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Testing and simplified modelling of deformation behaviour of battery cells

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Abstract

The deformation and failure behaviour of cylindrical, prismatic and pouch cells were characterized under different load situations like compression, bending and indentation. A special testing method with measurement of force, displacement, cell voltage and temperature was used to determine the relationship between mechanical responses and internal short-circuit. It was found that in many load cases the short circuit takes place just after a mechanical instability, which can be determined from the recorded force vs. displacement curve. A great challenge for modeling battery behavior in crash simulation is the development of an efficient method which enables a reliable prediction of battery deformation with indicators for short circuits by using a reasonable calculation expense. Based on experimental results a simplified model was developed to capture the essential deformation character of a pouch cell under different loadings. Instead simulating the complex cell layer structure a homogenized model was suggested and applied to simulate cell tests under compression in different cell orientations. Shell and solid elements in conjunction with compressible plasticity model were used to take into account the orientation dependence of the mechanical behavior and the volume change of the pouch cells.

Keywords: cell testing, battery safety, deformation behavior, short circuit, simplified modeling, crash

1 Introduction

The mechanical and electric behavior of batteries under crash loading is an essentially information for the construction and evaluation of electric vehicle concerning crash safety. An internal short circuit in a battery pack caused by large deformation of cells can result in smoke generation or combustion of the battery pack. Due to the lack of knowledges about cell behavior under crash loading most battery packs are protected with a massive and very stiff battery housing which is in opposition to the requirement on weight reduction for a compensation of heavy batteries. Until now there are only limited experimental results about the interaction between cell deformation and the internal short circuit [1, 2]. The most available numerical models for batteries are still not applicable for crash simulations of battery packs due to huge computation expense and limited prediction capability [3]. This circumstance is mainly related to the necessity of sufficient considerations to simulate a high number of sublayers with significant different material behaviors for detailed predictions of critical states during crash scenarios. In this work special testing methods were used to determine the influences of cell deformation and damage on short circuit behavior. A simplified model was developed to model mechanical behavior of cells in crash simulation in an efficient manner.

2 Cell tests under different mechanical loadings

Cylindrical, prismatic and pouch cells were tested under different loadings and relationships between deformation, damage and short circuit of cells were established.

2.1 Cylindrical and prismatic cells

To characterize the deformation and damage behaviour of cylindrical and prismatic cells compression, indentation and bending tests were performed under static loading. Cylindrical Nickel Cobalt Oxide (NCA) Lithium ion cells (GAIA, HP 602030 NCA-45 Ah/162 Wh) were used in this study [1]. The cells were discharged at a state of charge (SoC) slightly greater than 0%, or to the recommended voltage limit for discharge, approximately 3 V, respectively. A nearly zero SoC was used to detect internal short circuit and heat generation, but at the same time allows avoiding severe cell reaction like smoke and fire development. Three temperature sensors were applied on the cell mandrel shown in Figure 1 and the cell voltage was recorded during the test.

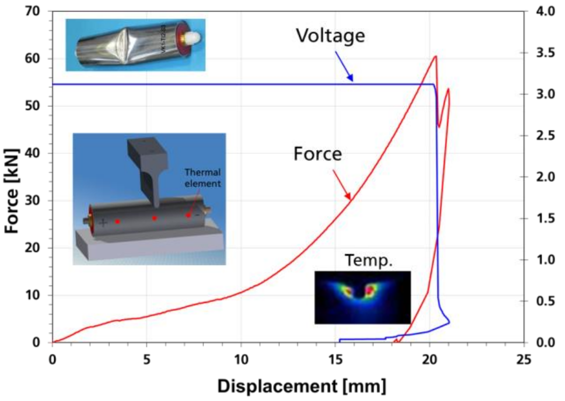

Figure 1: Measured force and cell voltage as function of punch displacement of an indentation test on a cylindrical cell

