



Licentiate Thesis in Solid Mechanics

# Discrete element modelling of the mechanical behaviour of lithium-ion battery electrode layers

AXEL LUNDKVIST

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Academic Dissertation which, with due permission of the KTH Royal Institute of Technology, is submitted for public defence for the Degree of Licentiate of Engineering on Friday the 19th April 2024, at 13:00 in 4303, seminarierummet, Teknikringen 8, Stockholm.

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## **Abstract**

Since their introduction in the late 20th century, lithium-ion batteries have become the leading battery technology for portable devices and electric vehicles due to their high energy density and rechargeability. However, the increasing demand for a longer battery life span is hindered by the fading of the battery's charge capacity over prolonged use. This reduction in charge capacity stems from electrochemical and mechanical degradation of the battery cells. The main research focus in the literature has been on the chemical degradation of battery cells. However, the mechanical degradation also substantially contributes to the battery's capacity degradation. Therefore, it is crucial to understand the mechanical properties of the battery cells to be able to mitigate mechanical degradation. The battery's mechanical degradation stems from the electrode layers' constituents. This thesis aims to model the positive electrode's mechanical properties by recreating its granular microstructure using the discrete element method.

In Papers 1 and 2, a discrete element method modelling framework is developed, which can reconstruct a positive electrode layer of a lithium-ion battery, simulate manufacturing processing steps, and determine the mechanical properties of the electrode layer. The framework uses two contact models, representing the positive electrode material in the form of particles and a binder agent, which gives the electrode layer its structural integrity. The framework is used to link the mechanical behaviour of the electrode particles and the binder agent to the mechanical behaviour of the entire electrode layer. The framework is able to capture the layer's pressure sensitivity and relaxation behaviour, properties which have been displayed in the literature through experimental testing.

## **Keywords**

Lithium-ion batteries; mechanical characterisation; simulations; contact mechanics; discrete element method.



## Sammanfattning

Sedan de introducerades i slutet av 1900-talet har litiumjonbatterier blivit den ledande batteriteknologin för portabla enheter samt elfordon på grund av deras höga energidensitet och återladdningsförmåga. Den ökade efterfrågan på utökade batterilivslängder är dock hämmad av redueringen av uppladdningskapacitet över längre användningstider. Denna reduering av laddningskapacitet kommer från elektrokemisk och mekanisk degradering av battericellerna. Det största forskningsintresset i litteraturen har varit på den kemiska degraderingen av battericellerna. Dock ger den mekaniska degraderingen ett betydande bidrag till batteriets kapacitetsdegradering. Därför är det viktigt att förstå battericellens mekaniska egenskaper för att kunna förhindra mekanisk degradering. Batteriets mekaniska degradering beror på elektrodlagrets beståndsdelar. Denna avhandlings målsättning är att modellera den positiva elektrodens mekaniska egenskaper genom att återskapa dess granulära mikrostruktur med hjälp av diskret elementmetodik.

I Artikel 1 och 2 utvecklades ett ramverk för modellering med användning av diskreta elementmetoden, vilket kan återskapa det aktiva lagret för en positiv elektrod, simulera tillverkningsprocesser, samt fastställa elektrodlagrets mekaniska egenskaper. Ramverket använder två kontaktmodeller som representerar det positiva elektrodmaterialiet i form av partiklar samt ett bindemedel, som ger elektrodlagret dess strukturella integritet. Ramverket används för att undersöka hur de mekaniska egenskaperna för det hela elektrodlagret beror på egenskaperna för de aktiva partiklarna samt bindemedlet. Ramverket kan fånga lagrets tryckkänslighet samt dess relaxering, egenskaper som har påvisats i litteraturen genom experimentell provning.

## Nyckelord

Litiumjonbatterier; mekanisk karakterisering; simuleringar; kontaktmekanik; diskret elementmetod.



## **Preface and acknowledgements**

The work presented in this licentiate thesis has been performed at the Division of Material and Structural Mechanics, Department of Engineering Mechanics, KTH Royal Institute of Technology between September 2021 and Mars 2024. The work was made possible through the generous financial support of the Swedish Energy Agency [grant 46558-1].

First and foremost, I would like to extend my deepest gratitude to my supervisors, Professor Per-Lennart Larsson and Associate Professor Erik Olsson. This thesis would not have been possible without your excellent support in solid mechanics and DEM modelling, your ability to move the project forward, and by pushing me to do my best work. I would also like to thank Professor Peter Gudmundson, Professor Artem Kulachenko, and the current and former PhD students and postdocs of the battery research group for your continuous discussions, feedback, and support.

