Modeling the Mechanical Behavior of a Li-Ion Pouch Cell under Three-Point Bending

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1 Abstract

Short-circuits caused by external forces, as they occur in crash situations, may lead to uncontrolled discharge of battery cells. As a consequence, the battery heats up locally, which, if it comes to the worst, results in an explosive reaction of the cell. However, the detection of critical deformations, for example in car crash simulations is very challenging: On the one hand, local indentations in the range of a few millimeters often result in a breakup of the inner structure and consequently in a short circuit. On the other hand, battery cells can also withstand surprisingly large deformations with the internal structure remaining intact. Thus, a reliable battery cell model has to capture a variety of different deformation modes.
Simulation models with different degrees of complexity are available for predicting and evaluating local indentations (e.g. [1]-[4]). Though, up to now more structure-dominated deformations of pouch cells like buckling or bending are not yet fully understood, what makes the derivation of sound modeling approaches for theses deformation scenarios especially challenging (e.g. [5]-[7]).
Within the present work a FE-model for simulating the bending behavior of a Li-ion pouch cell is developed based on the layered structure of the cell and validated against experimental results. Modeling assumptions necessary to consider the different involved length scales are discussed and the impact on the deformation behavior is evaluated. The developed numerical model provides a detailed insight into the cell behavior and may help to improve battery cell models in the future, to better predict their behavior in bending dominated deformation scenarios.

2 Introduction

Li-ion batteries are the key for the safety of electric vehicles in crash situations. If it comes to the worst, a short circuit, for example caused by failure of the internal structure of the battery cell due to mechanical deformation, results in a thermal runaway potentially leading to fire or explosion. Therefore, for analyzing the safety of electric cars in potential crash situations, understanding and modeling the integrity of battery cells is inevitable. Besides prismatic and cylindrical shape, pouch cells are widely used in electric vehicles. In contrast to the two other types, they consist of a thin and flexible casing (pouch), which gives them a weight advantage. Another aspect of the comparatively weak casing is that the resistance against mechanical deformation is strongly determined by the inner structure. For that reason, within the BATTmobil project a detailed experimental setting to determine both the material and the structural behavior of a selected pouch cell was realized [8].
Two different approaches to develop macroscopic models were outlined in the project: a) development of detailed models for selected loading scenarios and step-wise simplification leading to (partly) homogenized models. b) Application of a parameter-optimization process on selected parameters on an a priori chosen model set-up for different loading scenarios. In the herein presented study we demonstrate the approach in a) on the example of a three-point bending test. Work along b) is presented by Trondl et al. in [9].

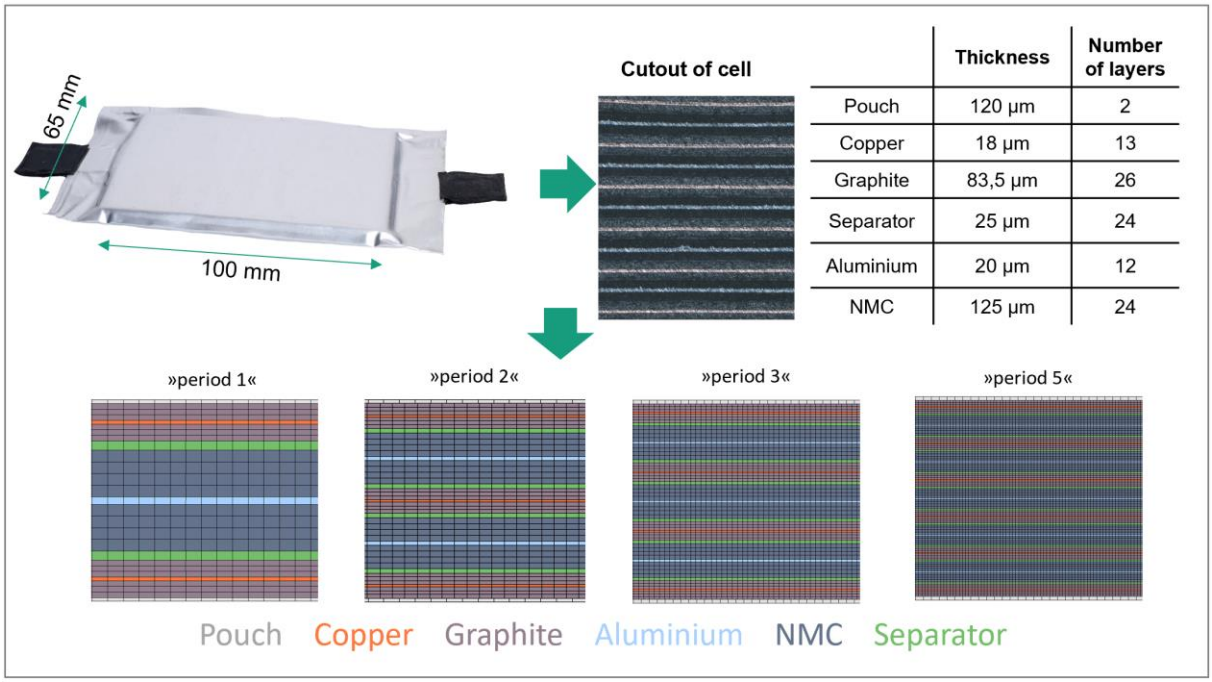
3 Development of a detailed numerical model