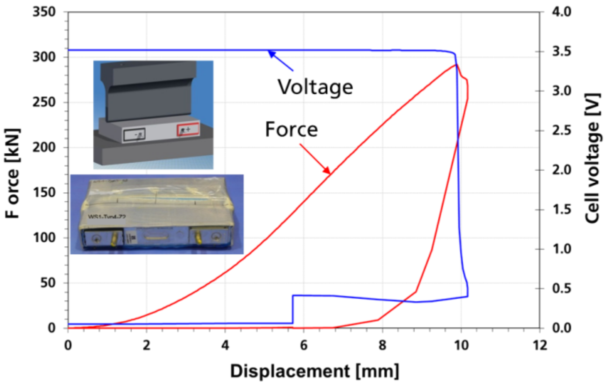

Figure 2: Measured force and cell voltage as function of punch displacement of an indentation test on a prismatic cell

The cells were located in a windowed cave featuring a gas exhaust device and loaded at a hydraulic tension/compression testing device quasi-statically. An infrared camera was used to determine the temperature distribution at the front of the cell during the test. The mechanical test was interrupted and the specimen is unloaded, as soon as the cell voltage dropped to zero, indicating the appearance of a short circuit. Figure 1 shows the measured force and cell voltage as function of displacement during an indentation test on cylindrical cell using an indenter with a radius of 5 mm. Figure 2 shows the experimental results of indentation test on a prismatic cell with the same indenter. In both cases it can be recognized that a sudden drop of the force occurs just before initiation of the internal short circuit or at the same time. The temperature rise after the internal short circuit in the cylindrical cell is shown in Figure 1. Although the housings of both types of cells underwent large plastic deformation, no fracture did occur in the housings. The sudden drops of the force were caused by rupture of inner structure of cells, which results in contact between the anode and the cathode.

2.2 Pouch cells

The individual encapsulated cylindrical and prismatic cells are beneficial for the requirements of crash safety and also lead to heavier structures and furthermore to less charge- and energy densities. These circumstances counteract lightweight constructions, which are important for larger ranges of electrical driven vehicles. Therefore alternative concepts of cell structures were developed, which results in the presently more and more applied weak pouch cells, also known as coffee bags.

A closer look to the orientation of the installed pouch cells in relation to the driving direction of the presently developed vehicles shows two principal alignments. For one orientation the driving direction is perpendicular to the in-plane region of the cells and for the other one the driving direction is parallel to the in-plane region of the cells. Therefore in representative crash scenarios not only the pressing or piercing normal to the plane of pouch cells are important load cases, also the crushing parallel to the plane of the pouch cell (lateral compression) represents an essential setting, which is also relevant for side crashes [5]. In most of the published papers this lateral compression or crushing of pouch cells is not treated.

A pouch cell delivered from the company li-Tec with a dimension of 220x180x10 mm was characterized under compression in lateral and thickness orientations. For the compression tests in lateral direction (crushing) notched holders (mounting and punch) were used to keep vertically the pouch cell standing. Figure 3 shows the measured force and cell voltage as function of punch displacement under lateral compression.

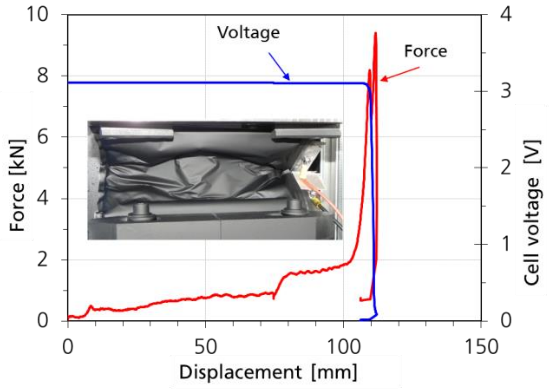

Figure 3: Measured force and cell voltage as function of punch displacement of a lateral compression test on a pouch cell

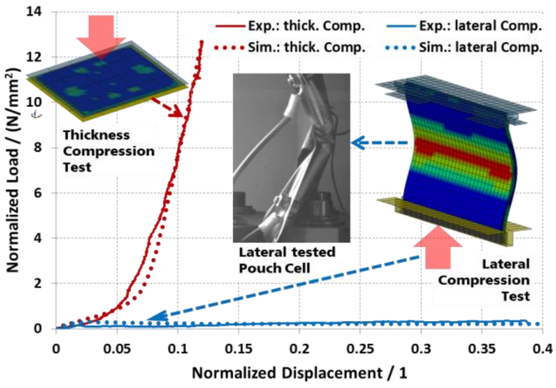

Figure 4: Measured (solid lines) and calculated (dashed lines) normalized force and displacement curves of compression tests on pouch cells in thickness and lateral direction

The short circuit observed during the test was caused by an electrode related contact of the deformed pouch cell with the screw, which was used to fix the holder. Without the external intervention of the screw no internal short circuit would occur under compression.