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Stockholm, Mars 2024

*Axel Lundkvist*





## List of appended papers

### Paper 1

A discrete element analysis of the mechanical behaviour of a lithium-ion battery electrode active layer

*Powder Technology*, vol. 425, 2023, 118574

Axel Lundkvist, Per-Lennart Larsson, Erik Olsson

### Paper 2

Discrete element modelling of the elastic-plastic and viscoelastic properties of a lithium-ion battery electrode layer

*DiVA*, id: diva2:1837654. Submitted for international publication.

Axel Lundkvist, Per-Lennart Larsson, Anand H.S. Iyer, Erik Olsson

In addition to these appended papers, the work has resulted in the following conference presentations:

### **Structural and mechanical simulation of a negative electrode active layer in lithium-ion batteries using discrete element modelling**

Conference presentation at *Svenska mekanikdag*, 2022, Luleå, Sweden.

### **A discrete element analysis of the mechanical behaviour of an electrode active layer**

Poster presentation at *BATTERY 2030+ annual conference*, 2023, Uppsala, Sweden.

### **A discrete element analysis of the mechanical behaviour of an electrode active layer**

Conference presentation at *PARTICLES 2023 VIII International Conference on Particle-Based Methods*, 2023, Milan, Italy.



## Contributions to papers

The author's contributions to the appended papers are as follows:

**Paper 1:** A. Lundkvist is the principal author. E. Olsson, P.-L. Larsson and A. Lundkvist conceptualised the problem to be analysed. E. Olsson developed the numerical code for the simulations, which A. Lundkvist further adapted for the analysis of the problem. A. Lundkvist performed the numerical analysis. A. Lundkvist, P.-L. Larsson and E. Olsson evaluated and interpreted the results. A. Lundkvist, P.-L. Larsson and E. Olsson reviewed and edited the final manuscript.

**Paper 2:** A. Lundkvist is the principal author. A. Lundkvist performed experimental measurements of particle size distributions with the aid of C. Hulme. A. H. S. Iyer performed the indentation testing. A. Lundkvist further developed the numerical code and performed the numerical analysis. A. Lundkvist, P.-L. Larsson and E. Olsson evaluated and interpreted the results. A. Lundkvist, P.-L. Larsson and E. Olsson reviewed and edited the final manuscript.



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## **Discrete element modelling of the mechanical behaviour of lithium-ion battery electrode layers**

The current shift towards renewable energy sources also places large requirements on energy storage systems. The energy previously stored in solid or liquid form, such as coal or oil, must now be stored in media that can be charged and discharged during short timescales by renewable energy sources, such as wind or solar power. For portable energy storage systems, for example, used in personal electronics or the automotive industry, the lithium-ion battery (LIB) has been a key player since its invention in the late 20th century. This is due to their remarkable rechargeability and energy density [1].

### **Introduction**

A LIB cell consists of a positive electrode (cathode), a negative electrode (anode), a separator, current collectors, and an electrolyte. The two electrodes are separated by the separator to avoid short-circuiting. Lithium ions move between the electrodes through the electrolyte, while electrons flow through an external circuit connecting the electrodes during the charge and discharge process. The two electrodes contain active material in which lithium is stored and can intercalate into/out of during the charging and discharging process. The negative electrode often uses graphite flakes as its active material, while the positive electrode can use a wide range of metal oxides, such as lithium ferro-phosphate (LFP) or lithium nickel manganese cobalt oxides (NMC), in the shape of spherical-like particles. The active material is held together by a porous and conductive binder agent, which gives the electrode structural rigidity, enables electrical connection to the outer circuit, and electrode wetting from the electrolyte. The binder agent which is considered in this thesis is composed of polyvinylidene fluoride (PVDF) mixed with carbon black. A schematic sketch of the LIB cell can be seen in Figure 1. This thesis will focus on the positive electrode, composed with NMC as its active material.

The development of the LIB technology is, however, still ongoing. The LIBs are currently limited by the fading of charge capacity over



prolonged use. This capacity degradation stems from both electrochemical and mechanical processes. An increased lifetime of the LIB is crucial in the automotive industry, where replacements of the large batteries are both expensive and cumbersome. Historically, the main research focus has been on the electrochemistry of LIBs. However, experimental observations have proved that mechanical degradation processes also play a significant role in the charge degradation. Therefore, understanding the mechanical properties of LIBs is a topic of interest [2]–[5].

The mechanical degradation phenomena seen in LIBs stem from the electrochemical-mechanical properties of the active material. During the charging/discharging process in the positive electrode, lithium ions intercalating into and out of the active materials cause mechanical swelling and shrinking. These dimensional changes cause internal stresses, which can fracture the active material. Already in the initial charge cycles, active material cracking is prominent.