For the study at hands experiments on a non-commercial pouch cell were used. The cell was manufactured at the Fraunhofer Institute for Silicon Technology (ISIT). Besides the pouch, the cell consists of in total 99 layers in the internal: 13 anodes, copper foils on both sides coated with graphite; 12 cathodes, aluminium foils on both sides coated with a lithium-based metal oxide (NMC) and 24 separator foils (see Fig. 1). Besides the cells, the manufacturer provided material of pouch, electrodes and separator separately. An intensive test-program to characterize the single components was performed at Fraunhofer Institute for Mechanics of Materials (IWM), documented in [10].

For the bending experiment on the pouch cell, the cells are horizontally placed on two supports (distance 6 cm) and loaded with a punch in vertical direction. Both punch and supports have a radius of 1 cm. The test was performed at velocity of v = 0.1 cm/s (in the simulation increased to 5 cm/s). Supports and punch are modeled as rigid. Furthermore, the symmetry in width direction is applied, so just a half-model had to be prepared and simulated. LS-Dyna version R11.1.0 with the explicit solver was used for all presented simulations.

3.1 Layer resolution in the simulation model

Besides homogenized models (e.g. [1] and [2]) and RVEs (e.g. [3]), also detailed models with reduced number of layers are used to model the mechanical behavior of pouch cells. So, in [7] the behavior of a pouch cell under in-plane loading (buckling) is modeled with a detailed model. In contrast to homogenized models, which are generally defined by calibrating material parameters to experiments on cell level. For both, RVEs and detailed models the cell's structure, though simplified, is integrated explicitly in the model. Therefore, if all parameters of the single components as well as their interactions were known, a calibration of a detailed model to experimental results on the cell level would not be necessary. However, due to the very complex material and structural behavior of battery cells, this is generally not the case. Furthermore, due to difference in the involved length-scales a compromise between layer-resolution and run-time has to be made.



	Thickness	Number of layers
Pouch	120 µm	2
Copper	18 µm	13
Graphite	83,5 µm	26
Separator	25 µm	24
Aluminium	20 µm	12
NMC	125 µm	24

Fig. 1: Size and layers of the experimentally investigated pouch cell (top) as well as layer resolution in the simulation model (bottom).

The simplest detailed model used in this study consists of one aluminum cathode with NMC coating on both sides, two separator foils, two copper anodes with graphite coating and an all-around pouch. This way the original 99 layers of the cell internal are reduced to only 11 layers. In the following, the different models are named based on their resolution. The mentioned model with 11 layers in the cell internal is called »period 1«; »period 2 (3/5)« is made up of 19 (27/43) internal layers. For higher resolutions, care was taken, that the length to thickness ratio of the elements remains constant. The resolution of the used models is demonstrated in Fig. 1. 3D simulation models up to »period 3« could be simulated in reasonable time, the »period 5« resolution was only used for 2D simulations.

3.2 Material and contact modeling

For the material modeling of pouch (aluminum-polymer compound) as well as copper and aluminum electrodes the elastic plastic material model ***MAT_PIECEWISE_LINEAR_PLASTICITY** is used. Material behavior of the separator (porous polyolefin) is modelled with ***MAT_ANISOTROPIC_VISCOPLASTIC**. The parameters were calibrated based on tensile tests on

single foils [10]. Due to low tensile strength and comparatively high strength under compression, the active materials (graphite and NMC) are modeled with the ***MAT_CRUSHABLE_FOAM.** Compression tests were performed on a stack of ten coated anodes and cathodes respectively, so, by knowing the behavior of the metal foils, the stress-strain behavior under compression could be calibrated using an optimization process [10].

The components of the cell internal are modeled with fully integrated solid elements (ELFORM 2), the pouch with fully integrated shell elements (ELFORM -16). Between the pouch and the cell internal as well as between the pouch on one side and the punch and the supports on the other side, a ***CONTACT_AUTOMATIC_SURFACE_TO_SURFACE** was defined with a friction coefficient of 0.2.