3 Simplified simulation of pouch cells

A simplified modelling approach is needed for crash simulations of vehicles because the detailed layer setup of a pouch cell, which consists usually of more than 200 individual plies (separator, electrodes and active material), is too complex and can’t be treated in an efficient manner. To setup an efficient analogous model, two principal ways were taken into account:

- A homogenized approach for the main internal cell-structure with a compressible plasticity model and furthermore a simplified cover of the cell.
- An approach based on the previously mentioned covered homogenization and additionally a composite layup in a simplified and consistent manner to the original structure.

The “pure” homogenization technique is very efficient but has no detailed information about the inner discrete layer setup, which is likely important to describe internal short-circuits for critical deformations (such as indentations, bending, etc.). The second approach with a simplified composite layup is more time-consuming and problematical due to the fact of the very different stiffnesses between the active material, the electrodes and separators. However this approach may be advantageous for the description of mechanical deformation driven internal short-circuits. Figure 4 compares the experimental results on the pouch cell under compression in thickness and lateral direction with those calculated using the homogenized approach. The force was normalized with the initial loaded area and the displacement with the initial thickness and width respectively. Obviously, the direction dependent deformation behavior of the pouch cells (which is not relatable to a true anisotropy in a continuum-mechanical manner) can be predicted with the simplified model. For modeling of short-circuits additional criteria have to be added into the approach.

3.1 Modelling and motivation

Typically, the cell units (also denoted as pouch cells or coffee bags) are collected in larger frames or boxes (also denoted as battery units), which should protect the weak cells against damage during possible crash scenarios. For weight restriction and other reasons (e.g. reduced space, etc.), however it is not possible to provide a highly protective casing for the pouch cells. Therefore it is necessary to model the battery units simultaneously during crash simulations of the whole automotive structure, which further necessitates the development of analogous models for the pouch cells to describe the mechanical and electrical behavior in a sufficient but also efficient manner. Due to the fact of the high number of individual stacked pouch cells in one cased or framed battery unit, a less complex analogous model of the individual pouch cell is required. This is further made necessary by the circumstance of several battery units in one typical automotive unit (such as a car), which leads in summary to a large number of pouch cells (up to a few hundred). On the other hand, this simplified analogous model has to depict the essential mechanical (and electrical) behavior as good as possible. In addition, the typical load cases such as compression in thickness and longitudinal direction, bending, piercing, indentation and others have to be described in a good agreement to experimental observations.

Presently available pouch cell models are too complex for the use in crash simulations of whole automotive structures (e.g. 150.000 elements in [6], up to 650.000 elements in [6a]). Therefore applicable simplified analogous models are needed to simulate the essential mechanical and electrical behavior. Critical short-circuits, which could lead to possible dangerous states (up to explosions), are in principle related to problematic deformations of the pouch cells during crash loading scenarios, such as piercing, crushing, etc. Therefore, a first step in developing simplified analogous pouch cell models is to describe the mechanical deformation behavior as good as possible. This local mechanical deformations should be used in a further step to derive the possible occurrence of critical short-circuits. The focus of the presented work is addressed to the mechanical deformation behavior.

3.2 Structural cell setup

Pouch cells are layered structures, which consist of different materials with significantly varying behaviors. The principal layer setup is shown in Figure 5. The tested lithium-ion pouch cell consists of the following materials:

- Solid copper anodes with a thickness of about 10µm.
- Solid aluminium cathodes with a thickness of about 15µm.
- Solid separator layers which are polymer structures with a thickness of about 25µm.
- Granular anodic active material which consists mainly of graphite. One layer has a thickness of 60µm.
- Granular cathodic active material which consists in principle of Lithium Metal Oxide (LiMOx, Li-Ions and Metal Oxide such as exemplarily Cobalt-Oxide). One layer has a thickness of 85µm.