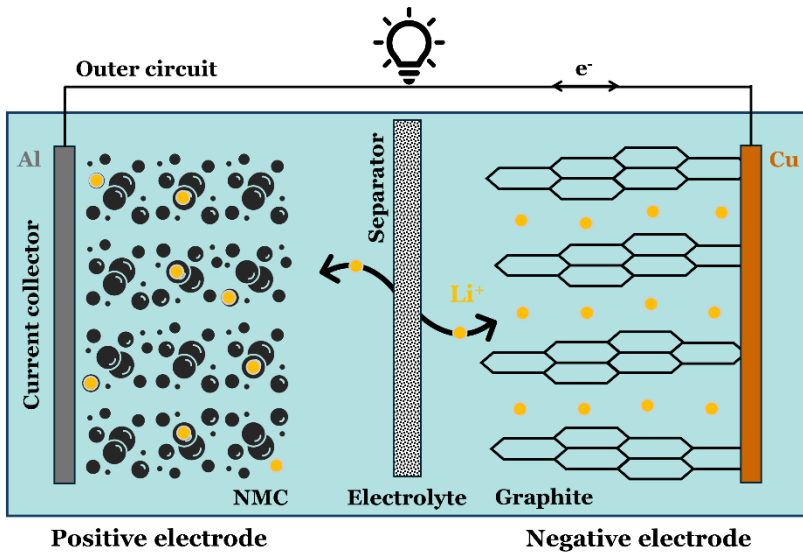


Figure 1 Schematic sketch of a LIB cell.

The consequence of active material cracking can both increase and decrease the function of the cell. Some argue that active material cracking increases the connectivity of the active material to

the electrolyte, while others argue that the cracking causes the active material to become inactive [3]–[6]. The swelling may also cause macroscopic failure of the positive electrode layer, such as delamination of the active layer from the current collector and island formation within the electrode layer. This leads to decreased connection or isolation of the active layer to the external circuit. To understand and mitigate these degradation mechanisms, experimental techniques have been used to characterize the mechanical properties of the active layer.

Various experimental methods have been utilised to characterise the active layer of the positive electrode. Nanoindentation has been used extensively to characterise the individual constituents of the positive cathode active layer, i.e. the active material and the binder domain. Other micromechanical testing routines have also been used, such as micropillar compression and microcantilever bending. These methods give insight into the constitutive behaviour of the different domains in the layer as well as other properties, such as interface strength between the binder domain and the active material or the binder domain and the current collector. Mesoscale testing techniques of the layer have also been performed to find the global properties of the active layer. These methods consist of indentation tests and U-shape bending tests, and from these, properties such as layer stiffness and time-dependent relaxation of the layer can be determined. Observational techniques such as x-ray computer tomography have also been employed to enable insight into the change of the microstructure of the LIB over its lifetime. [7]–[16]

To gain further insight into the mechanical properties of the active layer, computational methods serve as a valuable complement to the experimental techniques. They can reproduce experimental observations and help understand the link between length scales and coupling between physics, which indeed characterises this problem. Two methods used extensively for the modelling of LIB electrode layers are the finite element method (FEM) and the discrete element method (DEM). FEM has been used on multiple scales of the electrode layers, from electrochemical-mechanical modelling of the swelling and fracture process of active material to stresses in the full battery packs due to swelling, using homogenisation methods [17]–[19].

For modelling of the global electrode layer, DEM has proven to be a useful tool considering the granular microstructure that the active material and binder domain form. The manufacturing process of the cathode layer has been the focus of modelling, particularly the calendaring process, where the active layer is calendared in order to increase the final layer's energy density. However, DEM has also been used to simulate the heat flux and electrical conductivity in the active layer [20]–[24].

### **Motivation**

Despite thorough experimental testing and modelling of the positive electrode active layer, there remains a limited understanding of its mechanical properties. This mechanical behaviour must be fully understood in order to handle the mechanical degradation of the electrode. This thesis aims to increase the understanding of the mechanical properties of the positive electrode active layer. By developing a DEM modelling framework which can simulate the calendaring process of the active layer and determine various mechanical properties of the active electrode layer, such as stiffness and relaxation both in compression and in tension, a greater understanding of the link between local mechanical behaviour of the layer's constituents and the global behaviour of the layer could be found. This framework serves as an excellent base for further research on the mechanical degradation of the positive electrode layer stemming from swelling and fracture of the active material.

