Computational Materials Science 136 (2017) 297–305

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Crack detection in lithium-ion cells using machine learning

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ARTICLE INFO

Article history:
Received 3 February 2017
Received in revised form 5 May 2017
Accepted 6 May 2017

Keywords:
Thermal runaway
Lithium-ion battery
Crack detection
Machine learning
3D microstructure
Stochastic modelling

ABSTRACT

It is an open question how the particle microstructure of a lithium-ion electrode influences a potential thermal runaway. In order to investigate this, information on the structural changes, in particular cracked particles, caused by the failure are desirable. For a reliable analysis of these changes a reasonably large amount of data is necessary, which necessitates automatic extraction of particle cracks from tomographic 3D image data. In this paper, a classification model is proposed which is able to decide whether a pair of particles is the result of breakage, of the image segmentation, or neither. The classifier is developed using simulated data based on a 3D stochastic particle model. Its validity is tested by applying the methodology to hand-labelled data from a real electrode. For this dataset, an overall accuracy of 73% is achieved.

1. Introduction and motivation

Lithium-ion batteries combine several beneficial attributes, such as high energy density and low self-discharge. However, one of the biggest drawbacks is their vulnerability to thermal runaway [1]. This is when the temperature of the cell exceeds a certain threshold, e.g. through overcharging, and exothermic decomposition of the electrodes generates additional heat accelerating the process. Such catastrophic failures are rare, but devastating.

During the thermal runaway particles in the electrode material break, which then affects the reaction [2]. More precisely, it has been shown that smaller particle sizes (and thus higher specific surface area) lead to more intense heat generation with lower onset temperature (see e.g. [3,4]). However, information on the broken particles is required for a more detailed analysis of which particles are more likely to crack and thus worsen the safety of the cell. The main goal in this paper is to detect these particles and hence to pave the way for further research.

Finding cracked particles, i.e., particles that broke into two parts, has always been challenging. Typically this is done by visual inspection. This method however has several disadvantages. It is time-consuming and processing a large number of particles is infeasible. Moreover, it is tedious even for smaller particle systems and often leads to errors. Other approaches are based on advanced segmentation algorithms [5]. However, such segmentation algorithms often have to be specifically tailored in order to take into account the given features of the considered image data. In the present paper, an algorithm based on machine learning is proposed, where the complex, non-linear nature of our problem makes supervised machine learning [6,7] an appropriate tool, since the associated techniques possess the ability to make predictions based on previously learned sample data. The classifier, which considers pairs of particles of the post-mortem cell, decides whether they are the result of breakages. In case a particle broke into multiple pieces, every pair of (neighbouring) fragments is detected. To the best of our knowledge, this is the first work of using machine learning for crack detection in lithium-ion batteries.

To develop our classification model, we use simulated data. We generate a particle structure based on a parametric stochastic model (see [8]) and extract pairs of particles with their class labels, which describe the relationship to each other, e.g. if they are the result of breakage. Then, different features and classifiers are investigated. The resulting predictive classifier is retrained and evaluated on hand-labelled data to verify that it is also applicable to real-world data. This process is illustrated in Fig. 1. Note that, in contrast to full hand-labelling, for training of the classifier only a (relatively) small number of labelled particle pairs is necessary, and thus the enormous effort of hand-labelling is strongly reduced.

The algorithm distinguishes three classes. We have a class label for particle pairs which are the result of breakage and one for those which were already separated in the pristine battery cell. But

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http://dx.doi.org/10.1016/j.commatsci.2017.05.012
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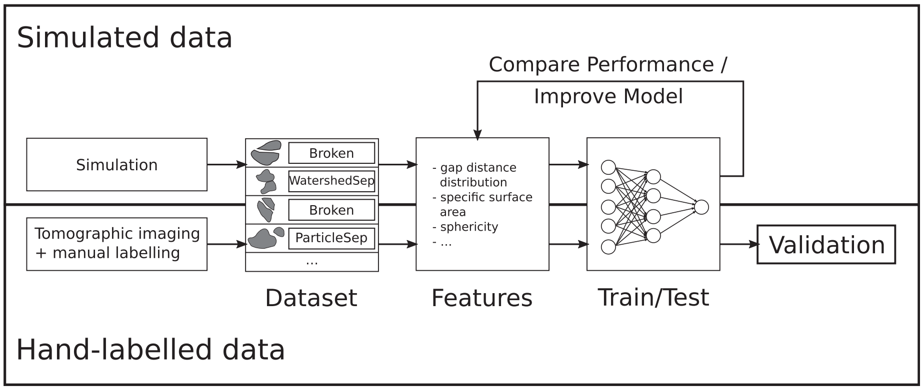