The typical thickness of an individual pouch cell is about 10mm, which results in a large number sublayer-systems as shown in the middle of figure 5 (colored schematic sublayer-setup).
A further important part of the pouch cell is the outer flexible casing, which is normally a thin aluminum laminated film and influences the mechanical deformation behavior especially under loading in plane, for example crushing. This outer aluminum laminated film (Figure 7), which has a thickness of about 0.1mm, stabilizes the whole inner layered structure of the pouch cell against critical mechanical loadings which could possibly occur during crash and cause electrical short-circuits.

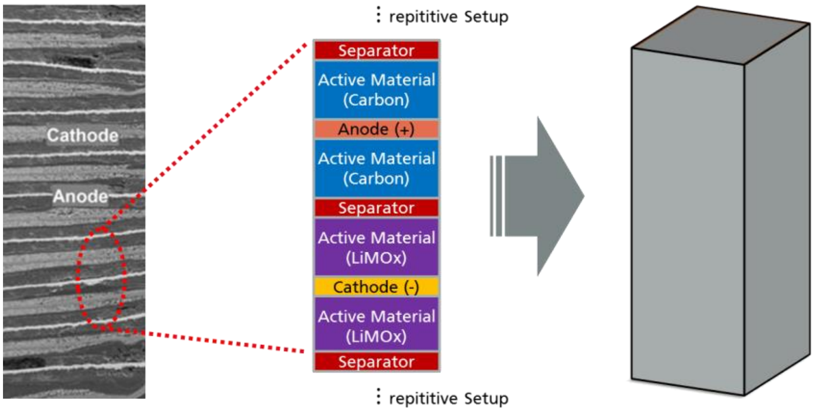

Figure 5: Typical setup of a pouch cell (left) and schematic structure of a representative (repetitive) sublayer system (middle) as well as a first simplified homogenized approach for modelling (right)

In a first approach the complex inner structure of the pouch cell is simplified by a single homogenized material model (Figure 6). This approach is motivated by several assumptions and reasons, which are listed below:

- The layer structure shows a dominance of the active material in the anodic and cathodic regions. About 80% of the pouch cell consists of granular active material.
- The very thin solid electrodes and separators have negligible bending stiffness and weak shear behaviour. Therefore in a first approach the stiffness portion of the thin solid layers (electrodes and separators) in relation to the overall deformation behaviour of the whole pouch cell has less influence and is not considered, which is additionally justifiable by the separation of all solid thin layers with limp active material.
- Only the thin outer aluminium laminated film for casing stabilizes the weak and granular-dominated inner layered structure of the pouch cell which motivates a modelling of this part (Figure 7).
- The dominating active material has a granular structure which leads to the assumption of a single isotropic homogenized material inside the pouch cell (Figure 5 right, Figure 6).

Based on these reasonable assumptions of the above specified first approach a second additional improved analogous model was developed and compared to experimental investigations. This improved analogous model consists of solid and intrinsic shell elements (Figure 8). The principal structural setup of this improved approach is similar to the first one with the difference that for this case a simplified (consistent) layer-setup of the electrodes and separators is considered. The motivation for the additional inclusion of a simplified layer-setup is explained in the following.

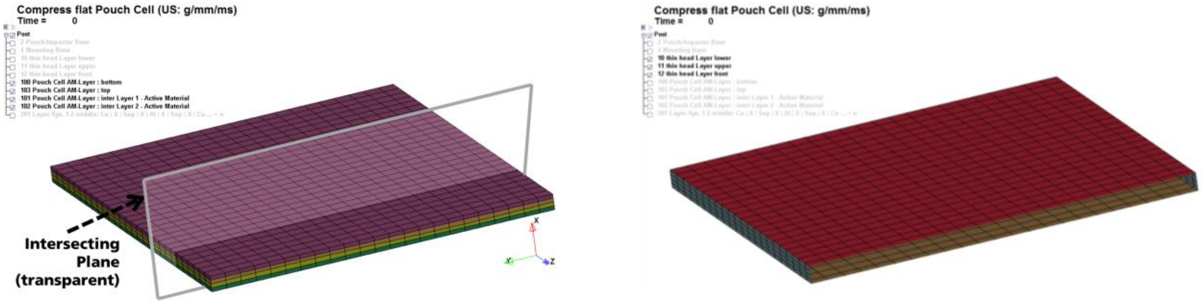

Figure 6: Solid elements in structural setup of pouch cell (transparent face represents cutting region for Figure 7)

Figure 7: Shell elements which represent the outer thin casing of the pouch cell

The solid elements contain the homogenized inner behaviour of the pouch cell, which is shown in Figure 6. As one can see in Figure 7, the structural stabilizing outer thin casing is modelled with membrane elements by using the same surface nodes as the underlying solid elements (Figure 7 shows only the casing without the inner solid elements). For efficiency reasons reduced integrated elements and a medium size for the discretization are used.