### **Modelling of the mechanical behaviour of LIBs**

As mentioned in the Introduction, modelling of the mechanical behaviour of LIBs has addressed several problems using various methods. As the lithium-ion battery system ranges over multiple length scales, from the active material scale on the micrometre scale to the entire battery module on the metre scale, it is impossible to capture all phenomena acting on the various length scales with today's computational methods. Therefore, the focus has been on modelling on individual length scales and bridging phenomena across adjacent length scales.

On the active material scale, the focus has been on capturing the swelling and fracture of the active material due to the lithium-ion

intercalation and determining an appropriate constitutive model for the porous binder domain. This has often been achieved using FEM [17], [25]. On the cell scale, modelling has addressed deformation and damage of the electrode layer due to outer mechanical loads stemming from crush events and internal stresses arising from the swelling of the electrode layers over charge cycling [5], [19], [26], [27]. On the electrode scale, the calendaring process during electrode manufacturing has been a topic of focus. Processing parameters such as calendaring pressure have been related to parameters linked to cell performance, such as porosity and conductive paths in the electrode. DEM has been proven to be a remarkable tool for modelling on the electrode scale, as it links the properties of the electrode constituents, i.e. the active material and the binder agent, to the properties of the full electrode layer [22], [23], [28], [29]. DEM has also been used for various applications with a granular nature, such as modelling of asphalt, mineral processing, and powder compaction for sintering [30]–[32]. However, there is a knowledge gap in the modelling of the electrode layers' mechanical properties post-manufacturing, which is the motivation of this thesis.

As stated previously, this thesis focuses on modelling the mechanical behaviour of the positive electrode active layer. In particular, how the mechanics on the active material level affect the mechanical properties of the electrode layer. A DEM modelling framework was developed to link these two length scales, where the discrete elements constitute the active material. Two contact formulations were stipulated for the active material, one for contact between individual active particles and one for the case when the binder separates the active particles. This framework allowed us to investigate how the mechanical properties of the active particles and the binder influence the mechanical properties of the entire electrode layer. The mechanical behaviour of the individual constituents of the electrode layer is expressed through a stipulated contact relationship. The influence on the full electrode layer, from the local mechanical behaviour, could be predicted by varying the properties of the contact models, e.g., by introducing plasticity or viscoelasticity.

## Summary of paper 1 and 2

**Paper 1.** The DEM framework for the reconstruction, production processing, and mechanical testing of a positive electrode layer was developed. The framework consists of three main steps. Initially, an uncalendered electrode layer is created by random packing of active particles and particles separated by binder. The layer is thereafter calendered to a prescribed calendering height. Finally, the in-plane unloading stiffness of the layer is determined at various strain levels, both in compression and tension. The influence of the properties of the binder domain on the electrode layer properties was investigated by varying the stiffness of the binder and including plasticity. The main achievement of the study was capturing the pressure sensitivity of the electrode layer, where increased compression levels lead to a stiffer layer, a behaviour which has been observed in experimental studies. Through the DEM framework, the increase of stiffness in compression was shown to be a result of an increased number of particle contacts at higher compression levels.

**Paper 2.** The framework, established in Paper 1, was further developed by implementing a new contact model for the active particles based on advanced contact mechanics. The new contact model followed the constitutive properties of the elastic-plastic active material. The results for the calendering process and the measurement of in-plane stiffness using the new particle contact model were comparable to the modelling results from the previous study. Viscoelasticity was also implemented for the binder contact model, and relaxation simulations were performed and compared to experimental measurements. The main finding of the work was reproducing the relaxation behaviour of the active layer, both in compression and tension, and showing that the relaxation behaviour was affected by the compression level.

## **Conclusions and future work**

In this thesis, a DEM modelling framework for the evaluation of a LIB-positive electrode layer's mechanical properties was developed. The framework reconstructs the full electrode layer by modelling the interaction between the active material and the binder agent. The framework can capture the mechanical characteristics of the layer, in particular its pressure sensitivity and relaxation behaviour. Through this understanding of the link between the mechanical properties of the electrode layer and its constituents, it may be possible to optimize the composition of the electrode layer to increase the battery's performance. The framework also proves an excellent base for further assessment of the electrode layer's mechanical behaviour.

The continuation of this work will consist of further development of the modelling framework. Firstly, the effect of charge cycling will be investigated by implementing swelling of the active particles and variations of the active material properties, dependent on the battery's state of charge. Thereafter, the mechanisms for mechanical degradation within the battery will be investigated by implementing fracture of the active particles and the binder and coupling it to the previously investigated mechanical behaviours. These developments will lead to a more complete model of the mechanical behaviour of the electrode layer throughout its lifetime.

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