A controversial issue is the modeling of the interaction between the layers within the cell. In [7] it was assumed that the layers are detached from each other, in this case a contact between all neighboring layers has to be defined. However, in [3] and [4] the coatings were tied to the respective metal foils, the interaction between the separator and the coatings is modeled with a contact. For the analysis at hand it was decided to model the cell internal as fully bonded. Two considerations led to that assumption. First, the cell itself is under negative pressure, meaning that in reality separation of layers is unlikely. Second, the shear strength of the coatings is very low and furthermore cannot be measured experimentally up to now.

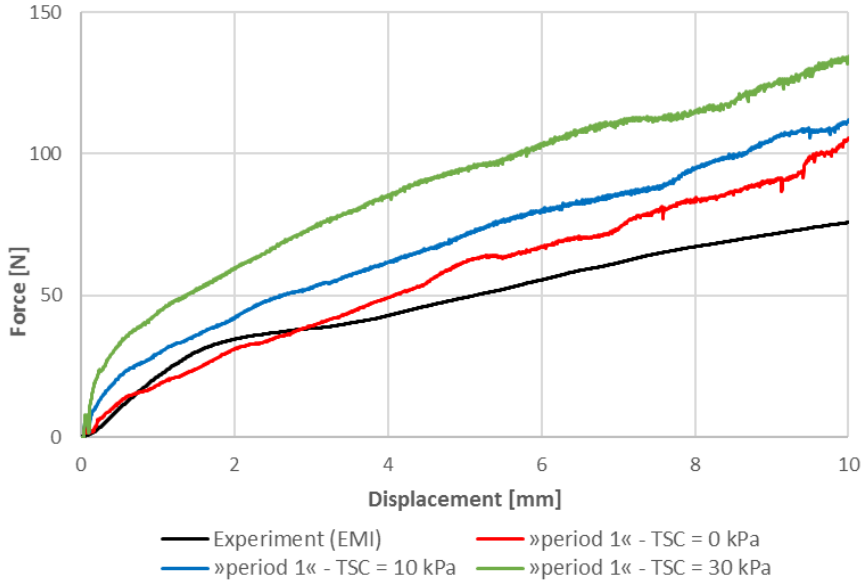


*Fig. 2: Variation of the tensile stress cutoff (TSC) in the ***MAT_CRUSHABLE_FOAM** influences the force in the simulated bending-test. Simulations with »period 1« resolution of the layered structure.*

Hence, the stress cutoff (TSC) in the ***MAT_CRUSHABLE_FOAM** is used as a calibration parameter to determine both, the shear or rather the tensile strength of the coatings and the interaction between the coatings and the separator. Fig. 2 demonstrates that for different values of TSC (0, 10 kPa and 30 kPa) the force level varies, with TSC = 0 kPa giving the best accordance with the experiment.

3.3 Side remark on the geometry of the pouch

In a first step, the casing was modelled as a box closely surrounding the inner layers. That approach led to high stresses within the edges and an early failure of the pouch, which was not observed in the experiment. Thus, according to Fig. 3, the pouch was adapted at the edges, so that the cell internal could be deformed easier without larger stresses in the pouch. The better accordance with the experimentally measured force supports the chosen approach.

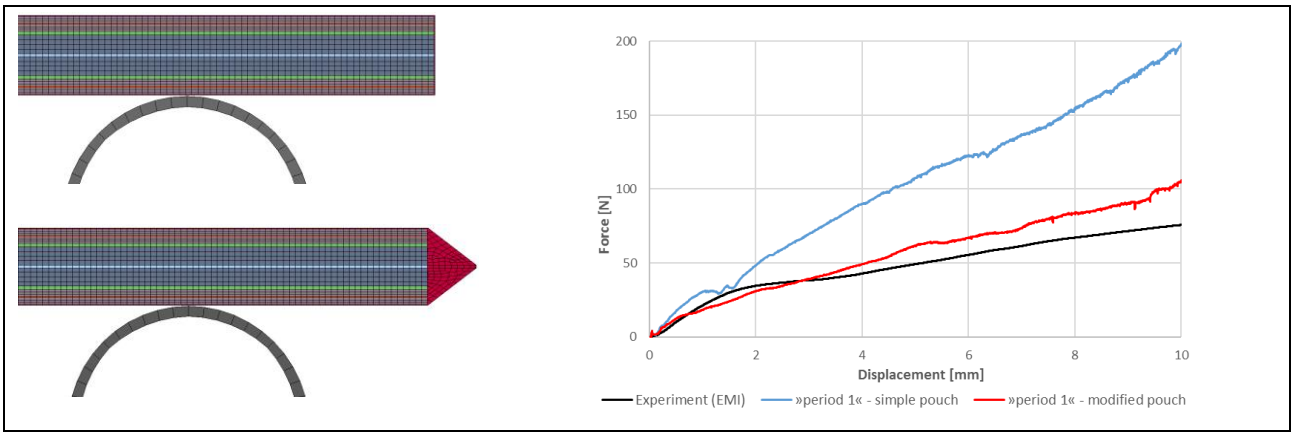


Fig. 3: Influence of the geometry of the pouch (colored in red on the left) on the simulated force-displacement curve (right). Closely surrounded box (left top) leads to higher forces compared to a more realistic approach (left bottom). Simulations with "period 1" resolution of the layered structure and TSC = 0 kPa.