The following reasons motivate the introduction of a simplified (consistent) inner layer-setup for the second analogous pouch cell model:

- For the prediction of electrical short-circuits a simplified approximation of the inner structure is probably (very) useful in comparison to a homogenized material model, because the local states of stresses or strains and their gradients (possible localizations) are probably much better representable, which supports the predictions of local electrical collapses.
- Possible directional dependent deformation (anisotropic) effects of the whole pouch cell can be described by introducing a simplified internal layer-setup.
- For severe deformation states during lateral crushing of pouch cells it is expected, that strong bending effects in conjunction with local pronounced compaction of the active material leads to a significant influence of the high number of very thin electrodes and separator layers, which is for most other load cases insignificant. This circumstance is observed during calibrating the analogous models to experimental measured data and described in a following section.

The simplified approximation of the inner layer setup of electrodes and separator films is based on the compatibility of the area moment of inertia, which should be similar to the original structure. Additionally, the simplified inner structure should have comparable quantities in relation to the shear weakness and bending flexibility in comparison to the real setup, which are mainly caused by the weak connection of the many stiff electrode and separator layers with the granular active material.

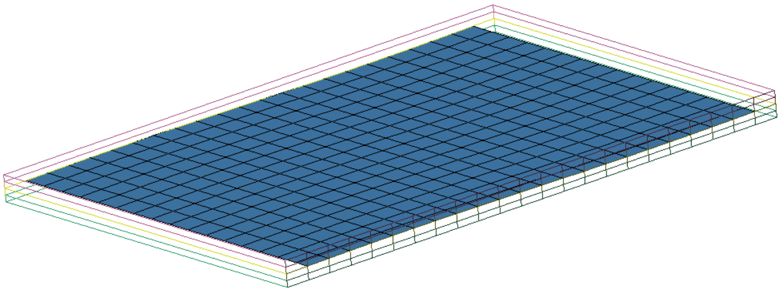

Figure 8: View through and cut of the improved analogous model with one additional inner composite shell plane in the middle (blue; remaining active material is transparent and not visible in this figure)

The consistent map of the inner layer setup is modelled by using shell elements with a convenient composite layup structure, which is calibrated to the experimental measurements and the above mentioned restrictions in relation to the original layer setup (area moment of inertia, shear weakness, etc.). To keep the computational costs in the improved analogous model as less as possible, the usage of a minimal number of layers was intended, because the number of integration points in shell thickness direction influences the performance significantly. In addition, different versions of improved analogous pouch cell models with one (Figure 8) or exemplarily three additional composite shell planes are tested and calibrated to the experimental results.

The inner shell plane(s) use the same nodes as the solid elements of the active material and influence the lateral contraction for compression testing in thickness direction. This leads to a recalibration of the compressive plasticity model for the active material in relation to the analogous pouch cell model without the additional simplified (consistent) inner layered structure.

3.3 Material models

The granular structure of the active material motivates the usage of material models, which are typically used in powder technology for applications such as powder compaction in cavities. For such applications pressure dependent compressible plasticity models are widely used, which describe the yielding (second invariant $I_{D,2}$ of deviatoric portion of the Cauchy stress tensor) as a function of a measure of the hydrostatic pressure (first invariant or trace of the Cauchy stress tensor I_1). A convenient choice in that relation is the Drucker-Prager-Cap model (Figure 9), which has the advantage to describe different yielding behaviours for compressive and tensile stress states.

