

## Physics-based registration applied to battery degradation observed using X-ray tomography

Sonia Ait Hamouda <sup>1,\*</sup>, Alexandre Dufour <sup>3</sup>, Peter Moonen <sup>1,2</sup>

<sup>1</sup> Universite de Pau et Pays de l'Adour, E2S UPPA, CNRS, TOTAL, LFCR, Pau, France

<sup>2</sup> Universite de Pau et Pays de l'Adour, E2S UPPA, CNRS, DMEX, Pau, France

<sup>3</sup> TotalEnergies, Pau, France

\*Speaker: Sonia.ait-hamouda@univ-pau.fr

### 1. Introduction

The lifetime of a Li-ion battery is limited by microstructural degradation that evolves over the course of successive charging and discharging cycles [1]. The non-destructive nature of X-ray computed tomography renders the technique well-suited to investigate these (and other) dynamic processes. By comparing datasets acquired at different points in time, insight in the degradation process can be gained. Typically, affine or non-affine registration of successive datasets is used to assess the local strain field. However, such approach is unaware of physical limitations, such as material properties or conservation laws. We present a proof-of-concept study showing that physics-based registration enables accounting for these constraints and could be a useful tool in battery research.

### 2. Materials and Methods

We develop our method based on a scan of a classical rechargeable 18650 lithium-ion battery. As a starting point, the middle slice from the stack was selected and artificially deformed. In a next step of this study, the battery will be cycled and the dynamic dataset will serve as an input to the model.

The 2D slice before and after deformation is given as an input to Bioflow. This is a plugin for Icy, an open-source collaborative bioimaging informatics platform [2]. Bioflow was initially developed to investigate biophysical mechanisms inside living cells, and implements a similar philosophy than the one envisaged for the study at hand [3]. In a first step, an active contour method tracks the boundary of the battery before and after deformation. A finite element mesh is automatically generated based on this contour and properties are assigned to each

element based on the grey level of the image. Next, the weak form of the governing equations is solved by the finite element method (FEM) using FEniCS. This package enables users to quickly translate scientific models into efficient finite element code [4]. The difference between the deformed FEM-model and the deformed slice is minimized, hereby respecting the governing equations and specific properties of the different battery components. After minimization, the FEM model provides the stresses, strains, and other quantities of interest at all points of the sample, as well as their evolution over time.

### 3. Results and Conclusion

A physics-based registration model is developed that takes into account physical processes underlying battery degradation. By matching the numerical model to the X-ray tomography data we ensure that the model closely represents reality. The proposed method offers wide-ranging advantages such as applicability to large-scale applications that allow a better understanding of physical phenomena such as material fatigue and failure analysis.

### 4. Acknowledgements

This research was financially supported by the European Doctoral programme on ENergy and Environment (EDENE) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 945416). The authors also thank TotalEnergies for financial support.

### 5. References

- [1] J M. Allen, et al. (0.1016/j.jpowsour.2021.230415)
- [2] F. De Chaumont, et al. (10.1038/nmeth.2075)
- [3] Boquet-Pujadas, et al.(10.1038/s41598-017-09240-y)
- [4] HP. Langtangen, et al. (ISBN 978-3-319-52461-0).