4 Analysis of the layer-resolution in the detailed simulation model

The approach descripted in chapter 3 can now be used to analyze one of the major aspects in battery modelling: how coarse the inner structure of the cell can be resolved to still correctly describe the deformation behavior? To answer this question for the bending scenario, the layer resolution of the internal structure is increased step by step, starting with the »period 1« model with 11 layers. However, the simulation time also increases significantly with a higher resolution of the cell.

4.1 Comparison of the force-displacement curves (3D)

Fig. 4 shows the force-displacement curve for different layer resolutions and the experiment. Due to the very long runtime of several weeks, the curves with the resolutions »period 2« and »period 3« end already at lower displacements. Despite the earlier termination of »period 2« and »period 3« a comparison between the simulated curves and the experiment is possible. It shows that the initial stiffness between all simulated curves and the experiment is quite similar. Although for »period 2« and »period 3« the force for displacements > 0.5 mm is smaller than in the experiment and in the simulation with »period 1«, the differences (especially between »period 2« and »period 3«) are still acceptable.

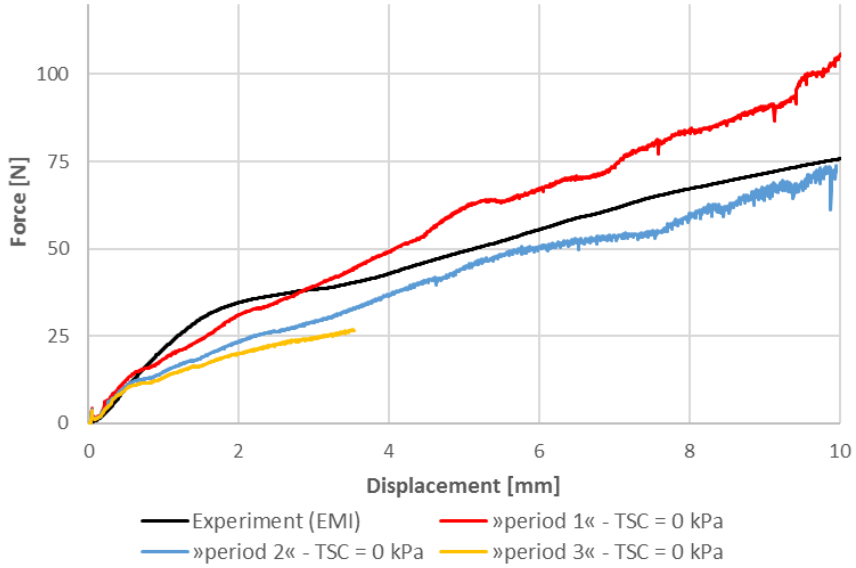


Fig. 4: Force-displacement curve simulated with different layer resolutions (3D) in comparison with the bending experiment.

4.2 Mechanical behavior on the layer-level

For a simple beam (one material) classical bending theory implies a linear stress distribution over the thickness with (beneath the punch) compressive stress on the top and tensile stresses on the bottom.