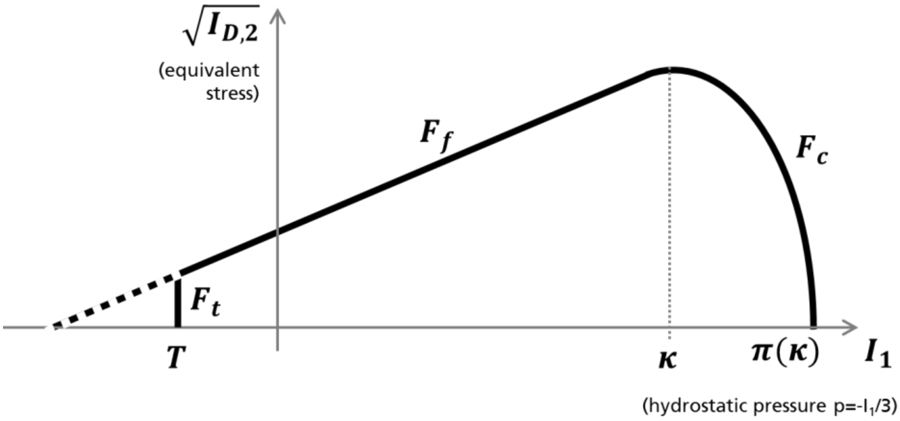

Figure 9: Principles of the Drucker-Prager-Cap model

It is obvious, that the active material has a significantly less tensile yield stress in comparison to compression, which could play an important role for some deformation states in different crash scenarios. Mentionable examples in that context are bending loadings during crushing pouch cells, which lead to development of tensile and compressive stresses on opposite sides of buckled regions.

In a rough simplified description, the Drucker-Prager-Cap model consists of a so called failure line F_f for tensile and lower compressive pressures respectively, as well as of an ellipsoidal cap F_c, which limits the yield stresses for higher compressive pressures as shown in Figure 9. Additionally, there is a cut-off for tensile stress T applicable to limit the yield stress for such kind of loadings (F_T). For the herein used isotropic hardening, the failure line (1) depends on material parameters (a, b) only and doesn't change during all deformation states.

$$F_f(I_1) = a + b \cdot I_1 \tag{1}$$

Only the ellipsoidal cap depends on the hardening, which is controlled by volumetric strain (and additional material parameters). The cap for higher pressure yielding is described by an ellipsoidal function

$$F_c(I_1, \kappa) = \frac{1}{R}\sqrt{\left[\pi(\kappa) - \langle\kappa\rangle\right]^2 - \left[I_1 - \langle\kappa\rangle\right]^2} \tag{2}$$

with a constant hardening independent aspect ratio R. The angle bracket operator in (2) represents the operand value for positive κ and zero for negative values of κ. Only the cap "pressure" $\pi(\kappa)$ – and therefore due to constant R also the midpoint of the cap κ (3) – depends on the hardening state.

$$\pi(\kappa) = \kappa + R \cdot F_f(\kappa) \tag{3}$$

The hardening itself is determined by the plastic part of the volumetric strain $\varepsilon_{p,v}$ (first invariant of the plastic strain tensor) over the cap “pressure” $\pi(\kappa)$ from (3) through the following equation (4)

$$\varepsilon_{p,v}(\kappa) = w \cdot \{1 - \exp(-d \cdot [\pi(\kappa) - \pi_0])\} \tag{4}$$

and additional material parameters w, d, π_0.

In summary, the yield surface in stress space is defined by the 3 previously mentioned functions, which are partially dependent on material parameters (failure line and cut-off tensile yielding) and the hardening (cap). For a detailed continuum mechanical description it is referred to [7, 8 & 9].

In principle there are also other pressure dependent compressible plasticity models available, e.g. the crushable foam model which is often used in crash simulations. But this approach has the disadvantage of symmetric yielding for compressive and tensile stress states.

For the second developed improved analogous model, which describes additionally the inner layered structure of electrodes and separators in a simplified manner, an ordinary incompressible isotropic plasticity model is used.