Fig. 1. Overview of the model development.

particles which touch each other can also be separated by the watershed algorithm [9] in the course of the image segmentation (cf. Section 2.1). Consequently, we differentiate the following three classes of particle pairs:

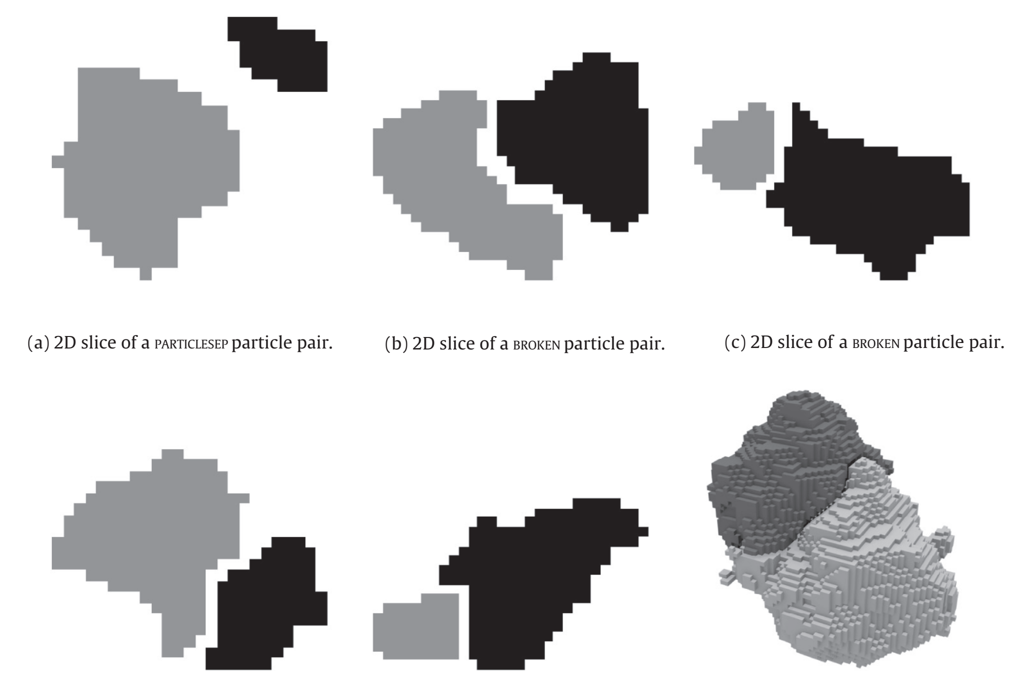
- BROKEN: The particle pair belonged to the same particle before it broke apart during the thermal runaway.
- WATERSHEDSEP: The particle pair corresponds to two touching particles in the tomographic image which are split by the watershed transformation.
- PARTICLESEP: The particle pair consists of unrelated, separate particles, i.e. a pair which is neither BROKEN nor WATERSHEDSEP.

Furthermore, these three classes describe the relationship of one particle to another one. It is hence possible that e.g. a particle which is part of a BROKEN-pair, can also belong to a (different) WATERSHEDSEP-pair. In Figs. 2 and 3 several examples of particle pairs are shown.

The rest of this paper is structured as follows. In Section 2, we describe tomographic imaging and the acquisition of the validation dataset. After that, in Section 3, we present our algorithm to simulate sample data and the classification model. In Section 4, we follow up with the evaluation results of the classifier on the simulated and on the validation dataset, and discuss its performance. The conclusion in Section 5 provides a summary and further research opportunities.

2. Description of tomographic data

The tomographic dataset used in this work was retrieved from [2] where a commercial $LiCoO_2$ cell underwent thermal runaway via high-rate overcharge electrical abuse. The $LiCoO_2$ sample was extracted post-mortem from an outer layer of the degraded electrode assembly, and exhibits a significantly reduced mean particle diameter, relative to an equivalent sample in its fresh state. This reduction in particle size is described in [2] as being due to the



(a) 2D slice of a PARTICLESEP particle pair. (b) 2D slice of a BROKEN particle pair. (c) 2D slice of a BROKEN particle pair.

(d) 2D slice of a WATERSHEDSEP particle pair. (e) 2D slice of a WATERSHEDSEP particle pair. (f) 3D rendering of a BROKEN particle pair.

Fig. 2. Examples of particle pairs from the hand-labelled dataset with their class labels.