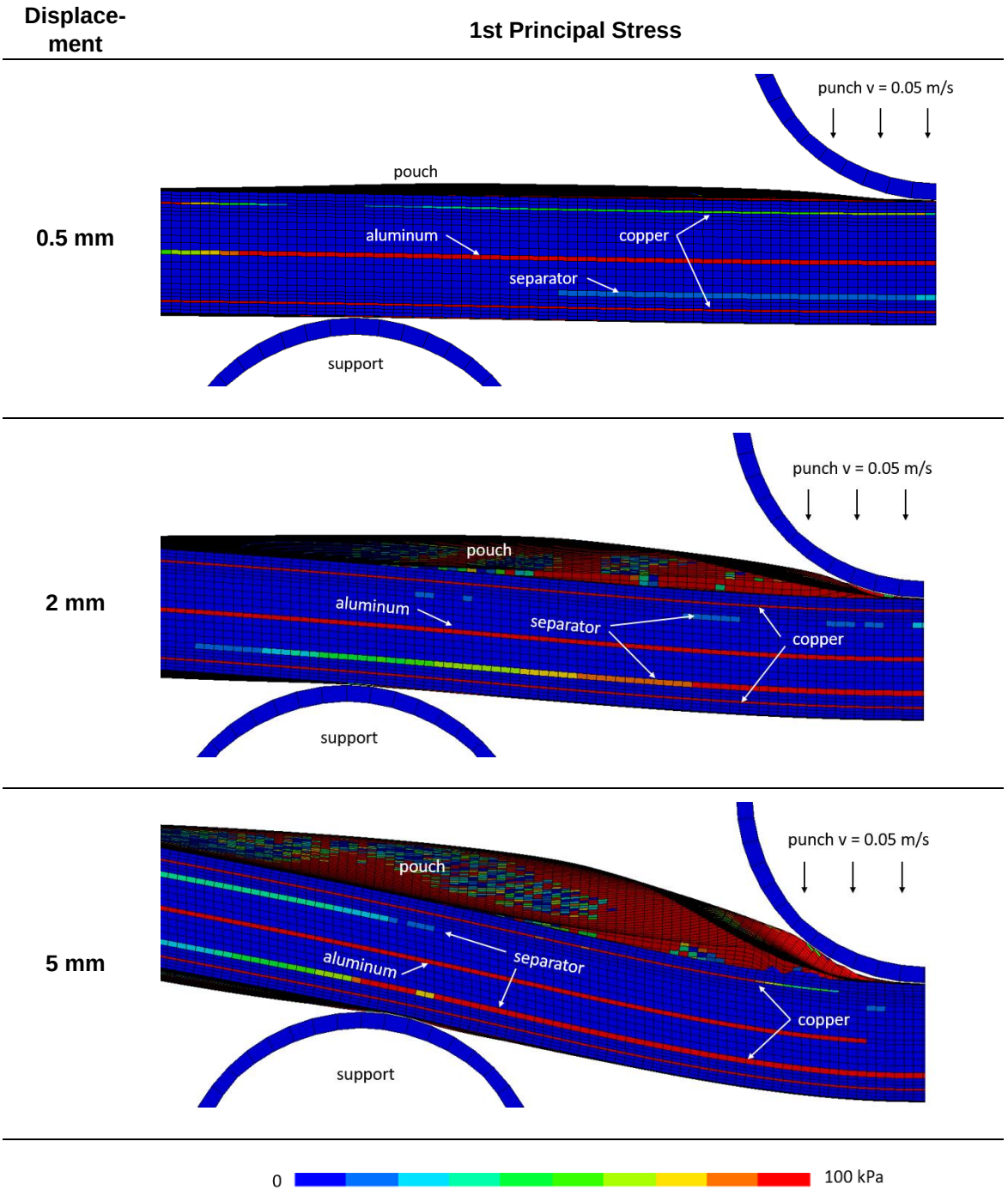


Fig. 5: First principal stress in the pouch cell for different displacements (cut-off at 0 and 100 kPa). Highest stresses occur in the stiff metal foils (aluminum and copper). Tensile stresses in these layers on top and bottom side of the cell.

Fig. 5 demonstrates that the stress state in the cell is different. Tensile stresses mainly occur in the stiffer layers of aluminum and copper, and to a much lower extend also in the separator. It is noticeable that, especially for displacements ≥ 2 mm, tensile stresses occur not only on the bottom, but also on the top side of cell, indicating that the tensile loading of the metal foils is the main load carrying mechanism for pouch cells in bending dominated scenarios.

4.3 2D Simulations with increased layer resolution

Major drawback of the 3D simulation is the runtime, which gives a strict limit to the resolution that could be simulated with the 3D model. Therefore, to investigate the effect of higher resolutions a 2D model is used. Table 1 summarizes the runtimes of the different 2D and 3D models, for a punch displacement of 2 mm. As an element formulation ELFORM 13, plane strain elements with full integration (NIP 4), is chosen. However, it must be noted that, due to the 2D inherent symmetry assumptions a closed pouch in width direction cannot be modelled.

Table 1: Runtime and used cores on EMI Unix-cluster for different models, evaluated for a punch displacement of 2 mm.

Model		Runtime (for 2 mm displacement)	Cores
3D	**»period 1«**	64 h	8
	»period 2«	206 h	16
	»period 3«	394 h	32
2D	**»period 1«**	2 h	1
	»period 2«	10 h	1
	»period 3«	27 h	1
	»period 5«	114 h	1

Fig. 6 shows the force-displacement curve simulated with a 2D model compared to cell bending experiments with and without a pouch cover (just the inner stack of layers was tested). A comparison between the two experiments show a pronounced difference in the force level, as already noted in [2]. In the simulation the 2D model behaves much softer than the 3D model, which is presumably due to the inadequate modelling of the pouch. As demonstrated in the figure, the behaviour of the 2D cell with high layer resolution is more similar to a cell without a pouch cover.