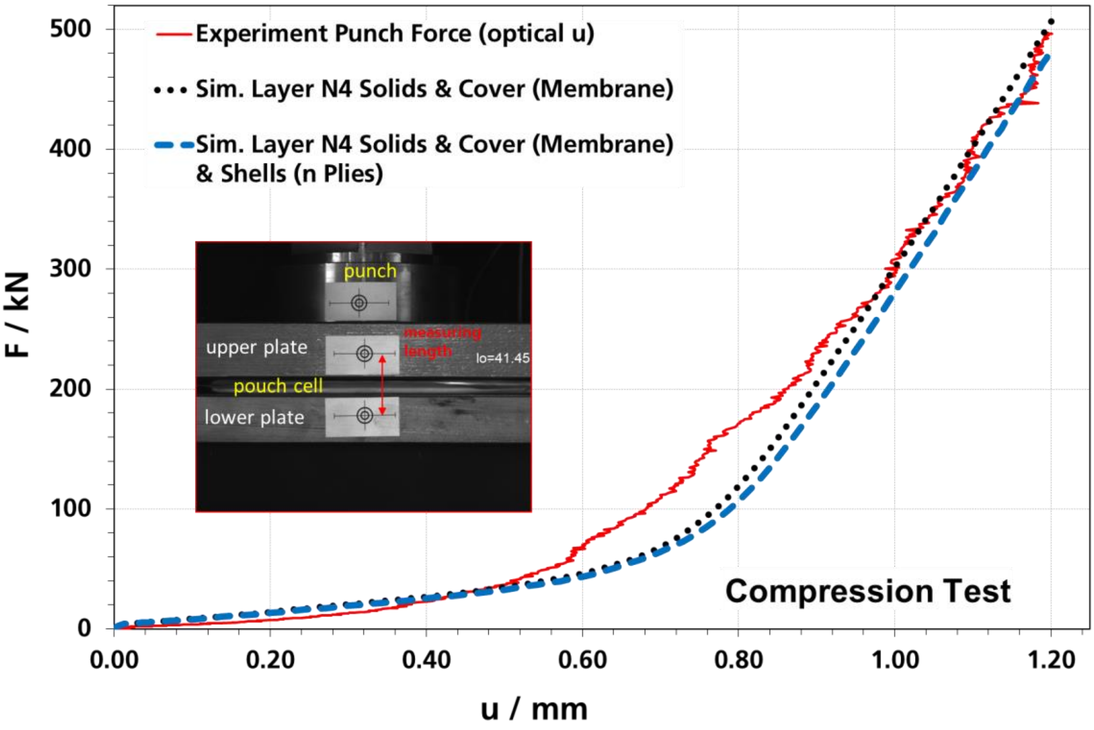

Figure 10: Force displacement characteristics during normal compression test

3.4 Comparison to experiments

For the calibration of the analogous models two types of mechanical tests are used and compared with respect to the global force-displacement characteristics.

- Normal compression test: The loading was applied perpendicular to the large main face of the pouch cell. The pouch cell was loaded between two large and stiff plates (Figure 10) in thickness direction.
- Lateral compression test: The loading was applied on the longer narrow head face. During the edge loading the upper and lower part of the pouch cell (shaft) was led in a notched punch and mounting tool. This type of experiment is similar to a crushing test and complex deformation states arise (bending) which could lead to delamination.

All presented results are related to quasi-static conditions for a punch speed of 0.01mm/s (normal compression test) and 0.1mm/s (lateral crushing).

Figure 10 shows the force-displacement curves of two developed analogous pouch cell models without and with additional inner composite shell plane in comparison to experiments. For both model types good agreements to experimental results have been achieved. Due to the fact of the incompressibility of the metallic electrodes and the polymeric separators, the main part of the thickness reduction is related to the compressibility of the dominant portion of the granular material (active material). Only a small portion can be related to the lateral contraction of the pouch cell, which has a medium influence on the calibration of the active materials for the two types of the developed analogous models (restrained lateral contraction for presence of additional inner composite shell plane).

