron microscopy measuring of the cathode

Results of the electron microscopy are summarized in Table 2.

Table 2. Summary of the cell geometry determination

	Quantity	Length	Width	Thickness
Cathode as a whole	23	118mm	95mm	0.1355mm
Cathode Aluminium	23	118mm	95mm	0.0155mm
Cathode LiMn ₂ O ₄	46	118mm	95mm	0.06mm
Anode as a whole	24	118mm	95mm	0.107mm
Anode Copper	24	118mm	95mm	0.011mm
Anode Graphite	48	118mm	95mm	0.048mm
Separator	1	4660mm	118mm	0.025mm
Pouch	1	130mm	105mm	0.15mm
Tape	6	10mm	10mm	0.04mm

Mechanical Component Tests

To obtain material parameters, the following experimental tests were conducted:

1. Tensile testing of pouch, separator, cathode and anode in longitudinal and transverse (cross) direction
2. Tensile testing of specimens in dry and moistened conditions

The moistened specimens were tested immediately after disassembling the cell. The dry specimens were stored to dry for a week under standard atmospheric conditions.

Figure 4 shows the force-deflection characteristics of the separator in the cross and longitudinal directions. Material anisotropy of the separator is obvious. Table 3 qualitatively summarizes the sensitivity of the test results to the test parameters.

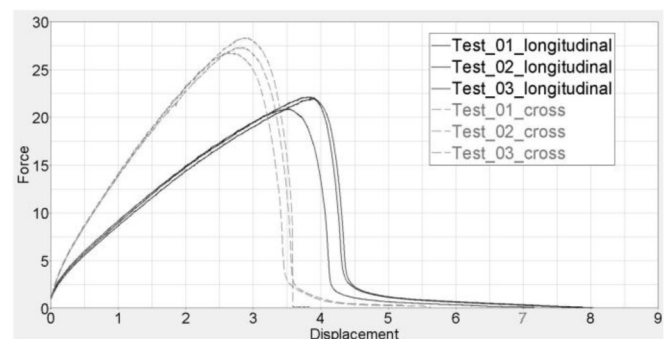


Figure 4. Force displacement curves of the separator under tensile loading in different directions

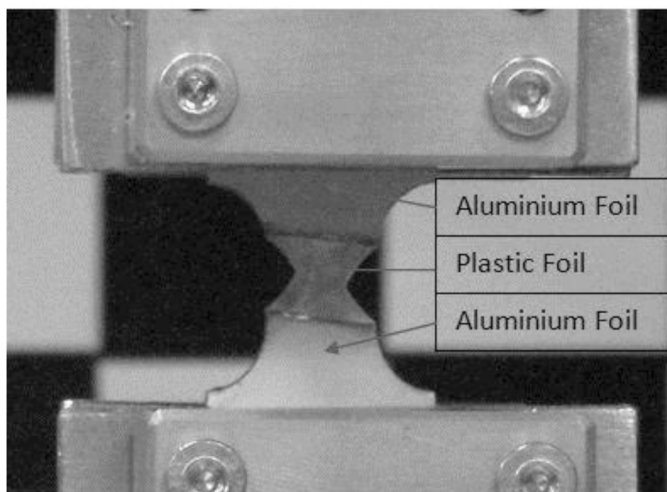
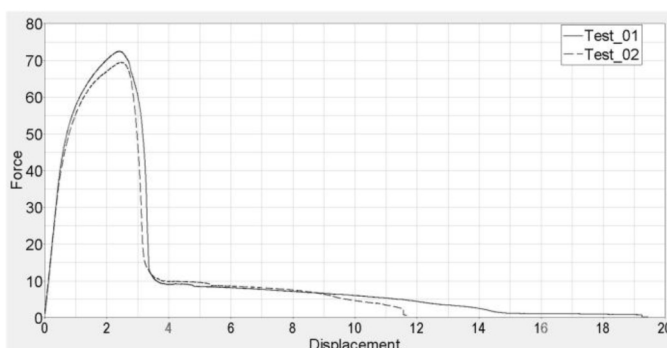
Table 3. Sensitivity to test parameters

	Sensitivity to Test Direction	Sensitivity to moisture
Cathode	Low	No
Anode	Low	No
Separator	High	No
Pouch	No	No

Sheidaei et al. [6] describe a significant difference between wet and dried separator test specimens in terms of mechanical properties. They found a 15% higher Young's modulus for the soaked test specimens. For the cell in this study, this was not the case.

Sheidaei et al. [6] also describe differences in force levels for tensile tests in the longitudinal and cross directions, i.e. anisotropy. This anisotropy was observed for the cell in this study.

The behaviour of the pouch in tensile tests is noteworthy. The cover is made of an aluminium sheet coated with synthetic layers. The aluminium fails and the plastic coating with small bearing capacity remains. [Figure 5](#) and [Figure 6](#) show the described phenomenon.

**Figure 5. Tensile tests of the pouch cover****Figure 6. Force displacement curves of the pouch cover under tensile loading**

Development of the Material Models

The results from the tensile tests were used to fill in the material cards and for the validation of the material behaviour in an explicit finite element solver. The model was developed and validated for LS Dyna Version 971 V5.1. All calculations were performed with the nonlinear explicit solver. Strain rate dependency was not considered. Quasi-static tests were performed at higher load rates in simulation than in experiments in order to reduce CPU time. Kinetic energies and material damping energies were monitored to avoid artefacts from dynamic effects in quasi-static load cases. The explicit solver was chosen to meet the requirements for highly dynamic simulations later in the project.

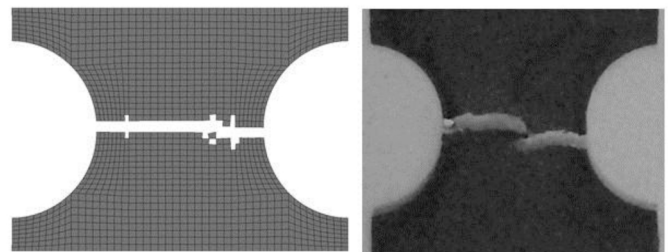
The following subchapters describe the material modelling in greater detail.

Material models for the electrodes

The anode and cathode were each modelled from three shell element layers sharing coincident nodes. One layer represented the metallic current collector (copper for the anode and aluminium for the cathode), and two layers represented the active materials (graphite for the anode and LiMn_2O_4 for the cathode). In this way it was possible to model the electrodes, which are composites (more precisely laminates). Delamination of the active material from the current collector was disregarded.

LS-Dyna offers more convenient ways to model composites (e.g. by applying the '*Part_Composite' or the '*Integration_Shell' keyword). It was found, though, that coincident shell layers are handy for the interaction modelling. This is more thoroughly described later.

Failures of the active material layers were detected as discontinuities in the force displacement curves. In this way it was possible to establish separate material cards for current collectors and active materials. For all layers, '*Mat_Piecewise_Linear_Plasticity (*Mat_024)' was used. [Figure 7](#) exemplarily shows a comparison between simulation and experiment for the anode. A very high correlation between simulation and experiment was found.

**Figure 7. Comparison between simulation and experiment for anode**