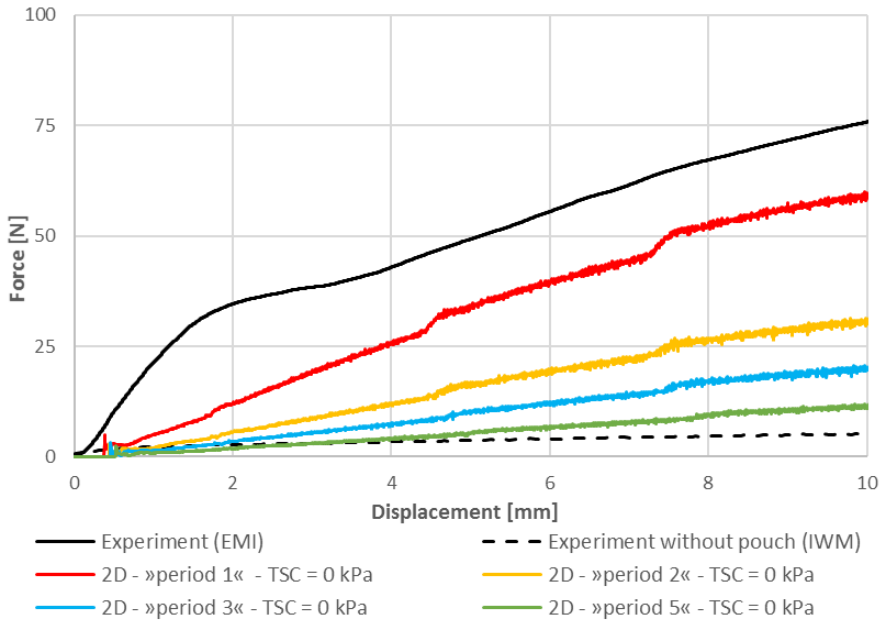


Fig. 6: Force-displacement curve simulated with different layer resolutions (2D) compared to cell bending experiments with (solid line) and without a pouch (dashed line).

5 Discussion of the detailed model

As already outlined in 4.3, forces in the 2D model are generally lower than in the 3D case. At this point, a more quantitative evaluation, based on fits on the curves, is aspired. As demonstrated in Fig. 7, a bilinear fit is performed on the 3D simulation and on the experiment. For the 3D »period 1« model, both slope 1 (initial stiffness) and slope 2 overestimate the experiment (slope 1 by 24%, slope 2 by 94%). The difference reduces for the »period 2« model to 9% and 36%, for the »period 3« model to 1% and 11% respectively (see also Table 1). The slopes seem to converge to the experiment, though in the simulation the intersection between the two lines diminishes with resolution and lies considerably below the experiment. This might be an indication, that the tensile strength of the active material (0 kPa, calibrated for »period 1«) is too low.

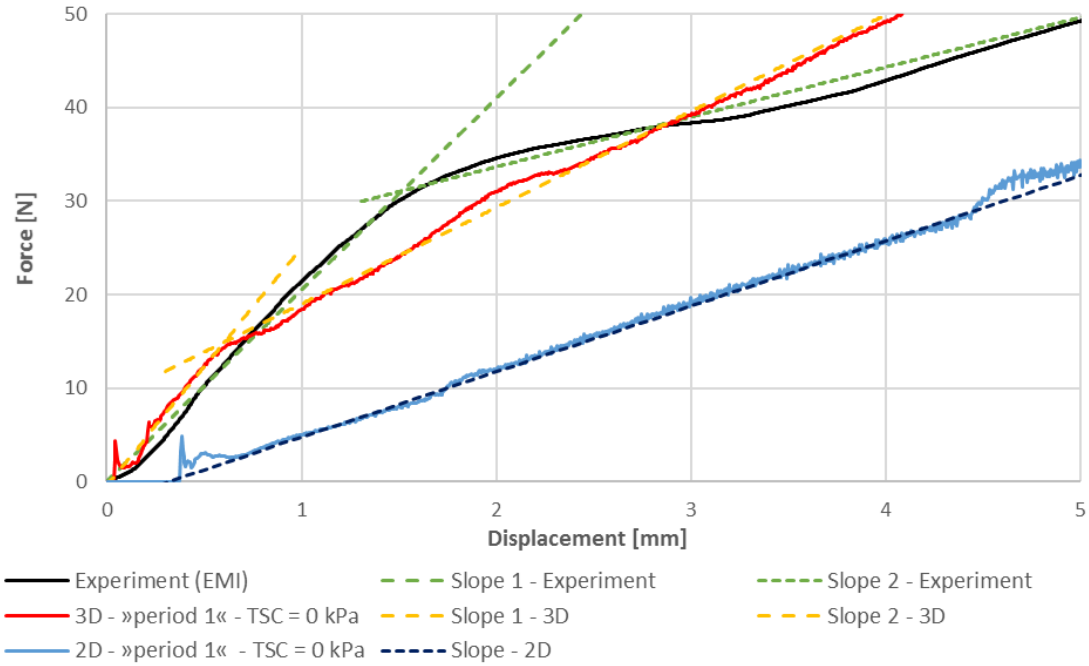


Fig. 7: Comparison of the slopes of the force curves for the first 5 mm of experiment, 2D and 3D model with »period 1«.