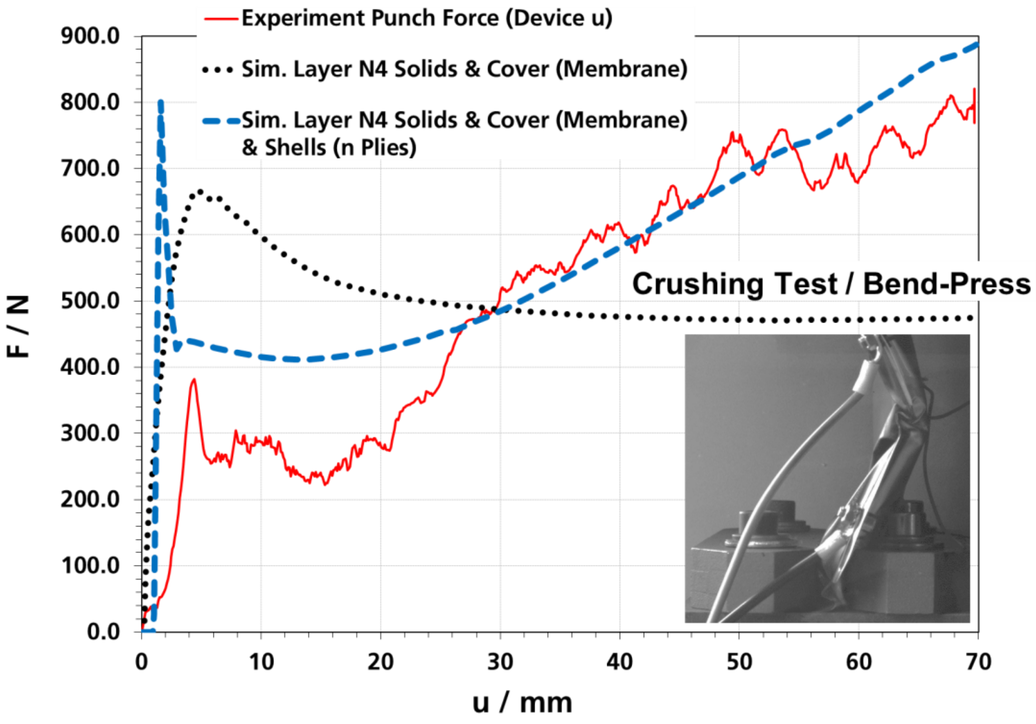

Figure 11: Force displacement characteristics during lateral crushing test

Figure 11 shows the force-displacement characteristic of the lateral crushing test, having a significant lower force level in comparison to the previously presented normal compression test in thickness direction, which is obviously related to the completely different loading conditions. The resulting behaviours of the two presented analogous model types are different, but the computed force levels for both model types show acceptable agreements to the experimental observation.

Related to the force displacement characteristics as well as to the comparison between simulation models and experiments, following consistent behaviours and remarks can be formulated:

- A force peak at the very beginning of the loading characteristic is present in the experimental observation and the simulations of both presented analogous model types. This peak is related to a buckling/stability phenomenon, which can be related to the thin metallic shells of the pouch cell. But the level of this force peak is different for all three curves. The overestimation of the peak force from both models is attributed to the simplification of the inner structure of the pouch cell. The most characteristic initial force peak in the improved analogous model can be explained by the additional inner composite shell plane, which is absent for the other model type.
- The expected decrease of the loading characteristic after the initial force peak is also present for all three curves, but also with different pronunciations. The improved analogous model shows a

significantly better agreement to the experiment in comparison to the more simplified model without the inner composite shell plane.

- In the experiments an increasing force characteristic for higher punch displacements is observed. This behaviour can be well simulated with the improved analogous model, which contains the inner composite shell plane. The absence of the simplified inner composite shell layup leads to a significantly less bending stiffness and further more to a constant force trend for the more simplified analogous model type,
  Furthermore, the presence of thin metal layers could improve the compaction of the active material during progressing crushing, which leads to a higher strength of the granular material and increasing bending stiffness, explaining the growing forces for higher punch displacements.

Finally it is remarkable, that a good agreement for both testing scenarios can be achieved by using the improved analogous pouch cell model, which takes the simplified inner layup structure into account. This fact could be promising for further steps in the development of expanded models for prediction of electrical short-circuits.

3.5 Outlook

One main goal in the further development of analogous pouch cell models is the prediction of short-circuits during simulations of crash loading scenarios for whole automotive structures (cars), which could be achieved by the following steps:

- Further experimental observations for impression, indentation and piercing tests with accompanying comparisons to simulations with the improved analogous pouch cell model.
- Detailed investigations and studies about mechanical conditions for different mechanical loading states by using the improved analogous pouch cell model to derive possible stress or strain based conditions for predicting internal short-circuits.
- Possible development of an advanced analogous pouch cell model by coupling the electromagnetic behaviour (Multiphysics problem).

4 Conclusions

Cylindrical, prismatic and pouch cells were tested with measurements of mechanical and electric responses. A strong relationship between mechanical instability and internal short circuit was found in different loading cases. For crash simulations simplified models were developed and calibrated, which show good agreements to experimental investigations.

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