

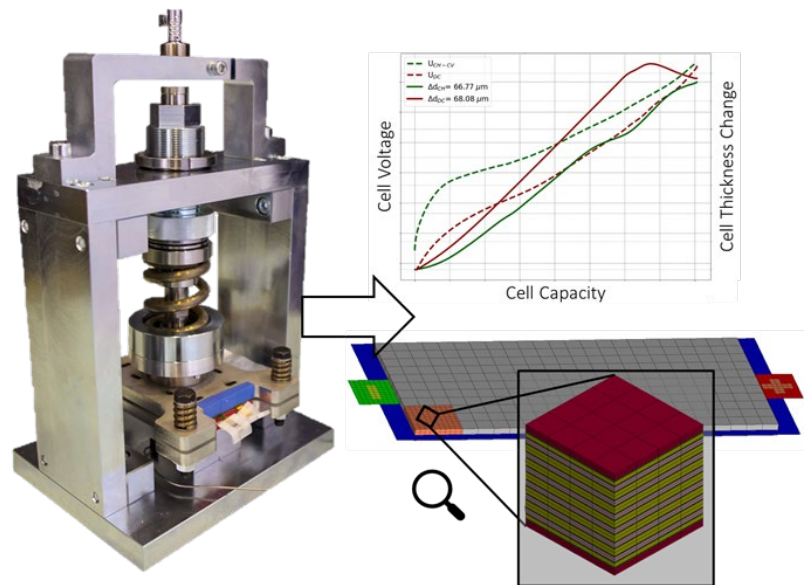
VIRTUAL VEHICLE Research GmbH

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INVESTIGATION OF THE EXPANSION BEHAVIOUR OF LITHIUM-ION CELLS WITH SILICON-BASED ANODES

MEASUREMENT AND SIMULATION OF CELL EXPANSION TO CHARACTERISE CELL CHEMISTRIES AND PREDICT MATERIAL BEHAVIOUR IN CELL PRODUCTION. THE TOOLS DEVELOPED HAVE THE POTENTIAL TO INCREASE THE EFFICIENCY OF CELL DESIGN AND THE PRODUCTION PROCESS.

In order to increase the acceptance of electric vehicles and their suitability for everyday use, their range must be increased above all. In recent years, silicon-based electrode materials have emerged as promising candidates. However, these materials show increased expansion when the cells are charged, which has a negative effect on the cell's lifetime and limits their use in e-vehicles.

For further development and subsequent commercialisation of such innovative materials, a precise understanding of the expansion behaviour is necessary. In recent years, there has been great progress in materials research and promising

material candidates have been developed. A major challenge here is the transferability of the properties from the laboratory to larger battery cells. This applies in particular to the expansion behaviour. Which parameters influence cell expansion and what does this mean for the performance and safety of the cells? These are the core questions that were investigated in the dissertation project *SimCP*. In order to be able to precisely measure the expansion of laboratory battery cells with a silicon-based electrode, a new measurement setup has been developed and built (see cover picture). In recent years, published studies showed that a certain pressure on the cells influences their performance.

SUCCESS STORY

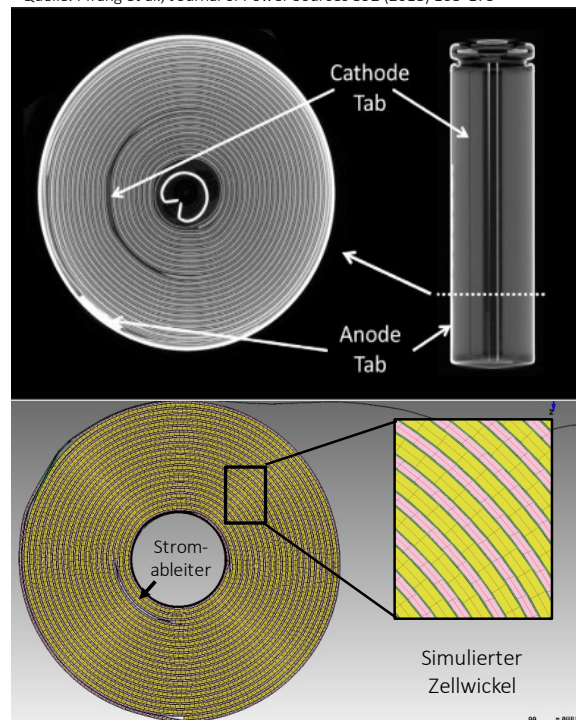
The setup is able to vary this pressure and investigate its influence on the behaviour.

Series of measurements were carried out which showed that the cells examined expand by approx. 3.5% when fully charged. It was also shown that cell performance can be increased by applying external pressure to the cell as well as by increasing the ambient temperature (45°C). Especially the behaviour at higher currents can be significantly improved in this way. Lack of pressure at low temperatures ($\leq 5^\circ\text{C}$), on the other hand, leads to a significant reduction in performance.

Parallel to the measurements, the behaviour of the cells was investigated by means of simulations. The model developed (see cover picture, bottom right) is able to visualise the mechanical stresses inside the cell under different load conditions. These quantities are very difficult to measure from the outside, which is why simulations are a useful tool here. With the simulations, it could be shown that expansion does not lead to negative effects within the cell (at electrode level and without ageing effects), provided it is allowed. If, on the other hand, the cell is fixed, this leads to a strong increase in mechanical stresses and can thus lead to cell failure in extreme cases.

The models can also be used to support the technology transfer to larger cells (so-called simulation-based upscaling). Cylindrical battery cells, as they are widely used in the consumer sector, are characterised by wound electrodes. The winding process also introduces mechanical stresses into the system and was therefore investigated simulatively in the project (see picture on the right). By varying production parameters in the simulation, it could be shown that above all the tensile force on the components during winding, as well as the size and position of the current collector, have a significant influence on the distribution of the mechanical stresses within the wound electrodes.

CT-Bild einer zylindrischen Lithium-Ionen Zelle
Quelle: Pfrang et al., Journal of Power Sources 392 (2018) 168–175



Simulation of the cell electrode roll and comparison with a CT image

Effects and impacts

The methodology developed in the *SimCP* project includes a measurement setup for detailed investigation of the expansion behaviour of battery cells. It also includes simulation tools to investigate the effect of expansion on cell performance and the influence of production steps on the cell.

What was demonstrated in *SimCP* on a specific cell chemistry can be used more generally to characterise new cell materials. This can support the development and production of battery cells and help to shorten development times - for example by pre-selecting certain configurations (material plus production or design parameters) through the simulations.

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Projekt coordination (story)

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This success story was provided by the consortium leader/centre management and by the mentioned project partners for the purpose of being published on the FFG website. Further information on COMET: www.ffg.at/comet