Table 2: Different slopes and intersections of the simulated force curves for 3D and 2D models of the cell in comparison to the experiment on cells with and without pouch.

	Slope 1 [N/mm]	**Slope 2 [N/mm]**	**Intersection [N]**
Experiment (EMI)	20.5	5.3	31.1
3D – »period 1« – TSC = 0 kPa	25.4	10.3	14.8
3D – »period 2« – TSC = 0 kPa	22.4	7.2	11.9
3D – »period 3« – TSC = 0 kPa	20.7	5.9	10.6
2D – »period 1« – TSC = 0 kPa	-	7	-
2D – »period 3« – TSC = 0 kPa	-	2.0	-
2D – »period 5« – TSC = 0 kPa	-	1.1	-
Experiment w/o pouch (IWM)	2.9	0.4	2.1

In contrast, the force-displacement curves of the 2D simulations can be fitted by single lines. Slopes of these lines are well beyond slope 1 in the experiment and therefore listed under slope 2 in Table 2. With higher resolution the slope decreases remarkably and goes well beyond the experiment. It can be assumed, that for a full resolved cell model, the slope approaches the experiment of a cell without a pouch. This obvious difference between the two models illustrates the importance of the closed pouch in a cell model and underlines that the 2D approach is insufficient to describe the deformation behavior.

6 Derivation of a partly homogenized model

For a reduced detailed model, or differently speaking a partly homogenized model, two major aspects have to be considered: pouch and metal foils. Based on the above findings a partly homogenized model could look like the one demonstrated in Fig.8. The model has a closed pouch (same as in detailed cell model), an inner block of active material (solid elements ELFORM 2), and shell-layers to represent the metal foils (shell elements, ELFORM -16). The thickness of the shell elements representing the metal electrodes is adjusted such that their total thickness represents the total thickness of both copper and aluminum foils in the experimentally investigated cell. For the curves demonstrated in the following the parameter set for copper was chosen for the metal foils (shell layers) and graphite for the active materials (solid elements). However, using aluminum and NMC instead makes practically no difference.

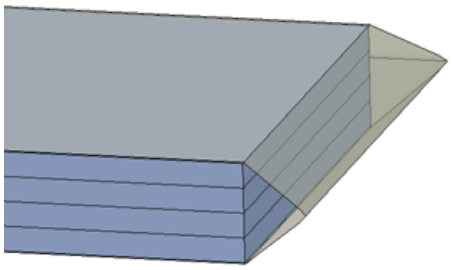


Fig. 8: Cutout of a partly homogenized model for a battery cell with a semi-transparent pouch.

For the partly homogenized model the simulation times decrease remarkably (40 h for the whole simulation). The force-displacement curves are shown in Fig. 9. It is easy to see, that the version with no metal layers in the inside is too weak and the force level only reaches about 20% of the experiment. Adding a single metal layer, leads to an overestimation of the experimentally measured curve. Though, with increasing number of used metal layers, similar to the detailed model, the force level decreases. However, already the version with 3 layers of metal foils (that corresponds approximately to the »period 1« detailed model) has a lower force level than the experiment.

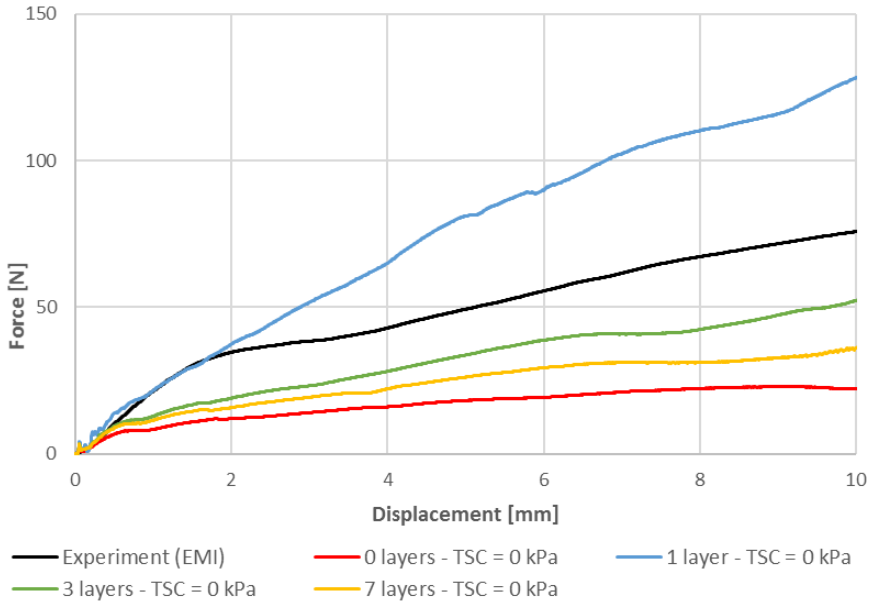


Fig. 9: Force-displacement curve simulated with a partly homogenized model for different numbers of internal metal layers.

As in the detailed model, also for the partly homogenized approach the tensile stress cut off (TSC) for the ***MAT_CRUSHABLE_FOAM** model, applied for the active materials, can be used as a fitting parameter to adjust the force level. Fig. 10 indicates that for this setting a TSC of 30 kPa was suitable to follow the experimental curve for a wide range (slope 2 being 6 N/mm in the simulation, compared to

5.3 N/mm in the experiment). On the other hand, the initial stiffness in the simulation model then strongly overestimates the experiment (slope 1 being 58 N/mm in the simulation and 20.5 N/mm in the experiment).

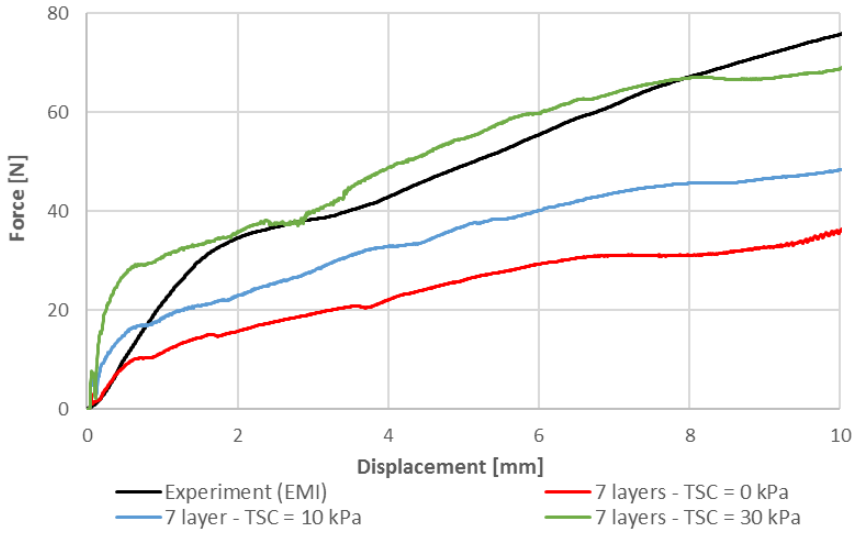


Fig. 10: Influence of the tensile stress cutoff (TSC) in ****MAT_CRUSHABLE_FOAM*** *for the partly homogenized model with 7 metal layers.*

7 Summary and Conclusion

Within the present paper, the development of a detailed simulation model for Li-Ion pouch cells under bending behavior is presented. Besides knowledge of the internal structure, number and thickness of the layers (pouch, separator, anode: copper and graphite, cathode: aluminum and NMC), in depth-knowledge of the material behavior of each component is necessary. It shall be noted that, except for the tensile behavior of graphite and NMC, all material parameters were determined by material tests on the respective material. The tensile stress cutoff (TSC) in the ***MAT_CRUSHABLE_FOAM**, used for the electrode's coatings graphite and NMC, is used as a calibration parameter considering both, the respective material behavior and sliding between the electrodes and the separator. In the model separator and electrodes are connected to each other by coincidence nodes. Main conclusions based on the detailed simulations are:

- The closed pouch cover is crucial for the bending behavior [2], the force level and the characteristic bi-linear shape of the force-displacement curve. It can not be modeled in 2D sufficiently.
- Low tensile and shear strength practically leads to a decoupling of the stress state within the different layers in the cell internal.
- During deformation, in the inner of the cell, the load is basically carried by the copper and aluminum foils under tension.

Based on these findings a partly homogenized model is proposed and compared to the experimental outcome. After recalibration of the tensile stress cutoff, also this approach could model the bending experiment sufficiently well. Focus of further improvement of both, the detailed and partly homogenized model, should be the decoupling of the layer interaction and the tensile strength of the active materials. To achieve this, a better understanding of the layer sliding and sticking in the experiment (especially for lower displacements) is considered essential.

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